

Supplementary Material

Unusual polarization properties of sub-nanosized magnesium clusters

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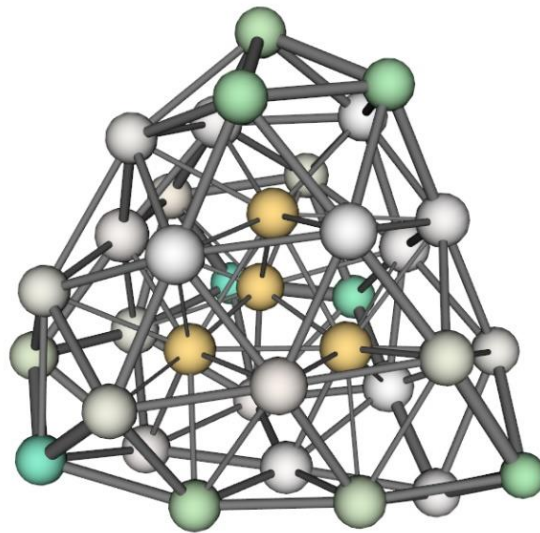


Figure S1. Global minimum structure of cluster Mg_{35} predicted by the MTP potential

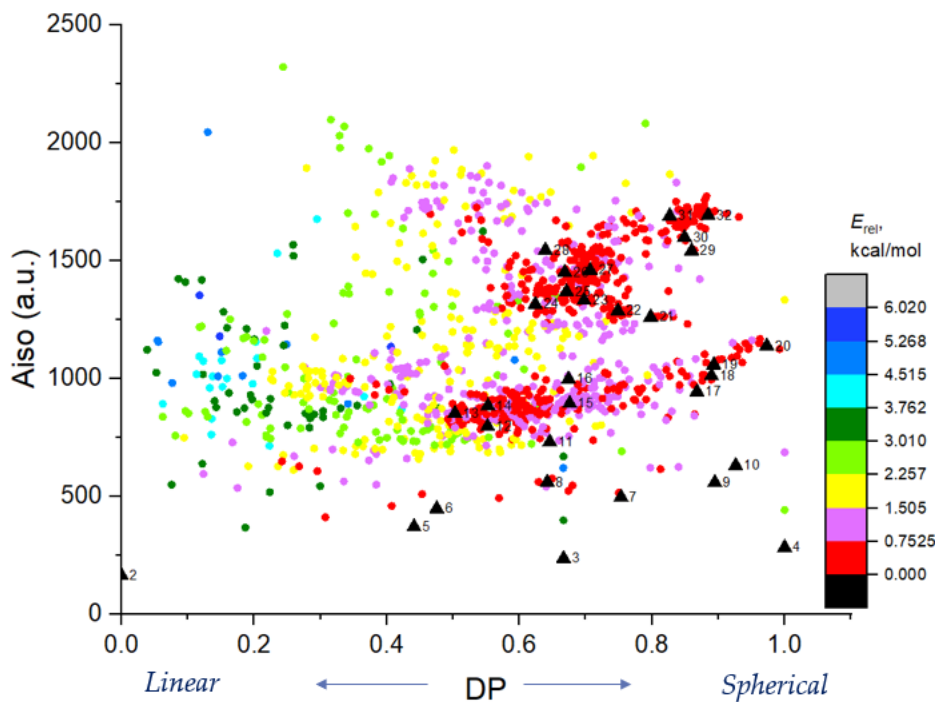


Figure S2. Dependence of DFT-calculated IEP of 1237 isomers of Mg_2 - Mg_{32} on the structure deformation parameter DP . Color designates the isomer relative energy. Black triangles correspond to the most favorable structures of nuclearity indicated by numerical labels.

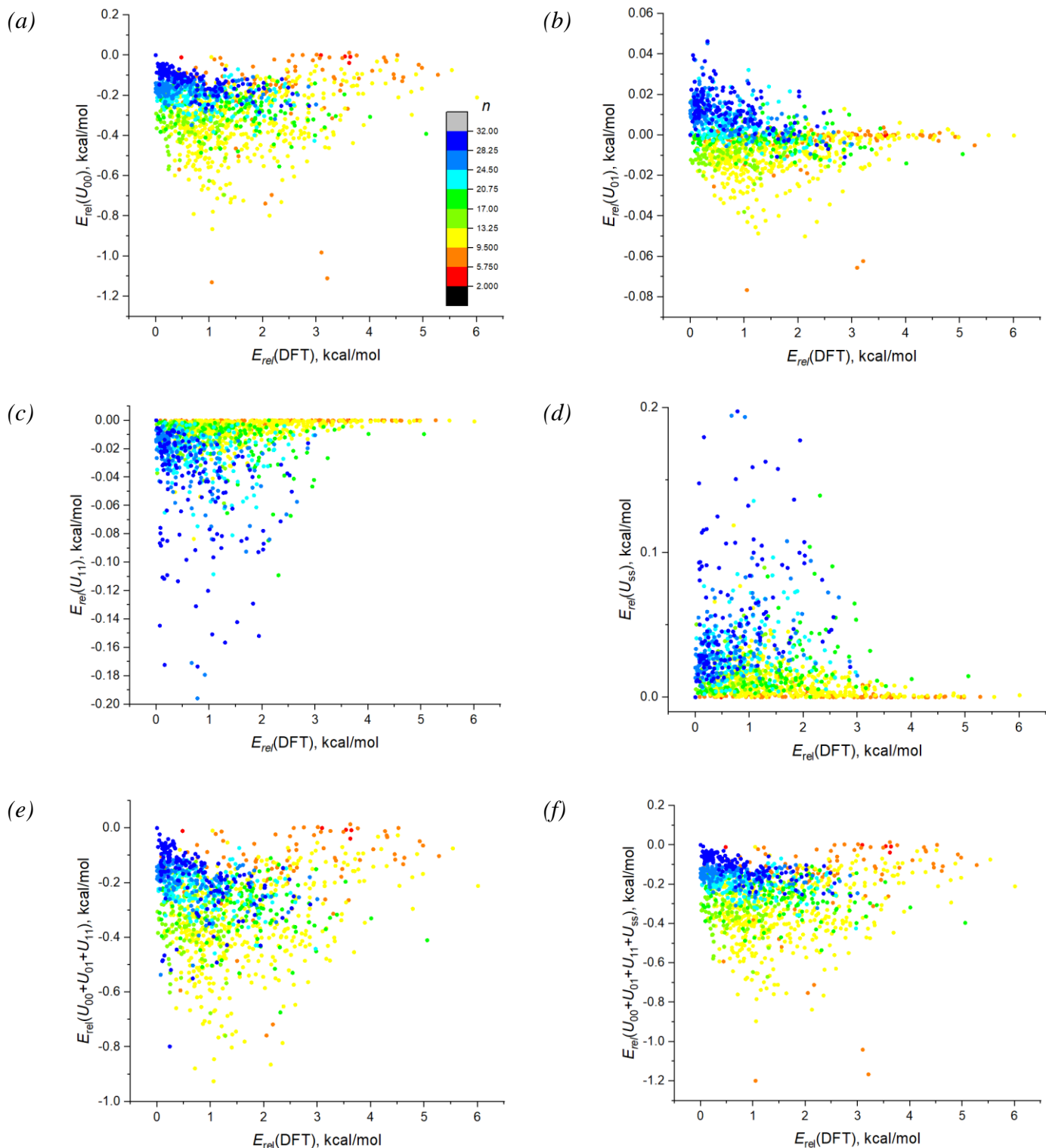


Figure S3. Correlations between the isomers' relative energies E_{rel} calculated by DFT and estimated on the basis of various energy components within the GD model (U_{00} , U_{01} , U_{11} , U_{ss} and their combinations) for 1237 cluster isomers $\text{Mg}_2\text{-Mg}_{32}$. Color indicates the cluster nuclearity (single scale for all charts). Some data points located outside of the vertical axis ranges are omitted.

Table S1. Energies and polarizabilities of 1237 isomers of Mg₂-Mg₃₂ calculated at the DFT level and within various induced dipole models. *n* is number of atoms; *E_b*, *E_{rel}* are the per atom binding energy and isomer relative energy in kcal/mol; *Aiso*, *Aaniso* are the isotropic polarizability and polarizability anisotropy, a.u.; *Etot* is the total energy of the optimized structure at the BP86/6-31G(d) level, Hartree. Most favorable isomers are marked with asterisks. *n*alp* is the idealized polarizability of *n* atoms at DFT level.

Polarizability models:					n*alp	DFT results			AM model		TL model		TE model		RP model		GD model		Etot	
<i>i</i>	<i>n</i>	<i>isomer</i>	<i>E_b</i>	<i>E_{rel}</i>	<i>Aiso</i>	<i>Aiso</i>	<i>Aaniso</i>	<i>Aiso</i>	<i>Aaniso</i>	<i>Aiso</i>	<i>Aaniso</i>	<i>Aiso</i>	<i>Aaniso</i>	<i>Aiso</i>	<i>Aaniso</i>	<i>Aiso</i>	<i>Aaniso</i>	<i>Aiso</i>	<i>Aaniso</i>	<i>Etot</i>
1	2	1*	-1.03	0.00	146.95	162.54	120.11	173.52	165.33	145.26	0.43	144.89	1.86	157.04	113.04	153.19	98.78	-400.142698		
2	3	1*	-3.18	0.00	220.42	235.82	124.35	331.14	291.19	215.28	0.58	213.88	2.63	230.53	133.88	225.25	122.40	-600.224345		
3	4	1*	-6.99	0.00	293.90	282.37	0.00	595.17	0.00	283.55	0.00	280.33	0.00	279.45	0.00	280.36	0.00	-800.323396		
4	4	2	-3.35	3.64	293.90	366.61	343.63	1145.51	2470.69	284.67	2.07	283.40	6.70	358.57	342.65	341.36	297.45	-800.300209		
5	5	1*	-7.04	0.00	367.38	370.33	216.82	775.73	180.02	350.87	1.45	346.80	5.29	359.22	205.34	354.01	178.17	-1000.404667		
6	5	2	-6.56	0.48	367.38	410.59	269.40	-1176.92	5434.92	351.67	2.16	348.76	6.32	411.98	279.81	404.12	251.40	-1000.400777		
7	5	3	-3.95	3.09	367.38	397.71	266.32	486.30	424.68	351.98	2.36	350.13	8.61	359.72	223.99	357.09	214.93	-1000.380032		
8	5	4	-3.50	3.54	367.38	516.40	545.84	-1186.09	5346.60	353.32	3.86	352.49	10.47	506.81	545.89	472.76	462.85	-1000.376405		
9	5	5	-3.42	3.62	367.38	549.12	750.24	-778.14	3460.91	353.93	5.24	353.16	12.62	535.93	736.05	491.80	607.83	-1000.375797		
10	6	1*	-7.38	0.00	440.85	447.27	244.94	1259.21	659.37	416.95	2.28	412.10	7.78	433.66	248.97	425.59	222.12	-1200.488831		
11	6	2	-7.21	0.17	440.85	458.61	284.78	1077.19	688.68	417.22	2.67	412.76	8.81	447.20	286.51	440.56	263.51	-1200.487224		
12	6	3	-6.68	0.70	440.85	491.97	238.05	-66.19	2482.60	417.76	2.22	414.17	6.74	481.18	235.30	469.44	213.07	-1200.482144		
13	6	4	-6.62	0.76	440.85	535.14	585.30	2926.90	6418.66	418.42	4.68	415.11	12.97	512.58	537.16	490.58	458.37	-1200.481561		
14	6	5	-6.28	1.10	440.85	549.16	385.94	1557.89	5984.69	419.00	3.50	416.73	9.03	555.80	409.97	537.16	363.09	-1200.478280		
15	6	6	-6.14	1.24	440.85	594.59	691.32	17.97	2000.98	420.13	6.18	418.06	13.75	599.81	718.13	568.32	615.45	-1200.476980		
16	6	7	-4.82	2.56	440.85	441.57	0.02	531.04	0.08	417.04	0.00	412.87	0.00	435.35	0.01	420.31	0.01	-1200.464364		
17	6	8	-4.31	3.07	440.85	637.50	742.31	-84.92	1868.51	421.07	7.06	420.20	15.60	643.37	793.98	597.81	673.26	-1200.459470		
18	6	9	-4.13	3.25	440.85	542.58	517.13	1940.00	4538.02	419.52	4.88	418.26	14.08	477.30	414.56	468.52	386.78	-1200.457757		
19	6	10	-3.62	3.76	440.85	668.43	578.35	-2130.43	3602.60	421.15	4.72	421.09	12.42	657.86	570.89	607.52	490.52	-1200.452844		
20	7	1*	-8.58	0.00	514.33	495.76	270.05	3132.18	1753.44	481.22	2.68	474.64	9.68	472.86	269.08	470.05	251.21	-1400.583646		
21	7	2	-8.30	0.28	514.33	508.61	244.99	1025.24	1015.70	481.77	3.23	476.05	10.13	499.83	258.93	494.24	240.31	-1400.580557		
22	7	3	-8.20	0.38	514.33	523.12	287.97	-35706.65	104825.68	481.98	3.09	476.60	10.50	505.59	287.97	503.63	274.11	-1400.579466		
23	7	4	-8.07	0.51	514.33	514.65	259.57	1439.32	135.35	481.74	2.88	476.04	10.00	493.61	270.60	489.28	252.74	-1400.577931		
24	7	5	-7.65	0.93	514.33	540.41	296.28	-5371.66	20382.74	482.24	3.29	477.28	11.12	522.94	284.86	520.82	274.87	-1400.573298		
25	7	6	-7.33	1.25	514.33	562.31	430.72	3170.03	6382.11	482.76	4.56	478.22	13.25	542.55	424.52	532.19	390.31	-1400.569708		
26	7	7	-7.03	1.55	514.33	611.24	566.64	-2178.33	12057.29	483.64	5.71	479.82	15.12	590.69	545.42	566.96	475.92	-1400.566380		
27	7	8	-6.96	1.62	514.33	626.75	632.39	-569.86	4693.85	483.94	6.19	480.41	16.37	608.40	614.59	588.91	553.68	-1400.565617		
28	7	9	-6.91	1.67	514.33	627.04	659.86	-3117.43	12206.67	484.27	6.80	480.81	17.10	614.32	659.55	592.76	590.31	-1400.565055		
29	7	10	-6.36	2.22	514.33	747.96	1102.30	-3347.98	12575.75	485.74	9.24	483.29	21.63	690.71	947.94	645.36	796.23	-1400.558857		
30	7	11	-6.33	2.25	514.33	674.66	601.98	268.57	1704.29	485.40	6.56	482.98	14.01	668.15	630.49	633.40	544.06	-1400.558521		
31	7	12	-6.25	2.33	514.33	756.81	1122.19	-231.59	3212.00	486.76	10.11	484.36	21.32	722.72	1042.26	665.99	856.37	-1400.557669		
32	7	13	-6.09	2.49	514.33	690.85	364.54	-290.12	2350.43	485.51	3.71	484.20	9.06	701.82	387.18	672.62	343.80	-1400.555887		
33	7	14	-5.97	2.61	514.33	751.45	811.76	-4860.56	14455.26	487.13	8.06	485.84	16.15	765.11	860.76	717.42	729.87	-1400.554529		
34	7	15	-5.83	2.75	514.33	836.76	1288.61	134.73	1789.96	489.40	12.42	487.72	21.54	847.87	1335.14	770.82	1093.28	-1400.552983		
35	7	16	-4.31	4.27	514.33	828.31	1052.26	283.92	2035.64	489.12	10.89	488.91	20.50	841.22	1131.25	766.18	936.27	-1400.536001		
36	7	17	-4.28	4.30	514.33	714.05	833.09	-3647.31	13769.68	486.79	8.46	486.30	20.43	614.91	648.01	597.77	598.01	-1400.535679		
37	7	18	-4.27	4.31	514.33	891.99	1376.42	15.47	1694.79	490.79	13.72	490.11	23.26	904.72	1454.55	807.27	1174.52	-1400.535580		
38	7	19	-4.13	4.45	514.33	761.66	1043.38	-59.94	1593.19	488.00	10.27	487.54	21.81	668.64	854.95	636.39	754.58	-1400.534056		
39	7	20	-4.06	4.52	514.33	620.16	489.60	1088.27	1213.98	486.19	6.14	486.43	17.30	549.24	389.58	540.54	369.54	-1400.533191		
40	7	21	-3.66	4.92	514.33	891.27	977.02	-1295.94	2778.00	489.77	8.86	490.44	17.95	879.29	970.97	789.27	793.65	-1400.528727		
41	7	22	-3.60	4.98	514.33	980.79	1659.23	475.88	3259.73	491.30	13.41	491.50	24.51	959.11	1629.47	839.57	1287.88	-1400.528069		
42	8	1*	-9.21	0.00	587.80	559.48	225.43	-901.66	19644.59	544.82	3.13	537.47	10.29	537.01	236.46	535.99	229.35	-1600.675118		

Polarizability models:				n*alp	DFT results		AM model		TL model		TE model		RP model		GD model		Etot	
i	n	isomer	Eb	Erel	Aiso	Aaniso	Aiso	Aaniso	Aiso	Aaniso	Aiso	Aaniso	Aiso	Aaniso	Aiso	Aaniso		
43	8	2	-9.13	0.08	587.80	575.20	208.43	1935.10	1261.16	545.35	3.20	538.86	10.05	559.79	214.82	558.94	208.41	-1600.674015
44	8	3	-8.85	0.36	587.80	560.13	213.58	2003.79	3218.01	545.10	3.13	538.26	9.88	536.35	212.63	536.71	206.67	-1600.670429
45	8	4	-8.77	0.44	587.80	606.69	504.25	-274.40	5208.38	546.18	6.45	540.24	18.46	585.35	482.24	574.72	434.90	-1600.669471
46	8	5	-8.77	0.44	587.80	544.56	197.99	639.50	1678.69	544.62	2.63	537.09	8.66	517.71	180.23	516.33	175.09	-1600.669410
47	8	6	-8.64	0.57	587.80	626.76	525.91	5595.52	15901.73	546.96	7.19	541.91	19.47	611.36	509.93	601.29	465.52	-1600.667789
48	8	7	-8.46	0.75	587.80	648.20	551.65	-2507.54	10077.25	547.74	7.94	543.44	20.34	630.11	534.56	622.35	497.98	-1600.665545
49	8	8	-8.16	1.05	587.80	651.46	543.26	8867.27	25032.08	546.73	6.07	541.37	17.06	620.97	517.24	606.72	470.61	-1600.661642
50	8	9	-8.01	1.20	587.80	670.31	600.30	-702.21	4802.87	547.61	7.45	543.03	18.89	661.41	611.33	645.17	561.24	-1600.659801
51	8	10	-8.00	1.21	587.80	727.87	653.39	474.31	1726.11	551.01	10.91	548.73	21.68	782.10	810.19	762.72	748.35	-1600.659626
52	8	11	-7.87	1.34	587.80	693.33	586.89	24972.38	79737.55	547.89	6.62	543.80	17.61	670.25	568.13	657.30	524.87	-1600.657976
53	8	12	-7.85	1.36	587.80	698.62	622.41	-2168.20	7927.92	548.30	7.28	544.31	18.11	679.98	621.95	667.32	582.25	-1600.657728
54	8	13	-7.73	1.48	587.80	679.39	535.48	-3070.54	13996.12	547.59	6.26	543.22	16.57	652.48	525.28	636.53	478.98	-1600.656142
55	8	14	-7.36	1.85	587.80	712.85	606.88	630.43	3567.02	548.45	7.11	544.86	18.20	692.46	593.04	677.90	548.84	-1600.651542
56	8	15	-6.77	2.44	587.80	788.38	811.06	40716.07	126492.47	549.96	8.97	547.31	20.87	762.12	783.41	719.33	672.98	-1600.644026
57	8	16	-6.74	2.47	587.80	815.17	994.85	340.05	3509.96	550.73	10.68	548.28	23.81	798.91	985.68	761.09	876.80	-1600.643629
58	8	17	-6.68	2.53	587.80	838.08	1109.49	1985.97	6114.24	551.59	12.05	548.81	24.03	809.80	1068.62	752.17	895.21	-1600.642793
59	8	18	-6.65	2.56	587.80	859.17	1185.62	346.12	2375.83	551.88	12.46	549.36	25.13	834.53	1152.78	784.25	997.32	-1600.642410
60	8	19	-6.60	2.61	587.80	851.56	1153.03	283.30	2234.62	552.73	13.77	550.75	26.79	842.39	1160.30	783.14	977.71	-1600.641804
61	8	20	-6.59	2.62	587.80	861.40	1229.70	106.59	2777.34	552.59	13.60	549.97	26.06	848.28	1231.96	792.41	1056.94	-1600.641643
62	8	21	-6.27	2.94	587.80	845.10	830.05	-2254.36	7474.38	553.03	11.27	552.25	20.73	887.47	967.49	837.02	840.35	-1600.637626
63	8	22	-6.20	3.01	587.80	877.07	1053.23	632.27	2239.63	554.15	13.68	553.21	24.46	920.78	1201.70	858.97	1032.19	-1600.636667
64	8	23	-6.09	3.12	587.80	1024.80	1806.99	-200.70	3288.30	554.09	15.79	552.47	30.69	932.92	1550.30	842.90	1261.78	-1600.635252
65	8	24	-5.72	3.49	587.80	1016.92	1460.75	-1882.68	5873.74	556.41	15.28	555.42	24.25	1040.96	1544.03	938.75	1249.08	-1600.630553
66	8	25	-5.59	3.62	587.80	1121.82	1998.78	205.76	1728.84	559.07	19.30	557.40	29.24	1122.80	2023.29	987.62	1605.46	-1600.628965
67	9	1*	-10.94	0.00	661.28	558.63	120.55	911.89	437.95	606.37	1.72	597.08	5.59	524.14	95.68	529.24	98.26	-1800.784275
68	9	2	-10.23	0.71	661.28	614.86	169.02	1258.28	1849.55	607.25	2.85	599.17	9.00	592.48	173.60	597.33	178.44	-1800.774042
69	9	3	-10.00	0.94	661.28	624.01	173.46	26252.53	39147.02	607.61	2.92	600.09	8.97	600.83	185.71	605.48	187.06	-1800.770778
70	9	4	-9.93	1.01	661.28	621.58	81.45	1348.39	494.87	607.11	1.82	598.92	5.70	587.95	95.85	590.36	106.71	-1800.769753
71	9	5	-9.44	1.50	661.28	660.00	440.98	1789.24	4743.58	608.18	6.34	600.96	18.47	631.05	431.27	623.90	399.60	-1800.762794
72	9	6	-9.39	1.55	661.28	658.20	435.58	7858.10	21959.61	608.09	6.11	600.80	17.95	628.26	436.98	620.82	403.99	-1800.761993
73	9	7	-9.15	1.79	661.28	694.49	505.43	-1310.43	7142.85	609.77	8.25	604.30	21.77	683.27	518.31	675.36	483.90	-1800.758576
74	9	8	-9.14	1.80	661.28	678.47	501.14	3358.83	7711.77	608.96	7.62	602.57	21.03	654.88	503.14	645.43	465.88	-1800.758383
75	9	9	-9.12	1.82	661.28	702.09	497.81	878.88	4525.41	609.65	7.47	604.01	19.76	671.78	466.10	670.59	451.04	-1800.758190
76	9	10	-9.09	1.85	661.28	680.29	437.37	-3212.69	13366.82	608.87	6.42	602.67	18.10	661.47	431.81	652.11	394.31	-1800.757765
77	9	11	-9.09	1.85	661.28	683.68	439.05	410.15	3085.88	609.03	6.56	603.00	18.30	668.98	433.32	659.80	396.61	-1800.757748
78	9	12	-9.07	1.87	661.28	689.68	437.22	1174.25	2237.44	609.10	6.16	603.27	17.78	669.03	426.78	661.02	393.23	-1800.757416
79	9	13	-8.90	2.04	661.28	703.37	586.41	885.49	517.94	609.74	8.90	604.02	23.49	679.54	572.86	663.25	518.72	-1800.754982
80	9	14	-8.89	2.05	661.28	711.08	540.54	-164.21	2387.66	609.45	7.50	603.43	19.77	688.23	552.40	680.58	528.03	-1800.754898
81	9	15	-8.86	2.08	661.28	698.52	483.52	-4261.30	15856.24	609.43	7.34	603.77	20.16	678.76	484.30	668.01	448.17	-1800.754427
82	9	16	-8.79	2.15	661.28	739.97	544.56	804.92	2184.75	610.46	7.74	605.42	18.90	723.42	558.02	715.81	534.46	-1800.753438
83	9	17	-8.77	2.17	661.28	718.63	481.20	-775.35	3624.88	609.53	6.26	603.73	16.64	686.21	451.13	673.36	412.97	-1800.753114
84	9	18	-8.76	2.18	661.28	742.82	519.63	19375.40	57605.86	610.43	7.09	605.48	17.61	725.67	514.62	715.09	481.58	-1800.752934
85	9	19	-8.68	2.26	661.28	744.69	725.14	7300.33	15852.63	611.16	10.82	606.59	26.64	732.22	720.74	712.24	653.67	-1800.751812
86	9	20	-8.57	2.37	661.28	727.86	566.55	290.18	2374.16	610.21	7.81	604.88	19.23	702.16	557.55	696.77	536.19	-1800.750247
87	9	21	-8.50	2.44	661.28	758.82	717.20	176.65	2718.01	611.97	11.39	608.06	26.79	751.69	738.75	734.88	681.50	-1800.749330
88	9	22	-8.45	2.49	661.28	788.31	844.47	-2182.38	9463.33	611.76	11.06	607.38	26.28	754.87	777.97	733.32	704.27	-1800.748505
89	9	23	-7.84	3.10	661.28	830.73	885.11	-7638.93	11263.12	611.91	10.36	607.90	25.24	786.22	815.88	757.96	733.15	-1800.739871
90	9	24	-7.79	3.15	661.28	853.92	947.56	2102.31	7460.75	613.27	12.01	609.94	26.63	848.82	964.39	818.25	878.07	-1800.739090
91	9	25	-7.73	3.21	661.28	873.56	1058.75	-2682.66	12456.20	613.89	12.93	609.95	26.60	836.75	1018.88	792.79	881.53	-1800.738193
92	9	26	-7.64	3.30	661.28	904.14	1162.40	295.15	2071.54	615.18	14.81	611.78	28.68	896.35	1181.02	851.85	1043.56	-1800.736913
93	9	27	-7.61	3.33	661.28	874.53	750.54	-917.90	1067.98	613.38	9.11	610.80	22.23	844.72	723.05	818.94	658.74	-1800.736492

Polarizability models:				n*alp	DFT results		AM model		TL model		TE model		RP model		GD model		Etot	
i	n	isomer	Eb	Erel	Aiso	Aaiso	Aiso	Aaiso	Aiso	Aaiso	Aiso	Aaiso	Aiso	Aaiso	Aiso	Aaiso		
94	9	28	-7.59	3.35	661.28	885.03	862.49	-2466.67	4592.86	613.93	10.48	611.34	23.81	861.06	850.98	835.94	788.23	-1800.736289
95	9	29	-7.49	3.45	661.28	930.02	1141.64	-1453.02	1361.96	615.47	13.76	612.59	26.86	902.09	1113.05	860.07	980.27	-1800.734760
96	9	30	-7.47	3.47	661.28	938.10	1192.07	-1410.65	5969.71	616.32	14.95	613.34	27.34	920.11	1198.15	878.97	1071.82	-1800.734463
97	9	31	-7.35	3.59	661.28	910.50	1072.44	512.32	3649.05	615.10	13.28	611.99	25.63	877.25	1046.72	832.30	911.93	-1800.732834
98	9	32	-7.14	3.80	661.28	870.40	694.78	-271.66	2189.29	613.33	8.49	611.05	19.39	841.28	651.02	815.54	588.49	-1800.729710
99	9	33	-6.89	4.05	661.28	959.80	1216.64	553.84	2037.81	617.46	16.83	615.61	30.72	962.15	1273.57	909.87	1124.17	-1800.726133
100	9	34	-6.48	4.46	661.28	1073.18	1589.02	1637.83	5442.28	619.03	17.98	617.37	32.48	1061.12	1601.00	982.41	1371.72	-1800.720265
101	9	35	-6.33	4.61	661.28	1155.15	1929.01	382.40	1992.29	623.04	23.42	620.81	35.59	1153.15	1961.44	1029.19	1582.13	-1800.718134
102	9	36	-6.31	4.63	661.28	1161.32	2001.07	335.94	2284.53	622.10	22.03	619.58	35.01	1149.83	2009.89	1033.68	1651.30	-1800.717925
103	9	37	-5.66	5.28	661.28	1135.24	1061.96	359.65	2738.01	620.97	12.36	621.88	20.53	1165.61	1132.48	1066.99	939.86	-1800.708469
104	10	1*	-12.26	0.00	734.75	630.77	40.26	1775.80	1734.91	667.45	0.69	657.03	2.00	577.61	48.55	588.50	53.87	-2000.892523
105	10	2	-11.22	1.04	734.75	686.16	0.00	-5611.82	1.78	669.05	0.00	660.98	0.00	663.38	0.00	674.39	0.00	-2000.875833
106	10	3	-10.45	1.81	734.75	709.29	424.42	200.98	1995.80	670.14	6.32	662.60	15.50	665.60	374.06	665.19	362.06	-2000.863680
107	10	4	-10.41	1.85	734.75	686.23	388.38	1559.71	3333.54	668.91	5.73	660.41	16.55	650.46	381.64	647.50	360.69	-2000.862955
108	10	5	-10.39	1.87	734.75	686.54	389.67	-2538.44	13366.95	668.89	5.53	660.39	16.01	649.29	365.89	646.23	345.56	-2000.862692
109	10	6	-10.24	2.02	734.75	699.61	376.78	1448.71	1874.94	669.02	5.82	660.55	17.08	669.39	367.69	666.99	348.53	-2000.860211
110	10	7	-10.13	2.13	734.75	702.67	437.58	81.97	2502.23	669.27	7.20	660.88	20.66	670.07	441.27	668.26	426.90	-2000.858469
111	10	8	-10.13	2.13	734.75	715.87	364.42	2945.65	3901.24	669.51	5.53	661.79	15.84	689.44	359.48	685.93	336.35	-2000.858427
112	10	9	-10.12	2.14	734.75	707.23	335.87	2309.81	5161.12	668.96	5.72	660.41	16.49	666.66	338.53	663.73	327.10	-2000.858417
113	10	10	-10.08	2.18	734.75	717.52	366.11	10057.93	26173.37	669.57	5.76	661.91	16.46	692.52	357.45	688.95	334.11	-2000.857750
114	10	11	-10.03	2.23	734.75	741.77	424.73	4944.06	15486.18	670.29	6.50	663.23	17.78	709.46	408.16	709.32	392.70	-2000.856888
115	10	12	-10.01	2.25	734.75	736.92	408.92	-40210.18	123327.02	670.20	6.44	663.05	17.37	704.05	390.87	703.53	374.68	-2000.856661
116	10	13	-9.94	2.32	734.75	719.58	405.44	2937.55	6514.10	669.74	6.84	662.09	18.96	690.27	410.11	686.17	394.39	-2000.855433
117	10	14	-9.90	2.36	734.75	722.46	357.66	3359.45	4314.35	669.55	5.24	662.03	15.05	690.64	347.27	684.50	316.70	-2000.854863
118	10	15	-9.84	2.42	734.75	781.85	496.63	-1703.96	7783.84	671.58	7.54	665.34	17.81	760.71	504.27	760.21	493.08	-2000.853941
119	10	16	-9.81	2.45	734.75	768.75	456.54	-5569.51	19459.58	671.06	6.90	664.66	17.42	743.32	445.71	741.61	430.65	-2000.853440
120	10	17	-9.81	2.45	734.75	737.39	402.95	2176.57	1854.38	670.33	6.82	663.50	18.59	716.60	404.86	712.15	382.54	-2000.853428
121	10	18	-9.81	2.45	734.75	750.18	413.77	1733.58	9337.19	670.62	6.28	664.04	16.53	714.14	395.29	713.91	378.07	-2000.853379
122	10	19	-9.78	2.48	734.75	754.34	432.22	5653.83	11789.63	670.85	7.13	664.42	18.61	724.23	416.55	723.60	404.09	-2000.852884
123	10	20	-9.75	2.51	734.75	732.12	450.81	9802.90	25355.68	670.61	8.09	663.98	22.05	707.43	462.91	703.72	444.42	-2000.852493
124	10	21	-9.73	2.53	734.75	734.08	445.73	-2706.80	10999.30	670.48	8.07	663.60	21.38	712.61	465.46	707.66	445.28	-2000.852151
125	10	22	-9.68	2.58	734.75	748.64	375.50	1730.85	1898.36	670.23	6.12	663.16	16.10	709.46	368.57	706.97	360.26	-2000.851385
126	10	23	-9.68	2.58	734.75	717.11	434.76	-2289.15	9375.32	670.26	7.51	663.34	20.92	691.11	448.78	685.55	426.20	-2000.851347
127	10	24	-9.67	2.59	734.75	739.00	538.35	-955.65	6089.26	670.57	9.16	663.57	25.04	710.32	537.52	700.95	501.16	-2000.851184
128	10	25	-9.64	2.62	734.75	793.73	508.30	-1748.52	5095.07	672.02	7.67	666.33	17.93	771.83	517.75	770.88	503.17	-2000.850757
129	10	26	-9.61	2.65	734.75	743.08	483.65	3379.22	7530.41	670.44	8.26	663.43	22.30	712.90	476.00	703.98	446.58	-2000.850217
130	10	27	-9.58	2.68	734.75	775.29	441.98	1938.76	1485.21	671.04	7.26	664.53	17.62	743.95	465.90	743.83	469.00	-2000.849783
131	10	28	-9.55	2.71	734.75	788.53	431.22	345.87	3661.45	671.34	6.47	665.02	14.66	752.25	425.71	746.67	408.23	-2000.849196
132	10	29	-9.47	2.79	734.75	740.08	400.35	3819.19	8829.47	670.27	6.98	663.46	19.11	718.72	414.32	711.89	389.52	-2000.848016
133	10	30	-9.42	2.84	734.75	748.24	470.37	-626.99	5258.57	670.95	8.74	664.58	22.81	722.40	479.54	711.85	446.51	-2000.847129
134	10	31	-9.40	2.86	734.75	772.93	567.25	1743.50	1745.63	671.52	9.67	665.56	25.36	746.91	566.15	734.22	523.73	-2000.846816
135	10	32	-9.40	2.86	734.75	766.00	558.51	1781.82	2308.76	671.69	10.30	665.74	25.85	744.80	564.06	732.52	523.87	-2000.846810
136	10	33	-9.36	2.90	734.75	781.86	560.50	1110.46	4146.15	671.77	9.44	666.19	25.07	757.94	558.56	747.55	519.01	-2000.846260
137	10	34	-9.35	2.91	734.75	792.77	612.13	-2333.52	12176.09	672.68	11.04	667.76	27.52	785.79	641.37	778.40	611.84	-2000.846072
138	10	35	-9.33	2.93	734.75	777.28	531.83	2122.82	8659.38	671.57	8.92	665.82	23.71	751.87	532.87	741.03	495.36	-2000.845689
139	10	36	-9.32	2.94	734.75	733.69	460.64	2887.91	4129.34	671.17	8.88	665.29	24.49	721.79	467.53	716.05	425.46	-2000.845638
140	10	37	-9.15	3.11	734.75	790.08	684.22	4189.28	6735.03	672.20	11.54	666.53	28.71	771.77	700.68	751.48	637.05	-2000.842865
141	10	38	-9.12	3.14	734.75	801.12	734.07	25337.15	73019.68	672.78	12.61	667.41	30.60	787.31	750.19	764.94	679.38	-2000.842383
142	10	39	-9.09	3.17	734.75	835.66	755.01	-2185.75	8163.60	672.84	11.16	667.31	26.33	795.34	721.70	776.81	660.27	-2000.841926
143	10	40	-9.06	3.20	734.75	841.50	825.39	-163.46	2091.45	672.60	11.60	667.04	28.15	792.37	762.92	773.97	700.37	-2000.841488
144	10	41	-9.02	3.24	734.75	847.92	824.77	52.77	2954.30	672.94	11.54	667.42	27.16	808.28	797.82	785.68	722.26	-2000.840795

Polarizability models:				n*alp	DFT results		AM model		TL model		TE model		RP model		GD model		Etot	
i	n	isomer	Eb	Erel	Aiso	Aaniso	Aiso	Aaniso	Aiso	Aaniso	Aiso	Aaniso	Aiso	Aaniso	Aiso	Aaniso		
145	10	42	-8.92	3.34	734.75	857.95	983.94	63628.43	186734.57	674.74	15.82	670.33	36.11	826.78	939.46	801.02	844.68	-2000.839170
146	10	43	-8.81	3.45	734.75	875.75	941.95	-1391.99	7039.63	674.18	13.91	669.42	31.51	838.67	903.51	814.57	824.90	-2000.837479
147	10	44	-8.80	3.46	734.75	861.39	813.17	94.40	3218.21	673.79	12.03	669.13	28.18	832.66	803.95	809.31	734.48	-2000.837312
148	10	45	-8.79	3.47	734.75	884.17	753.74	-87105.17	258756.84	674.42	11.12	670.51	25.73	850.28	717.82	838.94	680.92	-2000.837165
149	10	46	-8.76	3.50	734.75	873.00	822.89	-3607.71	9495.40	673.82	11.45	669.41	26.79	847.03	778.61	824.16	706.30	-2000.836672
150	10	47	-8.73	3.53	734.75	913.37	987.71	51.51	3771.39	675.51	14.43	671.29	30.24	862.98	907.04	844.64	840.92	-2000.836141
151	10	48	-8.72	3.54	734.75	851.02	870.38	610.50	2265.15	673.33	12.16	668.24	28.50	811.42	828.31	791.52	760.04	-2000.835966
152	10	49	-8.49	3.77	734.75	923.20	801.72	-178.41	4314.99	675.29	11.39	671.92	24.99	906.85	813.11	887.80	766.09	-2000.832335
153	10	50	-8.40	3.86	734.75	964.55	1243.33	-75.57	3252.25	676.92	17.76	673.57	37.27	941.26	1211.90	903.51	1092.16	-2000.831004
154	10	51	-8.38	3.88	734.75	977.47	1113.83	879.35	2006.39	677.71	16.05	674.01	29.35	964.39	1142.85	933.03	1046.09	-2000.830639
155	10	52	-8.21	4.05	734.75	999.12	1335.81	-865.47	5733.49	677.22	17.63	674.12	36.37	940.30	1196.11	905.39	1082.96	-2000.827924
156	10	53	-8.12	4.14	734.75	1008.46	1189.75	804.25	2037.02	681.26	20.98	679.31	36.15	1043.81	1325.71	1005.37	1206.76	-2000.826493
157	10	54	-8.06	4.20	734.75	1017.77	1231.35	729.99	1996.73	682.74	22.83	680.50	36.71	1058.41	1384.95	1014.97	1250.29	-2000.825526
158	10	55	-7.96	4.30	734.75	1093.72	1620.05	39.82	3369.31	680.73	21.34	677.83	38.37	1038.74	1484.60	982.80	1305.55	-2000.823953
159	10	56	-7.75	4.51	734.75	1076.57	1291.72	-7635.08	23773.34	683.10	21.74	681.84	35.38	1114.17	1419.26	1047.38	1223.07	-2000.820529
160	10	57	-7.72	4.54	734.75	1008.46	1201.20	506.50	1939.99	680.38	19.92	677.93	34.98	1025.91	1301.47	979.63	1171.80	-2000.820091
161	10	58	-7.48	4.78	734.75	1011.04	1105.26	778.88	3007.56	680.13	18.31	677.98	31.71	1004.19	1160.64	958.17	1035.29	-2000.816297
162	10	59	-7.47	4.79	734.75	1111.32	1535.22	-699.47	2750.44	680.84	19.77	678.63	36.02	1112.71	1578.41	1047.42	1389.70	-2000.816186
163	10	60	-7.39	4.87	734.75	1078.75	946.32	-727.78	1142.99	679.12	12.32	678.17	27.40	1046.27	919.19	1008.33	852.34	-2000.814879
164	10	61	-7.28	4.98	734.75	1144.14	1411.26	-763.78	714.09	681.52	17.64	680.06	32.31	1117.56	1398.12	1058.62	1239.80	-2000.813077
165	10	62	-6.72	5.54	734.75	1179.01	1596.20	2309.86	5899.79	684.25	22.42	683.33	37.29	1196.48	1698.69	1116.70	1482.14	-2000.804205
166	10	63	-6.25	6.01	734.75	1353.12	2136.35	3477.77	14717.35	687.29	24.62	685.71	37.96	1317.02	2092.17	1164.64	1661.99	-2000.796665
167	11	1*	-12.12	0.00	808.23	730.37	299.49	2512.16	4302.59	728.62	4.82	718.72	13.29	682.42	332.23	685.24	311.34	-2200.979169
168	11	2	-11.75	0.37	808.23	802.70	448.39	540.17	2101.63	730.92	6.99	722.69	15.11	739.94	422.33	747.16	416.52	-2200.972785
169	11	3	-11.69	0.43	808.23	785.76	347.71	1045.58	3248.36	730.43	5.47	722.10	12.09	722.90	307.07	727.67	289.30	-2200.971643
170	11	4	-11.66	0.46	808.23	737.70	257.02	1693.04	1327.52	728.83	3.91	719.32	10.65	688.20	255.07	689.10	227.92	-2200.971201
171	11	5	-11.62	0.50	808.23	744.76	318.50	364.65	1927.60	729.04	5.19	719.64	14.09	701.37	340.55	708.56	328.75	-2200.970553
172	11	6	-11.38	0.74	808.23	741.20	343.86	-19049.34	59724.06	729.14	5.92	719.81	16.18	692.53	350.51	699.22	345.72	-2200.966341
173	11	7	-11.37	0.75	808.23	762.65	343.91	1533.83	3549.60	729.79	6.19	721.00	15.60	706.88	334.02	715.18	331.35	-2200.966049
174	11	8	-11.36	0.76	808.23	755.00	259.23	639.90	1177.06	729.62	4.21	720.92	9.94	685.51	214.59	693.05	186.89	-2200.965980
175	11	9	-11.29	0.83	808.23	736.33	289.25	-1017.23	3907.89	728.64	4.98	718.73	14.27	692.49	287.47	698.64	281.54	-2200.964741
176	11	10	-11.18	0.94	808.23	769.30	259.54	-1034.60	16089.05	729.69	3.65	721.42	9.95	740.55	253.35	744.54	227.04	-2200.962744
177	11	11	-11.14	0.98	808.23	751.51	363.92	3380.30	7779.63	729.60	7.26	720.59	19.37	717.20	386.87	723.82	394.07	-2200.962013
178	11	12	-11.05	1.07	808.23	757.72	308.66	2839.10	3831.78	729.38	5.57	720.36	15.15	715.13	311.26	721.20	306.53	-2200.960516
179	11	13	-10.98	1.14	808.23	773.30	309.63	-1139.16	5086.11	730.03	5.49	721.96	14.61	744.12	309.01	747.42	295.89	-2200.959324
180	11	14	-10.95	1.17	808.23	754.94	372.71	975.45	1768.80	729.60	7.11	720.67	19.07	716.95	388.07	723.21	394.72	-2200.958725
181	11	15	-10.87	1.25	808.23	715.03	393.12	1122.91	873.24	729.34	7.37	720.29	21.03	680.04	368.32	676.58	349.27	-2200.957278
182	11	16	-10.80	1.32	808.23	858.82	413.89	-2160.88	2362.54	732.77	6.44	726.85	12.94	839.47	422.90	846.54	411.49	-2200.956095
183	11	17	-10.72	1.40	808.23	755.60	467.82	1048.35	476.07	729.78	8.86	720.89	24.96	722.43	466.21	720.54	449.50	-2200.954692
184	11	18	-10.64	1.48	808.23	769.48	291.30	1245.86	1646.11	729.91	5.29	721.90	14.31	731.71	285.45	743.11	285.13	-2200.953208
185	11	19	-10.57	1.55	808.23	756.52	467.77	1549.39	1893.72	730.60	8.93	722.73	23.98	717.87	440.74	720.25	438.05	-2200.952052
186	11	20	-10.53	1.59	808.23	739.87	390.81	1691.23	1363.61	730.07	7.65	722.03	22.15	706.21	375.48	705.74	356.83	-2200.951423
187	11	21	-10.53	1.59	808.23	745.20	371.99	-44890.96	139051.65	730.40	7.59	722.84	21.61	710.37	346.99	712.13	335.06	-2200.951349
188	11	22	-10.46	1.66	808.23	774.98	460.68	2229.91	3875.38	730.38	8.64	722.35	23.83	746.13	456.62	742.61	430.59	-2200.953094
189	11	23	-10.43	1.69	808.23	803.11	473.80	1892.34	11558.48	731.13	8.83	723.91	23.57	774.51	475.86	771.33	453.10	-2200.949547
190	11	24	-10.41	1.71	808.23	763.10	474.53	699.35	1318.75	730.05	8.51	721.76	23.45	728.17	474.95	724.43	456.15	-2200.949192
191	11	25	-10.39	1.73	808.23	786.03	502.91	18029.74	49658.02	730.68	9.35	722.82	25.57	751.21	502.02	748.01	480.08	-2200.948905
192	11	26	-10.39	1.73	808.23	778.06	436.10	2995.77	5897.16	730.95	8.67	723.67	23.44	738.72	417.48	739.50	405.68	-2200.948903
193	11	27	-10.32	1.80	808.23	801.69	488.05	6385.69	15560.52	731.20	9.18	724.04	24.47	775.62	489.97	770.17	462.76	-2200.947679
194	11	28	-10.27	1.85	808.23	774.41	379.68	1593.58	1614.50	730.44	7.71	722.73	20.64	730.98	388.99	729.21	381.95	-2200.946740
195	11	29	-10.19	1.93	808.23	801.70	412.95	1214.41	4028.04	730.41	6.92	722.80	19.96	772.26	417.61	761.89	393.99	-2200.945397

Polarizability models:					n*alp Aiso	DFT results		AM model		TL model		TE model		RP model		GD model		Etot
i	n	isomer	Eb	Erel		Aiso	Aaniso	Aiso	Aaniso	Aiso	Aaniso	Aiso	Aaniso	Aiso	Aaniso	Aiso	Aaniso	
196	11	30	-10.18	1.94	808.23	811.71	478.99	47163.85	136243.69	730.99	8.12	723.81	22.25	781.79	473.34	774.13	441.28	-2200.945197
197	11	31	-10.18	1.94	808.23	820.48	487.65	-16918.07	56879.88	731.90	9.56	725.51	24.60	799.44	493.26	793.23	464.90	-2200.945192
198	11	32	-10.16	1.96	808.23	766.22	404.19	711.56	3242.27	730.80	8.63	723.51	23.69	748.17	415.50	744.14	384.87	-2200.944921
199	11	33	-10.16	1.96	808.23	797.39	413.38	2106.08	2041.30	730.32	7.08	722.56	20.55	767.05	416.93	756.84	392.78	-2200.944805
200	11	34	-10.13	1.99	808.23	796.49	506.34	134.04	3906.70	731.38	10.40	724.28	27.04	771.42	525.76	764.76	500.31	-2200.944316
201	11	35	-10.09	2.03	808.23	823.24	549.93	-5407.66	21169.56	732.38	10.78	726.35	27.47	799.88	566.19	797.39	550.97	-2200.943623
202	11	36	-10.07	2.05	808.23	871.60	624.47	-341.07	1566.91	733.50	9.58	727.90	21.74	815.08	549.08	809.28	529.79	-2200.943252
203	11	37	-10.05	2.07	808.23	834.01	515.62	3563.80	6866.03	732.38	10.33	726.32	25.94	811.86	521.25	804.28	491.84	-2200.942870
204	11	38	-10.02	2.10	808.23	816.74	551.29	-4059.45	15737.15	731.89	10.95	725.10	27.95	785.66	547.55	778.04	517.63	-2200.942491
205	11	39	-9.98	2.14	808.23	826.73	503.87	-1042.59	3239.05	731.79	9.08	725.42	23.80	804.90	499.98	794.96	463.29	-2200.941653
206	11	40	-9.97	2.15	808.23	817.80	429.33	1647.87	5849.99	730.98	7.21	724.04	20.27	791.39	405.26	780.24	376.68	-2200.941612
207	11	41	-9.93	2.19	808.23	816.15	551.39	-21937.84	68930.97	732.35	11.07	726.47	29.88	791.80	539.59	786.95	507.96	-2200.940797
208	11	42	-9.92	2.20	808.23	930.67	955.11	471.09	1321.82	736.38	15.12	730.71	27.53	876.12	879.87	855.52	804.12	-2200.940623
209	11	43	-9.90	2.22	808.23	822.87	568.36	1905.83	1925.74	732.07	10.96	725.77	29.39	796.88	578.70	786.17	543.60	-2200.940326
210	11	44	-9.84	2.28	808.23	886.57	739.93	-1594.58	5745.51	733.08	11.29	726.69	26.03	844.60	698.82	829.77	639.32	-2200.939320
211	11	45	-9.81	2.31	808.23	824.62	474.51	-3127.37	13340.80	732.32	10.34	726.28	25.42	793.35	469.32	785.46	442.73	-2200.938732
212	11	46	-9.79	2.33	808.23	881.93	485.91	2316.48	5412.48	733.10	8.04	727.52	19.72	858.43	498.80	848.17	480.40	-2200.938458
213	11	47	-9.77	2.35	808.23	874.98	740.12	985.63	2080.27	732.82	11.90	726.35	29.00	835.25	723.86	824.26	688.55	-2200.938107
214	11	48	-9.75	2.37	808.23	844.65	681.84	-309.63	5328.93	732.84	13.07	726.61	32.08	819.76	695.14	805.15	647.27	-2200.937683
215	11	49	-9.74	2.38	808.23	883.05	494.26	110.47	3889.38	733.16	8.27	727.64	20.47	860.87	507.50	850.24	487.87	-2200.937580
216	11	50	-9.72	2.40	808.23	837.31	593.64	-72.65	3504.48	733.03	12.51	727.25	29.84	819.40	614.69	811.49	588.91	-2200.937102
217	11	51	-9.70	2.42	808.23	854.09	528.88	-381.55	2988.59	733.11	11.00	727.76	27.07	832.31	545.77	823.48	514.88	-2200.936849
218	11	52	-9.70	2.42	808.23	870.62	815.09	-4542.98	16535.77	733.43	14.25	727.57	34.14	838.62	810.25	819.16	741.65	-2200.936791
219	11	53	-9.69	2.43	808.23	902.17	804.20	-6991.82	22584.46	732.98	12.60	726.50	29.41	844.90	762.25	825.96	701.28	-2200.936572
220	11	54	-9.67	2.45	808.23	891.01	951.52	1414.42	1939.31	734.99	17.44	729.65	39.93	864.57	930.64	841.21	843.93	-2200.936305
221	11	55	-9.65	2.47	808.23	857.90	629.07	2768.71	4439.84	733.52	12.88	728.11	30.82	840.31	650.21	829.28	615.34	-2200.936014
222	11	56	-9.56	2.56	808.23	908.66	815.76	-1792.46	8520.66	734.10	13.33	728.43	29.76	870.79	801.15	852.90	745.38	-2200.934422
223	11	57	-9.40	2.72	808.23	941.80	951.40	-223.02	3714.94	735.36	15.80	730.38	34.20	908.09	934.25	888.74	870.25	-2200.931479
224	11	58	-9.34	2.78	808.23	1000.01	1004.79	273.71	2723.70	737.40	15.50	732.80	28.67	972.44	993.14	947.19	902.99	-2200.930545
225	11	59	-9.34	2.78	808.23	897.92	827.48	-3445.05	15094.42	735.86	16.17	732.04	37.10	856.52	775.77	852.23	730.08	-2200.930488
226	11	60	-9.29	2.83	808.23	912.98	766.14	3454.48	9335.78	734.28	12.65	729.31	30.90	876.35	743.46	853.11	680.98	-2200.929657
227	11	61	-9.29	2.83	808.23	938.96	844.34	187.54	3288.09	734.84	13.75	729.73	30.62	896.89	804.87	874.51	741.50	-2200.929601
228	11	62	-9.26	2.86	808.23	870.21	631.16	598.43	6980.83	733.38	12.25	728.38	30.26	859.10	657.36	842.12	609.15	-2200.929151
229	11	63	-9.26	2.86	808.23	957.08	715.31	1891.02	6571.44	735.03	11.34	730.51	24.22	924.63	731.18	915.47	713.71	-2200.929096
230	11	64	-8.98	3.14	808.23	976.72	825.81	2866.39	8340.38	736.47	13.35	732.81	29.83	949.30	825.95	922.67	755.66	-2200.924178
231	11	65	-8.79	3.33	808.23	1052.68	1292.98	-2071.14	7949.74	737.31	18.49	733.35	38.48	980.01	1171.01	947.46	1065.30	-2200.920944
232	11	66	-8.41	3.71	808.23	1139.88	1321.73	-1298.73	3179.71	741.65	19.57	738.99	34.99	1103.97	1293.81	1063.24	1169.02	-2200.914179
233	11	67	-8.35	3.77	808.23	1085.70	1131.34	617.36	4111.00	742.32	21.01	739.94	34.51	1097.26	1220.65	1058.11	1111.59	-2200.913080
234	11	68	-8.33	3.79	808.23	1154.70	1490.40	544.96	1116.98	741.41	20.72	738.49	37.32	1121.50	1429.21	1066.24	1258.44	-2200.912731
235	12	1*	-12.02	0.00	881.70	795.78	369.70	2593.20	4538.64	789.44	8.13	780.49	20.69	746.01	360.50	752.91	360.23	-2401.066331
236	12	2	-11.88	0.14	881.70	798.05	380.02	1018.38	1199.72	788.62	7.46	778.99	20.06	751.27	401.17	752.29	382.83	-2401.063762
237	12	3	-11.87	0.15	881.70	782.02	307.94	3524.06	7657.26	789.02	6.98	779.95	18.59	736.59	306.70	743.51	290.15	-2401.063484
238	12	4	-11.77	0.25	881.70	787.86	301.90	2630.81	3954.54	788.69	6.21	779.30	16.67	745.97	300.15	745.25	271.73	-2401.061643
239	12	5	-11.76	0.26	881.70	767.98	346.06	2184.11	3254.78	788.21	7.40	778.07	20.56	709.74	346.15	716.32	341.65	-2401.061334
240	12	6	-11.75	0.27	881.70	840.14	423.28	-1041.25	7476.18	790.09	8.46	781.76	20.82	783.10	414.92	787.74	402.29	-2401.061262
241	12	7	-11.74	0.28	881.70	782.17	351.78	8014.20	14961.08	788.71	7.76	779.16	21.05	734.93	352.27	739.15	346.84	-2401.061060
242	12	8	-11.73	0.29	881.70	834.63	446.45	7798.99	20037.16	789.65	8.48	781.01	21.40	780.84	473.19	780.77	448.62	-2401.060746
243	12	9	-11.65	0.37	881.70	826.65	369.95	26031.20	73198.86	789.78	7.54	781.38	18.72	772.39	356.81	776.55	341.45	-2401.059249
244	12	10	-11.60	0.42	881.70	883.22	334.15	1564.89	6937.12	790.78	5.73	783.25	13.78	826.85	325.01	823.33	306.96	-2401.058340
245	12	11	-11.57	0.45	881.70	834.79	288.07	3045.01	3934.94	789.04	4.88	780.26	13.25	792.89	321.37	785.08	296.40	-2401.057710
246	12	12	-11.56	0.46	881.70	929.51	779.03	39.44	3205.27	792.21	12.54	784.74	27.25	876.61	792.05	861.54	717.98	-2401.057585

Polarizability models:					n*alp	DFT results		AM model		TL model		TE model		RP model		GD model		Etot
i	n	isomer	Eb	Erel	Aiso	Aaiso	Aaiso	Aaiso	Aaiso	Aaiso	Aaiso	Aaiso	Aaiso	Aaiso	Aaiso	Aaiso	Aaiso	
247	12	13	-11.53	0.49	881.70	828.06	389.35	3567.01	6343.23	789.65	7.69	781.14	19.36	772.29	391.12	773.56	369.51	-2401.056938
248	12	14	-11.52	0.50	881.70	837.48	441.08	3058.10	5124.37	790.01	8.60	781.76	21.42	785.74	447.98	786.29	428.53	-2401.056853
249	12	15	-11.50	0.52	881.70	839.14	398.31	4309.38	7113.76	789.48	6.92	780.91	18.04	794.39	399.62	792.75	372.92	-2401.056377
250	12	16	-11.48	0.54	881.70	818.90	365.58	4462.49	5298.83	789.09	6.94	780.25	18.44	775.88	379.90	779.61	359.97	-2401.055959
251	12	17	-11.47	0.55	881.70	834.54	387.27	397.99	2454.93	789.60	7.80	780.98	20.06	792.59	413.03	795.21	395.47	-2401.055867
252	12	18	-11.46	0.56	881.70	800.39	458.62	26419.77	76808.45	789.11	9.34	779.84	24.71	743.58	479.41	750.35	480.70	-2401.055562
253	12	19	-11.42	0.60	881.70	839.76	400.73	34870.78	101818.68	789.92	8.52	781.51	21.56	803.90	418.75	807.61	407.27	-2401.054945
254	12	20	-11.42	0.60	881.70	785.81	288.11	1847.15	2919.72	788.64	6.33	779.23	17.78	751.64	286.33	757.69	273.65	-2401.054857
255	12	21	-11.41	0.61	881.70	823.62	420.25	-28481.21	88176.29	789.77	9.33	781.13	23.64	776.45	430.25	781.38	426.73	-2401.054615
256	12	22	-11.40	0.62	881.70	814.68	360.13	2555.56	5245.56	789.01	7.31	779.87	19.59	774.92	364.95	779.01	348.42	-2401.054506
257	12	23	-11.40	0.62	881.70	812.29	347.13	2686.10	4551.01	788.96	7.36	779.74	19.77	779.12	355.68	782.55	344.27	-2401.054459
258	12	24	-11.39	0.63	881.70	817.73	422.51	3296.11	7448.36	789.24	8.43	780.27	22.12	776.58	444.11	782.21	437.52	-2401.054390
259	12	25	-11.39	0.63	881.70	847.55	287.27	1023.76	114.66	789.18	4.45	780.69	12.08	809.70	304.68	806.14	282.08	-2401.054240
260	12	26	-11.36	0.66	881.70	833.34	400.73	14034.74	33773.45	789.66	7.40	781.24	19.49	789.88	386.03	792.55	373.49	-2401.053700
261	12	27	-11.33	0.69	881.70	834.89	408.24	257.79	6423.24	789.43	7.36	780.77	19.39	790.00	422.10	791.90	405.21	-2401.053071
262	12	28	-11.31	0.71	881.70	784.21	394.43	3080.40	6226.92	788.56	8.26	778.76	22.18	720.46	384.75	727.68	384.02	-2401.052825
263	12	29	-11.28	0.74	881.70	835.72	375.75	2908.37	5043.91	789.75	7.72	781.42	20.08	800.95	385.46	802.12	365.21	-2401.052191
264	12	30	-11.27	0.75	881.70	812.15	438.94	-10216.96	33891.12	789.53	9.68	780.65	25.39	777.74	453.61	781.41	451.44	-2401.052099
265	12	31	-11.27	0.75	881.70	825.07	408.48	655.62	1490.26	789.23	8.31	780.09	22.16	780.85	421.11	783.85	409.16	-2401.052001
266	12	32	-11.27	0.75	881.70	824.49	457.93	-5780.63	20404.49	789.58	9.04	780.84	23.41	776.32	463.35	779.06	452.77	-2401.051954
267	12	33	-11.27	0.75	881.70	804.54	445.68	15.25	3721.78	789.13	9.09	779.90	23.90	752.11	442.29	757.64	442.39	-2401.051950
268	12	34	-11.26	0.76	881.70	961.72	434.37	-297.14	2521.47	793.34	7.12	787.46	15.01	886.59	400.36	887.44	389.53	-2401.051860
269	12	35	-11.25	0.77	881.70	910.36	400.51	818.13	2763.75	791.59	6.62	784.53	14.42	852.95	396.80	849.43	384.50	-2401.051624
270	12	36	-11.22	0.80	881.70	842.20	233.76	3989.03	4477.58	789.28	3.72	780.94	10.15	798.79	227.53	790.99	197.71	-2401.051098
271	12	37	-11.21	0.81	881.70	952.27	516.49	454.66	3196.22	793.04	8.26	786.98	16.89	876.52	453.01	874.88	424.65	-2401.050853
272	12	38	-11.19	0.83	881.70	920.50	680.05	574.46	6932.76	791.61	10.37	784.38	23.32	850.52	605.46	840.46	548.21	-2401.050506
273	12	39	-11.19	0.83	881.70	845.97	407.08	-2318.01	10129.86	790.07	8.53	781.92	21.96	812.43	417.43	815.04	405.75	-2401.050498
274	12	40	-11.19	0.83	881.70	1048.01	1057.42	673.23	1786.80	797.25	17.27	790.84	28.25	971.77	999.58	961.45	938.04	-2401.050470
275	12	41	-11.17	0.85	881.70	917.46	553.58	-548.07	3049.39	792.06	9.01	785.28	20.04	842.06	494.10	839.56	465.16	-2401.050179
276	12	42	-11.17	0.85	881.70	847.12	368.42	-7754.18	29643.22	789.90	7.47	781.81	19.34	814.11	369.84	817.60	352.77	-2401.050046
277	12	43	-11.16	0.86	881.70	796.95	311.32	1190.42	1628.97	789.01	7.23	779.91	19.30	768.45	334.31	773.70	318.14	-2401.049983
278	12	44	-11.16	0.86	881.70	927.66	700.60	998.57	1772.52	792.38	11.73	785.27	25.61	876.58	701.83	877.66	671.84	-2401.049971
279	12	45	-11.16	0.86	881.70	858.87	322.41	518.66	3082.98	790.10	5.51	782.24	13.57	799.53	316.72	794.50	293.76	-2401.049949
280	12	46	-11.15	0.87	881.70	822.19	313.09	298.67	325.16	788.45	6.11	778.75	17.71	775.12	330.47	775.97	327.05	-2401.049784
281	12	47	-11.13	0.89	881.70	845.27	401.40	23554.17	69211.34	789.86	8.07	781.63	21.26	811.42	408.18	812.13	394.81	-2401.049397
282	12	48	-11.10	0.92	881.70	843.81	345.16	2415.72	7039.00	789.32	6.17	780.66	16.47	804.74	343.78	803.91	319.75	-2401.048791
283	12	49	-11.10	0.92	881.70	884.27	312.61	-8572.12	26651.29	790.81	5.15	783.63	12.69	830.32	300.95	830.18	277.59	-2401.048744
284	12	50	-11.09	0.93	881.70	1013.90	905.36	1275.69	2876.50	796.26	15.21	790.01	25.33	938.09	833.75	921.33	747.56	-2401.048601
285	12	51	-11.09	0.93	881.70	849.51	411.59	3038.02	3207.67	789.78	7.74	781.43	20.09	810.28	422.69	811.44	406.45	-2401.048595
286	12	52	-11.08	0.94	881.70	847.45	285.69	-38.61	5426.19	789.71	4.99	781.75	13.43	809.75	300.41	804.91	280.69	-2401.048396
287	12	53	-11.08	0.94	881.70	845.48	500.13	-505.15	4520.36	790.34	10.40	782.19	26.33	813.44	527.69	817.87	527.70	-2401.048347
288	12	54	-11.05	0.97	881.70	826.15	440.27	3154.00	6210.29	789.93	9.96	781.44	26.01	787.35	427.48	788.45	417.84	-2401.047778
289	12	55	-11.04	0.98	881.70	818.67	445.52	1070.12	529.51	789.81	9.43	781.50	26.62	778.27	424.94	779.81	417.77	-2401.047698
290	12	56	-11.04	0.98	881.70	835.77	352.81	2239.56	3626.64	789.64	7.03	781.38	18.41	807.80	348.51	809.97	325.46	-2401.047654
291	12	57	-11.04	0.98	881.70	860.57	259.13	-5900.27	25661.51	789.76	4.09	782.06	11.26	832.54	258.00	829.09	233.22	-2401.047594
292	12	58	-11.03	0.99	881.70	835.37	503.32	2437.63	3708.93	790.10	10.51	781.83	29.10	798.18	502.02	796.82	484.54	-2401.047389
293	12	59	-11.01	1.01	881.70	810.29	477.86	1296.41	1311.32	789.65	9.24	781.21	25.93	767.61	447.90	762.75	428.13	-2401.047004
294	12	60	-11.01	1.01	881.70	862.79	351.35	-514.55	30538.90	790.10	6.08	782.56	15.92	832.09	339.62	831.90	307.25	-2401.046994
295	12	61	-11.00	1.02	881.70	790.82	421.72	1561.83	1687.58	789.47	9.49	780.75	24.87	745.81	399.54	743.15	381.52	-2401.046915
296	12	62	-11.00	1.02	881.70	821.23	490.58	2551.18	4181.13	790.33	9.93	782.45	26.90	778.94	455.37	779.59	451.59	-2401.046844
297	12	63	-11.00	1.02	881.70	934.38	722.62	383.66	3236.21	792.57	11.97	785.53	26.20	877.09	709.49	878.05	689.57	-2401.046822

Polarizability models:					n*alp Aiso	DFT results		AM model		TL model		TE model		RP model		GD model		Etot
i	n	isomer	Eb	Erel		Aiso	Aaniso	Aiso	Aaniso	Aiso	Aaniso	Aiso	Aaniso	Aiso	Aaniso	Aiso	Aaniso	
298	12	64	-10.99	1.03	881.70	867.76	426.91	-13857.51	42119.90	791.01	9.22	783.91	22.85	839.67	436.22	838.49	415.16	-2401.046707
299	12	65	-10.99	1.03	881.70	845.08	470.50	6670.51	19491.98	790.54	10.71	782.53	26.54	809.54	493.53	810.42	484.65	-2401.046676
300	12	66	-10.96	1.06	881.70	794.68	302.23	78.15	2335.56	788.67	6.65	779.37	18.17	760.70	309.94	771.33	296.74	-2401.046122
301	12	67	-10.96	1.06	881.70	840.69	498.02	4560.79	10415.61	790.31	10.16	782.33	28.04	807.35	498.01	804.72	479.61	-2401.046114
302	12	68	-10.95	1.07	881.70	821.38	356.65	2.76	3693.94	789.67	8.15	781.47	21.55	777.47	348.86	786.00	353.10	-2401.045967
303	12	69	-10.93	1.09	881.70	809.66	485.82	-2197.45	4516.32	789.56	10.54	780.62	27.65	764.06	480.14	770.39	488.08	-2401.045585
304	12	70	-10.85	1.17	881.70	822.37	464.83	1616.12	1422.11	789.92	9.48	781.81	26.96	774.67	433.55	774.89	423.40	-2401.044049
305	12	71	-10.85	1.17	881.70	849.14	408.43	1318.66	7056.72	790.14	8.91	782.13	23.74	811.45	425.84	811.73	419.01	-2401.043935
306	12	72	-10.85	1.17	881.70	858.37	316.22	3431.21	4869.46	789.78	6.16	781.82	16.80	826.72	334.28	823.38	324.07	-2401.043918
307	12	73	-10.84	1.18	881.70	851.18	424.58	-15300.37	49319.84	790.54	9.94	782.71	24.57	812.20	441.30	813.28	437.19	-2401.043710
308	12	74	-10.79	1.23	881.70	887.23	707.23	1808.07	3189.59	791.31	13.12	783.59	32.11	842.31	705.35	839.38	683.74	-2401.042849
309	12	75	-10.78	1.24	881.70	845.53	441.65	-3489.46	14532.66	790.31	9.81	782.32	25.09	806.25	451.83	806.88	445.33	-2401.042624
310	12	76	-10.77	1.25	881.70	855.78	366.79	668.62	1625.95	790.30	7.09	783.01	18.64	813.23	350.60	819.29	344.58	-2401.042357
311	12	77	-10.76	1.26	881.70	844.12	485.11	926.27	6629.10	790.12	9.52	782.12	26.97	810.10	478.40	804.89	454.99	-2401.042327
312	12	78	-10.76	1.26	881.70	839.01	495.20	-187.03	5553.22	790.74	10.24	783.43	28.33	801.66	490.07	798.18	470.82	-2401.042296
313	12	79	-10.75	1.27	881.70	849.59	393.76	532.08	5079.35	790.32	8.27	782.75	22.30	812.38	407.47	815.58	396.72	-2401.042046
314	12	80	-10.74	1.28	881.70	857.92	524.12	-4248.08	24343.31	791.59	11.62	784.89	30.33	832.85	537.83	832.93	524.64	-2401.041856
315	12	81	-10.73	1.29	881.70	834.58	487.86	1654.84	2149.57	790.48	10.80	782.76	29.24	799.93	479.42	799.42	468.41	-2401.041717
316	12	82	-10.72	1.30	881.70	876.55	498.71	8854.74	25530.69	791.72	11.30	784.99	27.74	847.44	497.87	845.28	476.24	-2401.041479
317	12	83	-10.72	1.30	881.70	852.98	508.79	-3856.11	23929.26	791.03	10.56	783.97	28.84	822.38	503.55	817.38	485.59	-2401.041459
318	12	84	-10.71	1.31	881.70	849.84	490.52	2804.04	4076.58	790.94	10.26	783.86	28.38	812.75	485.09	811.78	467.53	-2401.041288
319	12	85	-10.70	1.32	881.70	948.74	838.52	-50.93	3246.70	793.63	15.40	786.89	33.11	907.72	842.64	901.80	811.58	-2401.041150
320	12	86	-10.70	1.32	881.70	925.16	405.43	1367.93	4055.86	792.13	7.21	785.53	16.71	882.28	416.70	885.09	418.19	-2401.041061
321	12	87	-10.68	1.34	881.70	926.04	625.96	1047.72	6177.55	792.09	10.78	785.23	24.92	881.95	624.03	882.80	608.40	-2401.040738
322	12	88	-10.64	1.38	881.70	863.34	513.96	548.50	5239.97	791.34	10.51	784.49	28.20	822.61	478.32	824.80	472.38	-2401.039941
323	12	89	-10.64	1.38	881.70	871.93	539.13	3439.90	8043.71	791.32	11.41	784.18	29.88	836.58	541.28	831.81	516.29	-2401.039874
324	12	90	-10.63	1.39	881.70	856.32	379.08	-1308.09	7016.65	790.42	7.90	783.11	19.97	816.78	375.46	824.56	357.54	-2401.039735
325	12	91	-10.63	1.39	881.70	855.45	503.63	2853.34	4374.12	790.88	11.01	783.40	28.05	824.93	504.77	819.10	475.02	-2401.039732
326	12	92	-10.62	1.40	881.70	953.67	620.38	872.67	2463.23	793.26	10.25	787.51	22.22	924.69	620.23	921.62	593.93	-2401.039566
327	12	93	-10.61	1.41	881.70	880.29	444.98	1772.07	3002.39	791.36	8.88	784.70	21.40	840.23	431.88	850.37	418.28	-2401.039399
328	12	94	-10.61	1.41	881.70	862.36	561.08	5145.91	11525.97	791.46	11.12	784.55	29.10	825.27	551.95	827.24	548.90	-2401.039344
329	12	95	-10.53	1.49	881.70	888.29	563.64	-706.44	5874.91	792.19	12.50	785.78	30.20	869.76	588.76	866.95	567.14	-2401.037824
330	12	96	-10.47	1.55	881.70	866.83	464.51	-905.29	6584.12	791.43	11.10	784.58	27.15	835.88	486.59	830.78	468.59	-2401.036761
331	12	97	-10.45	1.57	881.70	888.02	461.56	-779.37	8207.73	792.24	11.22	786.23	26.75	864.76	472.49	861.14	452.14	-2401.036408
332	12	98	-10.42	1.60	881.70	893.27	517.12	-9218.25	32605.05	791.75	10.37	785.38	27.55	863.22	514.87	852.65	483.14	-2401.035842
333	12	99	-10.41	1.61	881.70	917.94	863.74	-4824.83	17711.66	793.04	17.06	786.35	40.63	880.27	849.63	865.04	786.49	-2401.035638
334	12	100	-10.34	1.68	881.70	899.53	527.08	55181.47	159693.69	791.81	10.39	785.47	27.48	865.12	529.74	854.68	500.06	--2401.03424
335	12	101	-10.32	1.70	881.70	938.47	913.09	2262.91	3734.58	794.65	19.11	788.76	43.39	908.89	906.02	894.01	845.67	--2401.03384
336	12	102	-10.30	1.72	881.70	922.96	827.29	54216.24	159419.97	793.28	16.39	787.04	38.70	889.79	817.72	875.43	762.88	--2401.03345
337	12	103	-10.29	1.73	881.70	934.80	889.86	-62432.60	190541.84	793.99	17.95	788.01	41.80	906.37	882.32	889.87	817.72	--2401.03319
338	12	104	-10.25	1.77	881.70	926.91	846.27	-5341.11	19352.45	793.70	17.27	787.64	40.31	893.63	840.69	878.38	781.60	--2401.03258
339	12	105	-10.25	1.77	881.70	928.47	557.94	8495.32	19810.86	792.82	11.09	787.09	27.75	893.38	555.01	883.90	524.53	--2401.03246
340	12	106	-10.24	1.78	881.70	968.22	976.42	-6080.43	21091.32	795.36	17.63	789.51	37.04	920.22	918.24	919.78	908.04	--2401.03230
341	12	107	-10.22	1.80	881.70	899.91	573.68	-142.68	7148.89	792.51	13.15	786.41	31.83	876.40	604.16	869.48	583.02	--2401.03189
342	12	108	-10.20	1.82	881.70	919.21	605.76	979.61	8900.86	793.37	13.42	788.04	31.35	901.51	621.55	892.13	585.67	--2401.03148
343	12	109	-10.16	1.86	881.70	919.67	589.68	5529.64	17335.93	793.27	12.50	788.18	30.78	896.50	600.78	889.88	586.90	--2401.03078
344	12	110	-10.12	1.90	881.70	936.35	629.14	10327.25	58459.50	794.27	13.17	790.22	34.93	911.48	618.29	910.31	600.99	--2401.03002
345	12	111	-10.12	1.90	881.70	963.96	826.37	762.69	1189.18	794.02	14.71	788.20	33.24	923.24	789.45	910.38	735.90	--2401.03002
346	12	112	-10.07	1.95	881.70	1002.84	890.10	-2466.88	6250.93	795.18	15.87	790.07	34.36	964.99	866.67	950.24	811.25	--2401.02904
347	12	113	-10.06	1.96	881.70	967.82	921.00	105337.58	312124.81	795.74	19.52	790.81	42.98	944.96	922.12	926.78	851.46	--2401.02883
348	12	114	-10.02	2.00	881.70	955.45	874.15	3290.90	5946.12	794.96	18.12	789.91	40.83	929.69	881.08	912.44	813.57	--2401.02809

Polarizability models:				n*alp	DFT results		AM model		TL model		TE model		RP model		GD model		Etot	
i	n	isomer	Eb	Erel	Aiso	Aaniso	Aiso	Aaniso	Aiso	Aaniso	Aiso	Aaniso	Aiso	Aaniso	Aiso	Aaniso		
349	12	115	-9.96	2.06	881.70	997.52	983.96	273.76	3607.01	797.69	21.50	793.71	44.48	976.18	984.35	964.47	936.99	--2401.02699
350	12	116	-9.89	2.13	881.70	957.71	838.97	-665.56	5667.37	794.80	17.13	789.80	38.70	923.53	838.81	902.47	771.99	--2401.02570
351	12	117	-9.85	2.17	881.70	991.88	620.01	5658.93	16427.96	795.08	11.87	791.02	27.71	971.14	637.39	957.09	604.08	--2401.02491
352	12	118	-9.84	2.18	881.70	1007.48	801.47	565.63	4076.58	795.19	13.95	790.64	31.16	976.95	800.67	961.19	750.40	--2401.02473
353	12	119	-9.84	2.18	881.70	978.96	661.65	-471.50	2975.52	793.57	11.04	788.27	26.01	937.44	641.80	916.51	594.84	--2401.02469
354	12	120	-9.81	2.21	881.70	1030.68	1024.73	1031.80	3331.57	796.83	18.70	792.70	39.38	1001.00	1022.31	992.75	991.03	--2401.02408
355	12	121	-9.80	2.22	881.70	990.90	1014.73	-746.59	5345.81	796.47	20.75	791.80	44.81	961.64	1018.26	934.88	928.34	--2401.02380
356	12	122	-9.77	2.25	881.70	1028.91	1019.45	622.02	1297.48	800.08	21.60	796.01	36.87	995.27	1008.44	974.20	942.99	--2401.02335
357	12	123	-9.74	2.28	881.70	1008.04	890.09	904.96	2669.40	795.66	16.50	790.90	36.07	961.45	846.02	944.59	792.89	--2401.02273
358	12	124	-9.73	2.29	881.70	1013.98	671.87	5320.05	16083.33	795.65	12.45	791.92	29.14	990.28	670.69	973.27	629.69	--2401.02254
359	12	125	-9.55	2.47	881.70	1038.91	701.58	-175.11	2524.84	795.51	11.63	791.28	27.12	994.72	665.82	974.89	620.87	--2401.01916
360	12	126	-9.52	2.50	881.70	1008.29	610.90	-20517.95	62148.42	795.57	12.18	791.98	29.67	985.38	605.37	967.13	572.24	--2401.01857
361	12	127	-9.46	2.56	881.70	1080.16	968.32	1597.50	1881.80	797.78	16.42	793.26	31.37	1047.67	971.27	1019.72	905.69	--2401.01747
362	12	128	-9.46	2.56	881.70	1118.02	1459.77	503.48	3173.42	800.38	26.18	796.56	51.59	1084.69	1400.43	1045.74	1274.12	--2401.01747
363	12	129	-9.37	2.65	881.70	1047.09	1023.46	-790.33	4281.77	799.42	22.13	797.00	45.39	1034.03	1068.51	1021.53	1020.18	--2401.01564
364	12	130	-9.25	2.77	881.70	1169.75	1482.19	-1107.14	5017.90	799.84	23.39	794.83	42.26	1100.61	1408.19	1043.21	1228.70	--2401.01340
365	12	131	-9.24	2.78	881.70	1090.37	1029.60	-49.20	2923.60	802.89	24.42	800.56	40.73	1106.84	1124.31	1074.06	1023.47	--2401.01326
366	12	132	-9.16	2.86	881.70	1177.01	1482.43	-26.62	3639.95	801.39	24.11	796.89	41.34	1131.49	1448.15	1079.42	1287.99	--2401.01157
367	12	133	-9.15	2.87	881.70	1069.58	781.46	-10185.97	32127.30	798.08	15.07	795.61	33.33	1049.74	801.28	1019.87	734.30	--2401.01144
368	12	134	-9.05	2.97	881.70	1221.56	1611.10	689.25	1955.08	807.95	32.86	805.35	51.24	1237.94	1687.40	1191.38	1536.13	--2401.00956
369	12	135	-9.02	3.00	881.70	1163.30	1378.85	-14498.75	43622.01	801.49	24.56	799.29	47.86	1111.72	1276.54	1076.63	1158.59	--2401.00898
370	12	136	-8.92	3.10	881.70	1210.41	1542.66	857.58	2735.76	802.13	24.72	798.09	42.89	1165.52	1503.31	1108.62	1331.04	--2401.00700
371	12	137	-8.86	3.16	881.70	1166.56	1421.13	753.03	3806.38	801.68	25.24	800.04	49.37	1136.52	1362.12	1104.19	1254.23	--2401.00593
372	12	138	-8.85	3.17	881.70	1206.60	935.27	-3445.68	15355.04	801.51	15.20	799.03	24.88	1159.37	926.75	1117.85	830.58	--2401.00574
373	12	139	-8.70	3.32	881.70	1215.07	1518.37	836.47	1291.61	805.04	28.31	801.80	45.68	1192.55	1541.44	1137.87	1380.91	--2401.00276
374	12	140	-8.69	3.33	881.70	1282.93	1782.22	8729.04	22189.58	804.98	28.45	802.68	49.84	1270.84	1802.70	1220.35	1644.45	--2401.00270
375	12	141	-8.45	3.57	881.70	1224.52	1280.17	3606.60	9130.56	805.89	24.80	804.80	39.56	1231.50	1352.14	1173.63	1195.59	--2400.99815
376	12	142	-8.35	3.67	881.70	1408.90	2321.56	1110.85	3015.27	808.48	33.96	806.04	57.50	1334.34	2144.71	1248.68	1875.59	--2400.99612
377	12	143	-8.33	3.69	881.70	1418.29	2177.54	786.13	1678.98	809.32	31.33	805.09	45.87	1351.04	2071.60	1248.06	1759.32	--2400.99575
378	12	144	-8.32	3.70	881.70	1422.73	2064.24	-2324.16	9589.76	818.65	41.96	813.99	49.50	1511.49	2382.22	1439.50	2162.74	--2400.99554
379	13	1*	-12.43	0.00	955.18	851.76	393.29	-801.50	4975.32	848.47	11.07	839.61	27.03	809.92	409.12	815.49	401.10	--2601.163726
380	13	2	-12.30	0.13	955.18	835.14	375.26	-4415.42	17648.85	847.65	10.03	838.17	25.43	786.35	369.38	789.91	352.57	-2601.160974
381	13	3	-12.20	0.23	955.18	823.66	357.80	2678.54	3672.84	847.15	9.13	837.29	24.02	770.29	348.83	778.21	338.51	-2601.158862
382	13	4	-12.16	0.27	955.18	833.60	351.35	2160.21	2408.05	847.45	9.13	838.02	23.93	786.93	344.48	793.53	334.09	-2601.158034
383	13	5	-12.15	0.28	955.18	829.19	410.15	-2303.68	11031.06	847.24	10.00	837.27	26.07	772.72	415.12	780.90	412.16	--2601.157919
384	13	6	-12.12	0.31	955.18	828.18	448.75	-41969.69	128576.27	847.16	11.05	836.80	28.60	755.67	447.39	769.63	461.86	-2601.157248
385	13	7	-12.11	0.32	955.18	841.55	419.68	1724.35	1369.28	847.49	10.11	837.86	26.15	785.89	429.04	792.55	422.31	-2601.157006
386	13	8	-12.07	0.36	955.18	843.09	354.98	1225.98	1084.29	847.71	9.07	838.68	23.30	793.11	338.60	799.57	318.34	-2601.156178
387	13	9	-12.07	0.36	955.18	852.69	420.09	2188.64	3989.32	847.55	10.29	837.81	27.43	813.62	432.18	819.81	435.17	-2601.156169
388	13	10	-12.06	0.37	955.18	845.59	381.28	1399.81	1369.13	846.94	9.08	836.66	25.20	792.47	386.72	799.59	390.28	--2601.156023
389	13	11	-12.04	0.39	955.18	894.76	417.39	21382.27	58884.10	848.84	9.52	840.67	24.37	844.57	426.86	848.57	416.03	-2601.155712
390	13	12	-12.03	0.40	955.18	861.50	402.31	702.27	5659.23	848.27	9.96	839.53	24.76	815.21	407.55	815.20	384.43	-2601.155373
391	13	13	-12.02	0.41	955.18	892.79	437.39	-4911.00	19864.75	849.33	11.40	841.33	27.11	843.93	439.63	846.49	421.29	-2601.155196
392	13	14	-12.02	0.41	955.18	849.05	362.75	2983.68	4767.39	847.83	9.42	838.65	23.77	799.88	363.94	803.24	338.57	--2601.155178
393	13	15	-12.02	0.41	955.18	872.24	378.23	3788.04	7415.05	848.09	8.93	839.37	23.52	826.85	393.60	827.07	381.36	-2601.155158
394	13	16	-12.01	0.42	955.18	857.41	423.53	5387.22	11656.33	848.32	10.94	839.52	27.51	810.11	419.13	816.11	416.99	-2601.154950
395	13	17	-12.00	0.43	955.18	859.92	403.32	-16756.52	54646.40	847.63	9.35	838.26	25.50	804.60	438.62	809.85	435.26	-2601.154819
396	13	18	-12.00	0.43	955.18	810.87	379.81	874.68	4575.73	846.78	9.77	836.28	25.81	742.56	376.00	753.76	374.92	--2601.154755
397	13	19	-12.00	0.43	955.18	873.94	467.62	1680.20	2198.44	848.33	11.01	839.47	27.46	827.28	493.28	828.82	476.05	-2601.154742
398	13	20	-11.98	0.45	955.18	885.80	418.27	3284.23	6150.57	849.06	10.95	840.94	26.31	838.21	426.98	840.28	406.49	-2601.154411
399	13	21	-11.97	0.46	955.18	871.79	404.93	1925.08	1458.82	848.57	10.74	839.95	26.26	818.85	398.96	821.93	380.76	-2601.154261

Polarizability models:					n*alp Aiso	DFT results		AM model		TL model		TE model		RP model		GD model		Etot
i	n	isomer	Eb	Erel		Aiso	Aaniso	Aiso	Aaniso	Aiso	Aaniso	Aiso	Aaniso	Aiso	Aaniso	Aiso	Aaniso	
400	13	22	-11.96	0.47	955.18	861.87	393.92	2065.90	174.80	847.49	8.74	838.09	23.82	811.64	401.22	816.57	396.58	-2601.153932
401	13	23	-11.96	0.47	955.18	838.56	427.16	2266.03	3993.36	847.50	10.80	837.76	29.93	784.88	469.01	789.60	475.48	-2601.153872
402	13	24	-11.93	0.50	955.18	871.25	357.79	2161.80	4820.95	848.45	9.04	840.00	22.47	840.64	360.58	844.32	329.95	-2601.153390
403	13	25	-11.93	0.50	955.18	875.33	380.17	3993.42	6189.16	848.55	8.80	840.18	22.24	832.72	349.65	838.86	340.27	-2601.153356
404	13	26	-11.92	0.51	955.18	880.78	373.01	1446.53	864.52	848.74	8.64	840.79	22.64	836.03	368.18	835.58	349.36	-2601.153068
405	13	27	-11.89	0.54	955.18	865.83	386.74	-1767.53	5643.99	848.00	9.22	839.13	24.63	817.85	404.88	819.76	399.83	-2601.152575
406	13	28	-11.89	0.54	955.18	918.18	423.63	-13443.54	34589.75	849.68	10.03	842.22	25.19	861.67	411.14	868.35	407.04	-2601.152534
407	13	29	-11.89	0.54	955.18	848.76	407.44	52754.47	154307.88	847.61	10.03	838.21	25.64	797.93	411.66	803.30	400.12	-2601.152417
408	13	30	-11.87	0.56	955.18	868.50	381.82	1620.85	1547.19	847.76	8.72	838.69	23.45	818.18	393.38	821.28	383.46	-2601.152206
409	13	31	-11.87	0.56	955.18	864.10	398.57	2793.19	5324.00	848.01	10.03	839.08	26.87	808.94	428.77	811.63	428.81	-2601.152194
410	13	32	-11.87	0.56	955.18	853.34	400.32	1646.74	1509.21	847.03	9.44	836.80	26.34	800.68	416.55	807.00	417.27	-2601.152084
411	13	33	-11.87	0.56	955.18	856.81	390.72	3251.76	6889.26	847.65	9.16	838.32	24.80	798.81	406.81	802.72	401.00	-2601.152007
412	13	34	-11.86	0.57	955.18	857.98	375.58	735.30	2113.30	847.36	8.72	837.74	23.80	809.85	386.51	815.91	384.99	-2601.151878
413	13	35	-11.86	0.57	955.18	888.50	445.24	-1400.49	8166.29	849.02	10.14	840.97	25.44	839.45	461.15	843.91	457.87	-2601.151836
414	13	36	-11.86	0.57	955.18	880.81	383.38	2430.92	2679.89	848.58	8.46	840.47	22.09	834.49	387.85	836.80	368.02	-2601.151832
415	13	37	-11.85	0.58	955.18	846.41	419.46	58.33	7069.11	847.71	9.69	838.38	24.93	798.67	431.49	800.12	415.16	-2601.151669
416	13	38	-11.84	0.59	955.18	866.14	368.69	3184.53	4329.31	848.12	8.82	839.29	22.21	830.02	366.09	834.81	339.45	-2601.151412
417	13	39	-11.83	0.60	955.18	876.02	332.44	374.02	3985.59	847.72	7.56	838.70	20.37	843.48	316.36	848.00	304.84	-2601.151236
418	13	40	-11.83	0.60	955.18	862.21	414.09	2491.94	4149.00	847.92	9.45	838.91	25.38	810.02	420.44	815.97	416.24	-2601.151200
419	13	41	-11.82	0.61	955.18	879.95	449.26	26708.42	68677.76	848.76	10.16	840.41	25.62	837.74	432.88	843.03	424.64	-2601.151127
420	13	42	-11.81	0.62	955.18	871.36	336.00	1682.69	891.49	847.73	7.60	838.75	20.79	826.79	311.66	835.50	305.21	-2601.150767
421	13	43	-11.80	0.63	955.18	870.02	372.58	1818.54	1704.21	848.16	8.62	839.60	23.17	817.45	375.69	820.66	364.63	-2601.150658
422	13	44	-11.79	0.64	955.18	874.46	474.98	-305.70	3496.50	848.42	11.05	839.55	28.66	838.26	502.33	845.31	508.38	-2601.150463
423	13	45	-11.79	0.64	955.18	867.21	425.60	4526.26	10678.69	848.20	10.17	839.38	26.61	813.19	422.60	819.42	421.23	-2601.150389
424	13	46	-11.78	0.65	955.18	860.53	462.68	2859.50	5391.84	848.17	10.57	839.24	27.11	815.30	469.03	821.22	466.09	-2601.150322
425	13	47	-11.77	0.66	955.18	849.40	331.62	1429.13	2346.31	847.71	8.68	838.63	22.49	816.18	327.12	821.10	298.46	-2601.150081
426	13	48	-11.77	0.66	955.18	862.07	413.04	803.88	4082.26	848.48	10.92	839.86	27.33	821.36	409.76	827.58	406.31	-2601.149999
427	13	49	-11.76	0.67	955.18	910.89	389.86	74.47	5293.79	849.31	9.09	841.72	23.28	855.64	375.45	860.29	366.11	-2601.149921
428	13	50	-11.76	0.67	955.18	900.68	370.50	-2071.02	12720.04	848.96	8.45	841.11	21.49	849.87	350.58	851.06	336.12	-2601.149777
429	13	51	-11.76	0.67	955.18	874.04	348.43	2415.72	3360.32	848.38	7.83	840.12	20.28	839.56	332.50	842.70	309.84	-2601.149726
430	13	52	-11.75	0.68	955.18	884.98	413.06	962.84	3531.07	848.51	8.73	840.21	22.03	845.79	403.17	846.67	385.62	-2601.149715
431	13	53	-11.75	0.68	955.18	825.84	389.43	1844.19	1772.72	847.47	10.16	837.86	26.15	763.31	362.20	770.29	360.03	-2601.149694
432	13	54	-11.75	0.68	955.18	873.55	481.82	-2624.20	11569.46	848.30	11.02	839.45	27.76	826.97	511.32	832.85	503.54	-2601.149558
433	13	55	-11.74	0.69	955.18	880.75	340.95	1629.34	1981.22	848.04	7.23	839.53	19.37	840.06	331.48	837.33	304.76	-2601.149458
434	13	56	-11.73	0.70	955.18	872.19	339.76	1948.31	2017.62	848.47	8.18	840.34	22.30	825.11	338.40	827.01	328.40	-2601.149278
435	13	57	-11.73	0.70	955.18	897.35	457.67	2411.00	3972.37	849.34	10.00	841.73	24.51	847.44	456.60	848.19	432.31	-2601.149213
436	13	58	-11.73	0.70	955.18	856.49	360.27	389.01	4788.09	847.49	8.62	838.09	23.37	811.92	353.17	819.68	353.60	-2601.149169
437	13	59	-11.73	0.70	955.18	879.42	407.39	-219.62	8372.06	848.22	9.38	839.40	25.20	843.38	421.12	846.97	413.94	-2601.149144
438	13	60	-11.72	0.71	955.18	867.34	351.13	1502.95	1606.46	848.09	7.89	839.55	21.29	814.42	332.10	816.99	319.89	-2601.148979
439	13	61	-11.72	0.71	955.18	861.68	373.00	2145.01	2701.11	847.66	9.43	838.30	25.05	819.86	382.01	830.16	396.83	-2601.148896
440	13	62	-11.70	0.73	955.18	850.89	320.38	2759.96	5511.40	847.23	7.33	837.68	19.86	810.25	304.59	816.82	282.87	-2601.148658
441	13	63	-11.69	0.74	955.18	847.63	316.69	1363.48	814.28	848.10	7.63	839.79	19.93	811.02	289.64	816.74	263.33	-2601.148405
442	13	64	-11.69	0.74	955.18	851.55	337.63	-140.06	4340.73	847.73	8.35	838.67	21.96	796.77	322.29	802.67	317.75	-2601.148371
443	13	65	-11.68	0.75	955.18	881.23	367.60	-54558.17	173299.68	848.14	8.13	839.60	21.36	838.80	374.27	838.62	357.05	-2601.148117
444	13	66	-11.67	0.76	955.18	869.12	388.50	2021.39	2218.30	848.08	8.78	839.39	24.20	819.01	390.73	821.91	381.97	-2601.148025
445	13	67	-11.66	0.77	955.18	870.04	420.73	2827.10	4573.98	848.17	10.40	839.27	27.74	824.93	412.73	829.56	410.91	-2601.147751
446	13	68	-11.66	0.77	955.18	869.89	406.41	2858.30	4342.36	848.09	8.72	839.46	24.16	816.68	402.15	818.43	392.52	-2601.147717
447	13	69	-11.64	0.79	955.18	884.83	528.44	1792.29	1442.60	848.73	11.63	840.33	33.08	830.44	497.76	837.28	494.44	-2601.147425
448	13	70	-11.64	0.79	955.18	881.51	509.71	-149148.84	450099.27	848.81	12.65	840.23	31.32	847.62	544.63	854.71	554.27	-2601.147275
449	13	71	-11.64	0.79	955.18	884.16	423.83	4308.93	9173.89	848.78	10.06	840.50	25.89	849.80	451.95	856.52	456.57	-2601.147246
450	13	72	-11.62	0.81	955.18	886.50	277.19	3432.36	4977.94	848.06	5.62	839.70	14.51	851.43	301.49	841.12	275.96	-2601.146955

Polarizability models:					n*alp Aiso	DFT results		AM model		TL model		TE model		RP model		GD model		Etot
i	n	isomer	Eb	Erel		Aiso	Aaniso	Aiso	Aaniso	Aiso	Aaniso	Aiso	Aaniso	Aiso	Aaniso	Aiso	Aaniso	
451	13	73	-11.61	0.82	955.18	879.52	387.38	5360.60	15969.37	848.12	9.02	839.33	24.69	842.78	399.35	846.28	392.00	-2601.146776
452	13	74	-11.61	0.82	955.18	892.81	401.95	2869.54	5447.97	848.70	10.07	840.48	25.92	853.20	433.37	856.23	428.72	-2601.146708
453	13	75	-11.61	0.82	955.18	900.43	361.53	2058.50	7355.35	848.68	7.90	840.70	20.72	869.83	354.42	872.97	335.75	-2601.146701
454	13	76	-11.60	0.83	955.18	886.38	424.31	2189.55	2773.09	848.37	10.18	839.58	26.52	841.50	432.73	845.17	425.59	-2601.146604
455	13	77	-11.60	0.83	955.18	864.91	358.75	1478.18	1548.96	847.28	7.97	837.76	21.60	821.04	353.88	832.07	350.27	-2601.146483
456	13	78	-11.59	0.84	955.18	874.35	331.80	2347.47	1988.35	848.93	8.60	841.24	22.96	843.51	359.29	843.87	352.38	-2601.146335
457	13	79	-11.59	0.84	955.18	898.85	541.64	666493.941995171.93	848.97	11.78	840.74	33.04	853.98	523.59	856.49	511.91	-2601.146278	
458	13	80	-11.58	0.85	955.18	1010.06	896.72	-213.29	3938.87	853.69	17.85	847.02	35.47	948.25	850.50	951.19	838.12	-2601.146159
459	13	81	-11.58	0.85	955.18	880.94	377.22	4161.44	8329.57	848.21	8.70	839.65	23.11	845.36	389.66	848.93	376.28	-2601.146087
460	13	82	-11.57	0.86	955.18	899.45	423.72	3045.46	3552.92	848.91	10.29	840.87	26.84	866.23	438.71	868.90	431.86	-2601.145837
461	13	83	-11.57	0.86	955.18	957.47	470.35	1059.47	3170.37	851.33	9.64	844.96	21.74	904.32	452.96	903.51	439.29	-2601.145818
462	13	84	-11.56	0.87	955.18	905.03	406.90	2786.34	4097.61	848.92	8.63	841.07	22.25	855.18	401.06	860.59	384.74	-2601.145594
463	13	85	-11.55	0.88	955.18	897.52	385.12	7964.74	22159.64	848.47	9.26	840.08	24.44	860.11	405.50	862.02	396.76	-2601.145404
464	13	86	-11.54	0.89	955.18	927.30	321.03	2213.36	6326.06	849.26	6.92	841.93	16.72	880.76	329.53	875.50	314.25	-2601.145313
465	13	87	-11.54	0.89	955.18	894.81	356.79	2823.11	3622.44	848.36	8.31	840.07	21.87	861.37	357.52	863.91	343.91	-2601.145254
466	13	88	-11.53	0.90	955.18	896.99	309.68	3171.61	5116.88	848.99	6.90	841.39	16.81	848.92	305.27	846.05	300.64	-2601.144965
467	13	89	-11.48	0.95	955.18	902.90	329.11	-804.82	5594.22	848.49	6.92	840.50	18.85	869.95	303.85	871.31	279.31	-2601.144006
468	13	90	-11.46	0.97	955.18	994.98	841.89	424.08	2345.10	851.65	15.52	844.50	33.90	944.37	842.10	934.48	791.81	-2601.143666
469	13	91	-11.46	0.97	955.18	922.61	555.87	3638.09	3810.51	850.13	12.25	843.02	33.54	883.86	548.40	885.73	533.79	-2601.143545
470	13	92	-11.43	1.00	955.18	872.82	377.22	1931.98	1980.14	848.03	8.83	839.39	23.84	829.87	380.24	833.21	365.92	-2601.143091
471	13	93	-11.41	1.02	955.18	911.72	396.99	3125.47	4575.29	848.75	8.92	840.64	23.50	871.99	413.72	870.63	400.84	-2601.142503
472	13	94	-11.41	1.02	955.18	894.67	397.13	10877.80	28238.09	848.78	9.15	840.87	24.59	846.08	388.57	849.21	380.21	-2601.142488
473	13	95	-11.39	1.04	955.18	900.11	438.50	9733.04	25208.05	849.02	10.94	840.98	28.24	862.17	454.74	863.61	449.52	-2601.142113
474	13	96	-11.39	1.04	955.18	901.11	547.66	2391.00	2943.84	849.40	11.94	841.76	33.33	852.40	527.79	854.95	516.72	-2601.142074
475	13	97	-11.38	1.05	955.18	960.57	373.42	742.02	2468.15	850.82	6.77	844.18	14.88	914.79	390.80	907.97	369.41	-2601.141927
476	13	98	-11.37	1.06	955.18	1030.35	700.61	-3521.77	11423.06	852.87	13.02	847.09	28.03	962.29	664.29	961.58	640.58	-2601.141683
477	13	99	-11.37	1.06	955.18	899.95	309.66	2137.27	2903.72	848.11	6.39	839.83	16.77	858.96	336.93	849.24	317.50	-2601.141664
478	13	100	-11.36	1.07	955.18	960.08	731.53	136.21	2612.96	851.01	14.27	843.83	32.80	901.72	688.05	899.92	669.05	--2601.14158
479	13	101	-11.36	1.07	955.18	923.84	318.24	3759.79	4663.46	848.45	6.47	840.61	16.80	893.29	364.73	881.75	340.27	--2601.14149
480	13	102	-11.33	1.10	955.18	929.14	409.13	-796.26	8639.90	849.31	8.40	841.87	21.42	884.29	421.88	877.19	396.12	--2601.141084
481	13	103	-11.32	1.11	955.18	911.56	388.25	6142.61	11867.19	848.80	8.20	840.97	21.62	874.55	398.59	874.56	376.84	--2601.141079
482	13	104	-11.31	1.12	955.18	878.18	298.44	2201.91	2819.21	848.02	6.92	839.60	18.45	835.69	308.52	830.08	300.26	--2601.141045
483	13	105	-11.30	1.13	955.18	914.30	536.81	2297.54	3611.49	849.98	12.05	842.98	33.28	875.51	517.74	878.34	505.11	--2601.141031
484	13	106	-11.30	1.13	955.18	937.91	567.63	-5857.80	26107.24	851.28	13.03	845.35	34.64	905.80	567.43	909.66	558.45	--2601.141029
485	13	107	-11.29	1.14	955.18	877.18	311.18	-1495.36	7354.38	847.97	7.31	839.40	19.68	835.97	319.31	835.76	323.49	--2601.141010
486	13	108	-11.28	1.15	955.18	910.33	281.71	836.15	3861.91	848.23	6.48	840.05	16.80	883.65	307.09	879.34	290.89	--2601.139994
487	13	109	-11.27	1.16	955.18	926.47	420.65	3456.60	5897.57	849.36	9.04	841.86	23.11	885.39	451.84	882.47	435.88	--2601.13977
488	13	110	-11.26	1.17	955.18	902.93	541.88	-2504.30	13249.64	849.38	11.37	841.91	31.56	852.98	498.81	854.28	494.66	--2601.13952
489	13	111	-11.26	1.17	955.18	1001.97	403.99	1442.93	3951.34	852.01	7.83	846.34	17.12	941.60	412.23	940.36	400.12	--2601.13945
490	13	112	-11.26	1.17	955.18	920.21	411.62	2213.88	1991.28	848.79	8.82	840.73	23.17	879.03	429.04	877.08	413.98	--2601.13941
491	13	113	-11.22	1.21	955.18	940.87	771.20	8061.91	21716.49	850.56	16.48	842.88	39.44	901.08	766.23	897.22	738.21	--2601.13865
492	13	114	-11.22	1.21	955.18	925.66	410.93	7519.65	20172.61	849.26	8.64	841.73	22.49	881.21	436.16	878.33	422.14	--2601.13853
493	13	115	-11.21	1.22	955.18	928.75	432.57	24230.28	68434.12	849.66	10.24	842.37	25.40	894.19	440.86	894.68	426.82	--2601.13839
494	13	116	-11.19	1.24	955.18	923.96	449.56	474.47	9401.18	849.83	11.27	842.55	27.72	888.69	462.80	890.01	454.77	--2601.13808
495	13	117	-11.17	1.26	955.18	1007.75	588.52	1701.24	4457.94	852.04	10.75	846.13	23.68	944.88	585.87	942.22	567.54	--2601.13754
496	13	118	-11.17	1.26	955.18	945.45	765.46	-1481.39	6927.90	850.51	16.54	842.82	39.60	898.12	762.21	892.88	733.30	--2601.13754
497	13	119	-11.14	1.29	955.18	902.48	418.87	-1368.38	9667.38	849.68	10.61	842.72	27.65	864.50	431.63	866.74	420.83	--2601.13704
498	13	120	-11.14	1.29	955.18	962.42	848.42	12960.08	29992.48	853.09	19.55	846.81	43.21	913.45	801.17	915.62	788.64	--2601.13699
499	13	121	-11.14	1.29	955.18	982.28	153.37	2655.71	5579.72	850.32	2.60	844.14	5.48	931.95	136.16	917.65	132.76	--2601.13696
500	13	122	-11.11	1.32	955.18	990.33	368.38	2022.92	5617.34	851.16	7.10	845.05	16.55	942.95	380.77	941.41	370.67	--2601.13641
501	13	123	-11.11	1.32	955.18	917.52	539.59	-2966.64	13332.70	849.91	13.11	842.44	32.65	879.07	538.76	880.25	536.27	--2601.13639

Polarizability models:				n*alp	DFT results		AM model		TL model		TE model		RP model		GD model		Etot	
i	n	isomer	Eb	Erel	Aiso	Aaniso	Aiso	Aaniso	Aiso	Aaniso	Aiso	Aaniso	Aiso	Aaniso	Aiso	Aaniso		
502	13	124	-11.11	1.32	955.18	1032.35	684.54	628.65	3945.26	851.96	11.79	845.86	25.00	988.46	720.31	962.50	651.11	--2601.13630
503	13	125	-11.09	1.34	955.18	951.93	355.03	12551.34	629.61	849.73	6.81	843.17	17.93	916.70	333.92	911.96	309.07	--2601.13601
504	13	126	-11.09	1.34	955.18	966.22	472.39	-726.55	14523.96	850.77	10.07	844.26	24.08	923.87	497.50	921.69	483.26	--2601.13592
505	13	127	-11.08	1.35	955.18	924.25	533.04	500.16	3261.81	849.86	12.18	842.64	32.87	884.48	528.72	880.90	510.33	--2601.13575
506	13	128	-11.08	1.35	955.18	945.48	826.65	766.72	2344.70	851.46	17.72	844.65	41.64	901.42	803.04	893.94	763.80	--2601.13572
507	13	129	-11.07	1.36	955.18	954.75	835.08	-389.46	4405.69	851.60	18.64	844.36	43.81	915.21	817.64	909.90	783.66	--2601.13553
508	13	130	-11.06	1.37	955.18	925.87	279.56	943.95	19676.54	849.01	5.92	841.83	15.34	887.87	266.71	884.27	257.72	--2601.13541
509	13	131	-11.05	1.38	955.18	934.75	484.47	12145.10	23432.69	850.44	11.76	843.80	28.41	907.75	524.66	909.66	518.60	--2601.13512
510	13	132	-11.05	1.38	955.18	943.95	460.54	-105.40	4814.51	850.13	10.70	843.21	26.74	908.68	481.87	903.87	464.62	--2601.13511
511	13	133	-11.02	1.41	955.18	1201.68	1469.05	522.29	1901.70	858.95	24.30	853.04	40.83	1143.73	1473.07	1090.12	1280.57	--2601.13453
512	13	134	-10.97	1.46	955.18	964.74	825.87	3305.02	6712.42	851.43	17.73	844.37	42.06	923.22	809.85	913.65	762.10	--2601.13344
513	13	135	-10.96	1.47	955.18	974.54	735.58	-5931.57	16274.02	851.58	15.40	845.38	36.00	943.11	733.18	935.61	689.05	--2601.13325
514	13	136	-10.95	1.48	955.18	968.93	821.97	1507.79	2636.72	851.90	17.83	845.39	41.70	935.84	808.89	926.94	759.55	--2601.13312
515	13	137	-10.93	1.50	955.18	979.73	842.86	4332.17	12118.56	852.60	18.87	846.26	42.97	944.29	831.46	935.95	785.13	--2601.13265
516	13	138	-10.93	1.50	955.18	975.04	551.41	-11875.54	37938.90	851.06	11.47	844.67	27.43	931.73	560.65	928.59	541.36	--2601.13263
517	13	139	-10.91	1.52	955.18	971.42	790.51	-1682.10	8547.80	851.95	18.08	845.27	41.65	930.18	789.48	922.30	754.93	--2601.13215
518	13	140	-10.88	1.55	955.18	1014.24	199.29	-15113.55	48271.40	851.33	3.45	845.71	4.48	964.21	202.77	951.20	209.31	--2601.13158
519	13	141	-10.83	1.60	955.18	1036.69	680.06	514.43	2755.12	853.00	12.96	847.40	28.41	1000.57	681.27	994.37	646.70	--2601.13061
520	13	142	-10.79	1.64	955.18	977.83	819.61	-2216.57	10558.01	852.83	19.58	846.69	44.75	943.52	822.77	935.49	786.65	--2601.12979
521	13	143	-10.79	1.64	955.18	975.69	813.84	11101.08	29788.13	852.30	17.99	846.02	41.33	940.51	794.17	929.99	743.03	--2601.12978
522	13	144	-10.79	1.64	955.18	1047.45	814.73	1482.30	6123.96	853.31	15.31	847.63	31.83	1008.83	795.02	1001.51	744.42	--2601.12963
523	13	145	-10.78	1.65	955.18	984.57	826.03	-18568.63	59550.88	852.66	18.27	846.82	41.80	959.17	824.59	948.11	772.77	--2601.12949
524	13	146	-10.74	1.69	955.18	981.70	857.39	-511.11	5067.25	853.10	20.03	847.15	45.12	949.41	863.75	942.41	832.70	--2601.12874
525	13	147	-10.71	1.72	955.18	945.61	367.07	2425.63	3872.46	849.97	8.21	843.68	20.44	905.51	345.30	907.03	330.44	--2601.12808
526	13	148	-10.71	1.72	955.18	992.07	822.37	68364.90	206404.58	852.81	18.16	847.11	41.46	959.98	810.73	949.58	759.48	--2601.12806
527	13	149	-10.71	1.72	955.18	1001.40	884.35	-1589.93	8528.50	854.07	20.92	848.51	45.66	968.37	885.28	959.47	849.63	--2601.12804
528	13	150	-10.68	1.75	955.18	1066.84	445.21	28313.24	86803.02	854.04	8.49	850.10	18.24	1041.13	449.02	1042.98	438.40	--2601.12744
529	13	151	-10.66	1.77	955.18	1043.70	569.24	-9749.12	31197.63	853.53	11.11	849.05	25.21	1017.50	585.72	1011.58	564.05	--2601.12699
530	13	152	-10.61	1.82	955.18	1067.45	875.71	-506.54	3231.49	854.65	17.32	849.84	35.28	1028.09	851.63	1013.63	791.56	--2601.12607
531	13	153	-10.56	1.87	955.18	1010.03	817.57	-433.81	6099.00	854.18	20.20	849.01	44.20	980.59	829.18	969.53	784.05	--2601.12502
532	13	154	-10.54	1.89	955.18	1004.40	868.76	-3779.24	15778.03	853.70	19.51	848.35	43.99	974.80	875.69	959.49	820.58	--2601.12461
533	13	155	-10.53	1.90	955.18	1030.76	891.28	857.59	5484.86	855.15	21.09	850.51	44.88	1004.43	887.30	991.97	834.80	--2601.12443
534	13	156	-10.53	1.90	955.18	986.25	574.49	-1441.19	6191.56	852.09	13.68	846.63	32.26	958.28	595.45	949.66	571.35	--2601.12429
535	13	157	-10.45	1.98	955.18	1033.42	838.36	1472.18	4220.46	853.71	15.96	848.78	36.85	979.09	787.60	970.77	754.97	--2601.12262
536	13	158	-10.29	2.14	955.18	1084.03	1047.12	-417.74	5997.42	856.00	19.92	851.24	41.12	1046.20	1037.44	1043.98	1027.71	--2601.11935
537	13	159	-10.26	2.17	955.18	1030.76	927.18	24.14	4826.45	854.88	21.55	849.97	46.49	993.77	940.52	975.04	878.07	--2601.11866
538	13	160	-10.24	2.19	955.18	1029.89	892.60	8282.32	20610.18	855.33	21.19	851.18	45.86	1007.70	917.41	987.37	846.97	--2601.11827
539	13	161	-10.22	2.21	955.18	1050.55	997.21	-612.38	5456.17	855.33	21.92	850.48	46.81	1009.99	993.50	994.26	938.08	--2601.11781
540	13	162	-10.03	2.40	955.18	1159.96	1364.54	377.73	3031.02	859.27	27.54	855.13	53.68	1120.61	1321.87	1091.94	1229.08	--2601.11407
541	13	163	-9.83	2.60	955.18	1251.18	1693.98	-137.03	3400.20	863.41	30.58	858.23	49.76	1195.83	1621.64	1177.66	1554.48	--2601.110982
542	13	164	-9.74	2.69	955.18	1217.79	1663.56	-543.89	5538.22	864.79	36.18	861.54	63.87	1208.28	1693.17	1175.03	1572.07	--2601.10800
543	13	165	-8.54	3.89	955.18	1531.22	1900.38	-791.52	3462.58	871.29	29.72	868.65	40.13	1504.52	1932.85	1417.58	1699.67	--2601.08303
544	14	1*	-12.62	0.00	1028.65	883.97	413.11	749.13	1589.30	905.20	11.69	895.46	29.80	822.01	399.62	832.70	405.18	-2801.257306
545	14	2	-12.61	0.01	1028.65	896.37	360.87	228.06	4624.30	905.84	11.06	897.08	27.33	845.80	354.94	849.65	345.94	-2801.257106
546	14	3	-12.58	0.04	1028.65	890.66	365.10	1456.61	1422.06	905.56	10.92	896.51	27.24	835.35	357.00	843.12	350.70	-2801.256413
547	14	4	-12.58	0.04	1028.65	887.34	370.73	1754.59	1974.04	905.34	10.86	896.03	27.27	830.35	367.18	839.57	362.70	-2801.256387
548	14	5	-12.57	0.05	1028.65	915.02	455.58	-627.76	2123.86	905.64	11.45	896.39	31.70	857.53	487.40	865.04	490.47	-2801.256272
549	14	6	-12.53	0.09	1028.65	910.53	438.42	1854.41	1684.93	904.83	11.08	894.53	31.19	852.37	448.68	865.03	457.06	-2801.255308
550	14	7	-12.52	0.10	1028.65	879.17	345.99	806.49	1996.60	904.94	9.98	895.28	25.68	827.05	347.35	832.72	338.08	-2801.255114
551	14	8	-12.50	0.12	1028.65	918.43	400.60	548.64	5758.16	906.35	12.02	897.86	29.33	868.31	402.27	872.63	396.78	-2801.254596
552	14	9	-12.50	0.12	1028.65	909.82	400.36	1025.72	2242.61	905.85	11.57	896.76	28.82	860.44	398.68	865.69	393.70	-2801.254551

Polarizability models:					n*alp Aiso	DFT results		AM model		TL model		TE model		RP model		GD model		Etot
i	n	isomer	Eb	Erel		Aiso	Aaniso	Aiso	Aaniso	Aiso	Aaniso	Aiso	Aaniso	Aiso	Aaniso	Aiso	Aaniso	
553	14	10	-12.49	0.13	1028.65	886.51	344.82	2948.07	5362.81	905.33	10.18	896.23	25.60	827.04	343.69	833.94	335.26	-2801.254308
554	14	11	-12.48	0.14	1028.65	881.91	326.64	1363.81	1401.15	905.35	9.92	896.27	24.94	831.18	314.47	835.79	301.22	-2801.254243
555	14	12	-12.46	0.16	1028.65	898.43	324.98	2242.96	2085.92	905.59	9.50	896.85	24.15	853.37	320.27	856.69	308.27	-2801.253784
556	14	13	-12.46	0.16	1028.65	910.32	374.85	5136.29	11927.12	906.20	11.33	897.77	27.79	858.62	367.84	862.16	355.53	-2801.253639
557	14	14	-12.45	0.17	1028.65	895.23	393.87	2629.28	4355.01	905.23	11.13	895.71	29.22	832.83	409.37	840.52	414.54	-2801.253480
558	14	15	-12.40	0.22	1028.65	999.04	777.23	194.38	4120.73	910.25	19.92	903.22	42.91	940.27	752.62	947.94	743.72	-2801.252357
559	14	16	-12.37	0.25	1028.65	865.33	306.45	1494.59	1412.04	904.68	9.31	894.90	23.75	837.33	302.01	842.06	274.46	-2801.251831
560	14	17	-12.37	0.25	1028.65	885.52	342.20	2808.40	3981.61	905.03	9.88	895.48	25.29	841.89	335.34	844.19	322.43	-2801.251769
561	14	18	-12.35	0.27	1028.65	932.53	391.12	2105.96	1785.38	906.81	11.15	898.96	27.18	886.79	380.22	888.90	359.16	-2801.251277
562	14	19	-12.33	0.29	1028.65	927.12	406.69	5043.33	10415.54	906.49	12.00	898.18	29.23	874.96	411.12	879.67	403.79	-2801.250876
563	14	20	-12.32	0.30	1028.65	911.10	431.40	3260.82	5601.46	905.88	11.30	896.99	28.61	855.59	429.34	862.99	424.00	-2801.250674
564	14	21	-12.32	0.30	1028.65	910.94	369.87	631.48	2941.22	905.65	9.27	896.86	25.31	862.28	369.45	864.41	355.67	-2801.250613
565	14	22	-12.32	0.30	1028.65	919.38	357.13	743.32	4147.63	905.86	9.77	897.20	24.74	881.64	366.74	885.70	344.68	-2801.250541
566	14	23	-12.30	0.32	1028.65	932.16	432.03	2796.65	4325.00	906.90	12.44	898.84	29.84	885.38	449.52	888.93	441.73	-2801.250126
567	14	24	-12.26	0.36	1028.65	894.63	374.68	2225.62	3072.85	905.48	10.79	896.27	28.00	845.20	382.62	850.06	377.54	-2801.249375
568	14	25	-12.20	0.42	1028.65	907.00	396.28	1803.30	1776.80	905.55	10.32	896.41	28.38	857.38	384.68	859.92	376.93	-2801.247950
569	14	26	-12.20	0.42	1028.65	933.58	413.65	2482.30	3209.92	906.19	11.21	897.49	28.54	893.03	426.09	899.33	420.35	-2801.247926
570	14	27	-12.19	0.43	1028.65	943.98	344.16	149773.99	443019.61	906.31	9.72	898.05	24.33	909.61	341.42	913.51	319.80	-2801.247769
571	14	28	-12.18	0.44	1028.65	940.28	422.81	2269.99	2205.38	905.87	9.80	897.24	26.74	883.81	426.15	893.10	423.59	-2801.247394
572	14	29	-12.16	0.46	1028.65	951.68	738.55	112943.23	336635.93	907.19	16.75	898.57	40.28	891.30	721.99	894.99	704.47	-2801.247150
573	14	30	-12.16	0.46	1028.65	959.55	479.76	1752.30	7718.77	907.17	11.90	899.34	31.37	921.80	498.44	929.70	499.78	-2801.247096
574	14	31	-12.12	0.50	1028.65	933.88	492.39	-10987.48	36573.13	906.35	12.86	897.64	32.01	884.52	509.86	895.57	521.89	-2801.246231
575	14	32	-12.10	0.52	1028.65	914.25	396.21	18697.01	49923.52	906.07	11.26	897.41	27.95	857.33	391.90	863.48	384.21	-2801.245807
576	14	33	-12.10	0.52	1028.65	943.15	668.13	3860.92	9191.78	906.91	15.80	898.15	37.95	885.11	653.02	890.42	637.57	-2801.245608
577	14	34	-12.09	0.53	1028.65	913.38	408.25	2262.98	3660.58	905.74	11.13	896.72	28.54	855.58	428.79	860.72	424.43	-2801.245413
578	14	35	-12.05	0.57	1028.65	958.23	422.84	8495.93	19312.11	906.85	9.82	899.26	26.21	904.82	425.19	909.66	413.66	-2801.244633
579	14	36	-12.02	0.60	1028.65	954.49	398.50	-13651.47	46390.05	906.86	9.48	899.34	25.43	902.83	384.26	906.71	374.69	-2801.243911
580	14	37	-12.01	0.61	1028.65	954.22	370.69	2802.30	2330.34	906.51	9.53	898.63	24.02	905.66	372.88	908.29	356.64	-2801.243800
581	14	38	-12.01	0.61	1028.65	907.51	396.10	-1452.66	10013.74	905.64	10.63	896.65	27.19	862.88	387.37	868.15	381.35	-2801.243698
582	14	39	-11.95	0.67	1028.65	959.47	381.04	2776.08	2761.63	906.40	8.66	898.54	23.60	913.42	363.48	919.88	352.05	-2801.242392
583	14	40	-11.93	0.69	1028.65	975.00	736.16	-85798.78	258254.23	908.25	17.86	900.35	41.53	917.05	711.07	922.67	692.92	-2801.241813
584	14	41	-11.72	0.90	1028.65	970.86	490.31	4202.18	13306.99	907.37	11.99	899.95	28.95	933.42	503.66	932.24	487.20	-2801.237177
585	14	42	-11.62	1.00	1028.65	973.90	194.11	3198.92	2232.29	906.37	4.57	899.02	11.59	943.93	207.90	931.70	189.22	-2801.234891
586	14	43	-11.43	1.19	1028.65	1019.41	718.59	2320.91	6857.03	908.98	16.73	902.33	39.91	980.32	721.70	975.62	691.88	-2801.230817
587	14	44	-11.32	1.30	1028.65	997.93	776.34	4974.95	11625.99	909.83	19.72	903.41	46.28	953.72	747.72	952.26	723.58	-2801.228306
588	15	1*	-13.53	0.00	1102.12	893.45	263.76	1423.95	343.40	961.38	8.88	951.85	22.22	841.01	253.60	849.04	236.72	-3001.368988
589	15	2	-13.37	0.16	1102.12	928.86	319.84	4597.08	10360.27	962.14	11.11	953.13	27.14	875.37	325.00	883.80	319.57	-3001.365066
590	15	3	-13.34	0.19	1102.12	941.88	340.18	698.65	1642.49	962.70	12.13	954.13	29.19	889.50	352.23	896.19	349.03	-3001.364408
591	15	4	-13.30	0.23	1102.12	912.05	329.26	1698.58	1485.53	960.94	10.50	950.31	26.93	874.14	325.93	884.80	321.35	-3001.363328
592	15	5	-13.08	0.45	1102.12	903.71	312.73	1399.48	1155.04	960.90	10.13	950.44	25.43	869.23	307.79	874.22	297.14	-3001.358222
593	15	6	-13.02	0.51	1102.12	905.97	326.86	525.90	3903.65	961.15	10.33	950.97	26.14	875.01	324.18	876.36	304.77	-3001.356777
594	15	7	-13.02	0.51	1102.12	947.46	359.18	1703.29	1971.91	962.64	11.79	954.04	28.79	895.24	360.50	902.28	358.09	-3001.356654
595	15	8	-12.84	0.69	1102.12	953.06	352.83	1688.04	2117.71	962.63	11.40	953.89	27.55	914.35	357.74	919.32	348.46	-3001.352278
596	15	9	-12.82	0.71	1102.12	951.49	367.75	1392.17	977.93	962.60	10.69	953.94	28.05	895.53	361.67	899.31	356.13	-3001.352016
597	15	10	-12.80	0.73	1102.12	950.25	413.78	3804.55	7977.07	962.99	12.99	954.52	31.87	894.16	426.02	903.35	435.57	-3001.351534
598	15	11	-12.78	0.75	1102.12	947.26	364.86	1392.87	1719.59	962.33	10.80	953.42	28.00	895.35	354.15	902.25	347.95	-3001.350995
599	15	12	-12.73	0.80	1102.12	985.46	432.27	1829.41	2450.26	963.81	12.25	956.02	31.59	925.41	415.62	936.89	424.15	-3001.349753
600	15	13	-12.69	0.84	1102.12	961.25	412.98	1361.80	1971.29	962.44	12.19	953.29	30.23	923.33	429.49	935.38	438.86	-3001.348769
601	15	14	-12.66	0.87	1102.12	982.62	364.11	32507.56	92409.43	963.12	10.76	955.00	28.17	925.49	351.75	931.26	343.79	-3001.348188
602	15	15	-12.66	0.87	1102.12	964.64	361.24	-2.74	5810.35	963.00	10.24	954.95	25.04	913.36	357.71	921.15	343.01	-3001.348056
603	15	16	-12.63	0.90	1102.12	966.40	376.85	1021.08	3696.63	962.05	10.72	952.62	28.31	923.07	390.66	931.87	390.16	-3001.347397

Polarizability models:					n*alp	DFT results		AM model		TL model		TE model		RP model		GD model		Etot
i	n	isomer	Eb	Erel	Aiso	Aaiso	Aaiso	Aaiso	Aaiso	Aaiso	Aaiso	Aaiso	Aaiso	Aaiso	Aaiso	Aaiso	Aaiso	
604	15	17	-12.62	0.91	1102.12	980.17	404.24	1517.10	7029.98	963.48	12.08	955.65	30.69	921.67	405.96	927.49	408.82	-3001.347092
605	15	18	-12.62	0.91	1102.12	958.60	437.01	5150.13	12665.74	962.23	12.50	952.91	33.80	899.12	451.91	910.66	465.22	-3001.347063
606	15	19	-12.59	0.94	1102.12	948.38	399.17	1658.47	2236.58	962.07	11.61	952.78	30.56	890.19	381.75	897.07	383.68	-3001.346439
607	15	20	-12.55	0.98	1102.12	963.70	326.54	2029.88	1447.80	962.65	9.18	954.34	23.99	914.23	313.05	919.28	299.14	-3001.345535
608	15	21	-12.55	0.98	1102.12	1003.53	359.00	2433.19	1630.64	963.53	10.44	955.85	27.14	954.52	333.66	961.43	324.10	-3001.345333
609	15	22	-12.50	1.03	1102.12	975.02	379.91	3146.21	3468.17	962.63	10.18	954.21	26.68	930.34	387.61	933.51	369.16	-3001.344298
610	15	23	-12.45	1.08	1102.12	1006.19	726.48	1916.76	5284.87	964.65	18.99	956.53	44.48	942.31	709.80	947.41	697.11	-3001.343148
611	15	24	-12.42	1.11	1102.12	1049.62	719.68	-6735.45	26314.12	965.72	18.91	958.75	43.22	998.82	734.27	994.78	702.60	-3001.342225
612	15	25	-12.39	1.14	1102.12	987.26	316.37	2609.18	1712.89	963.78	9.32	956.78	23.22	952.17	301.52	952.32	290.40	-3001.341684
613	15	26	-12.38	1.15	1102.12	1011.63	306.82	2994.09	2390.41	963.66	9.83	956.22	24.00	975.91	311.29	979.80	294.04	-3001.341337
614	15	27	-12.37	1.16	1102.12	1038.91	745.38	1340.03	1574.57	965.34	19.12	957.92	44.15	987.03	756.32	983.07	720.72	-3001.341173
615	15	28	-12.35	1.18	1102.12	1020.64	731.98	4943.03	14174.53	964.69	18.64	956.58	44.06	965.11	721.73	970.42	712.74	-3001.340723
616	15	29	-12.34	1.19	1102.12	1038.21	768.27	23354.14	67278.37	965.44	19.55	957.98	45.19	984.74	766.56	987.75	749.44	-3001.340546
617	15	30	-12.34	1.19	1102.12	1023.22	664.56	-698.99	6987.77	965.32	18.91	957.84	43.50	970.17	663.74	968.94	632.06	-3001.340405
618	15	31	-12.33	1.20	1102.12	1040.12	764.86	1090.06	1696.83	965.63	19.67	958.16	45.28	995.37	776.72	999.16	759.15	-3001.340233
619	15	32	-12.25	1.28	1102.12	979.65	310.07	1849.98	1795.05	962.33	9.14	953.70	23.18	931.03	300.18	940.54	302.72	-3001.338341
620	15	33	-12.24	1.29	1102.12	1044.06	739.35	-13427.09	50317.04	965.74	19.56	958.34	45.12	990.91	743.03	993.60	724.84	-3001.338115
621	15	34	-12.20	1.33	1102.12	1067.23	716.59	7236.90	22897.19	966.23	18.58	959.94	42.61	1017.20	716.64	1017.33	698.84	-3001.336996
622	15	35	-12.11	1.42	1102.12	1038.87	401.03	1629.32	2686.83	964.42	10.72	957.67	27.22	987.92	399.10	994.25	381.45	-3001.334961
623	15	36	-12.04	1.49	1102.12	1080.49	794.36	-10294.93	38058.83	967.29	20.38	961.28	44.79	1032.86	789.86	1029.09	752.13	-3001.333253
624	15	37	-11.86	1.67	1102.12	1096.16	743.11	-1238.46	6803.97	968.66	22.25	963.26	47.30	1058.86	766.18	1058.11	734.98	-3001.328999
625	15	38	-11.78	1.75	1102.12	1174.62	1161.56	510.86	6672.89	971.14	27.12	965.39	53.28	1103.50	1108.91	1089.43	1037.26	-3001.327049
626	15	39	-10.97	2.56	1102.12	1233.04	1198.28	1773.78	2913.41	973.03	27.93	969.09	56.88	1176.98	1151.83	1166.92	1115.06	-3001.307793
627	16	1*	-13.71	0.00	1175.60	997.75	232.71	3912.85	1847.98	1018.05	10.32	1009.35	24.40	936.27	256.82	944.03	235.21	-3201.464716
628	16	2	-13.69	0.02	1175.60	974.09	355.67	2072.02	1819.65	1016.98	11.20	1006.68	29.51	925.57	348.39	937.34	355.58	-3201.464233
629	16	3	-13.49	0.22	1175.60	1008.83	393.72	4744.23	12658.48	1019.00	12.35	1010.95	29.12	947.98	384.63	957.10	381.50	-3201.459142
630	16	4	-13.49	0.22	1175.60	974.21	243.48	1325.50	4653.88	1017.42	9.76	1008.07	23.48	918.60	244.97	921.36	229.22	-3201.458995
631	16	5	-13.47	0.24	1175.60	950.14	272.34	1229.72	2118.72	1016.31	10.52	1005.45	25.84	902.00	257.41	909.31	246.47	-3201.458660
632	16	6	-13.46	0.25	1175.60	993.62	317.15	-293.16	6033.30	1017.80	11.51	1008.46	27.33	949.00	319.90	955.38	309.92	-3201.458249
633	16	7	-13.45	0.26	1175.60	956.34	348.48	1307.79	1057.32	1016.88	11.42	1006.65	30.30	886.75	326.27	901.03	336.02	-3201.458040
634	16	8	-13.44	0.27	1175.60	947.85	313.20	1875.30	2277.95	1016.42	9.95	1005.82	25.88	914.09	302.07	916.76	279.13	-3201.457941
635	16	9	-13.28	0.43	1175.60	970.09	301.95	1263.72	1497.54	1017.45	9.52	1008.20	24.23	929.47	293.49	931.53	277.31	-3201.453783
636	16	10	-13.16	0.55	1175.60	1017.55	404.57	2419.41	2292.43	1018.29	12.62	1009.24	32.95	963.60	408.26	976.76	418.10	-3201.450791
637	16	11	-13.00	0.71	1175.60	1024.55	356.37	1480.91	2418.00	1019.65	11.53	1012.39	28.70	973.23	345.32	977.76	340.52	-3201.446702
638	16	12	-12.97	0.74	1175.60	1052.93	665.08	4760.94	10067.51	1020.27	18.52	1011.99	42.62	1007.11	654.44	1013.88	631.28	-3201.445957
639	16	13	-12.88	0.83	1175.60	1051.00	317.29	4362.64	7302.60	1019.54	11.08	1012.10	27.35	997.32	310.16	999.23	305.26	-3201.443499
640	16	14	-12.87	0.84	1175.60	1070.34	667.02	984.47	1370.21	1021.72	19.95	1015.02	44.55	1007.39	661.98	1013.13	651.06	-3201.443363
641	16	15	-12.79	0.92	1175.60	1089.48	682.25	2600.50	4419.59	1021.73	19.28	1015.22	43.62	1031.81	680.62	1034.05	660.84	-3201.441165
642	16	16	-12.54	1.17	1175.60	1097.14	473.63	-365.92	5816.44	1021.95	14.52	1016.10	34.82	1038.30	477.46	1050.08	490.26	-3201.434989
643	16	17	-12.46	1.25	1175.60	1105.41	668.68	4082.80	6725.41	1021.68	19.16	1014.97	44.01	1059.82	665.81	1063.07	649.63	-3201.432908
644	16	18	-12.41	1.30	1175.60	1116.04	752.37	2523.72	19360.66	1024.84	23.92	1019.92	51.63	1076.00	745.45	1072.99	696.21	-3201.431513
645	16	19	-12.41	1.30	1175.60	1108.02	851.66	-155.06	6108.13	1023.27	24.34	1016.75	53.29	1047.43	834.91	1056.22	838.95	-3201.431453
646	16	20	-12.12	1.59	1175.60	1135.42	670.96	2253.64	3283.64	1022.72	18.32	1017.07	44.17	1084.44	669.81	1088.79	660.00	-3201.424242
647	16	21	-11.98	1.73	1175.60	1179.30	850.11	-663.93	7422.84	1026.48	25.25	1022.07	52.44	1138.44	874.90	1139.57	861.04	-3201.420679
648	16	22	-11.94	1.77	1175.60	1198.27	756.89	1001.36	6987.16	1026.39	20.21	1023.15	42.54	1155.32	757.01	1154.45	727.01	-3201.419627
649	17	1*	-14.68	0.00	1249.07	944.16	270.06	1425.06	901.90	1070.20	8.76	1058.69	23.06	928.69	243.87	921.91	217.92	-3401.582481
650	17	2	-14.31	0.37	1249.07	972.81	259.36	1467.47	929.41	1071.18	8.27	1060.89	21.15	952.87	242.40	946.79	209.55	-3401.572397
651	17	3	-14.24	0.44	1249.07	971.98	232.56	1783.03	1093.93	1070.98	7.64	1060.53	19.47	950.59	213.70	945.78	182.66	-3401.570567
652	17	4	-14.08	0.60	1249.07	1009.63	304.76	1771.57	1242.01	1072.53	10.73	1063.45	27.37	957.36	303.33	961.78	297.02	-3401.566267
653	17	5	-13.91	0.77	1249.07	1007.93	288.28	1520.72	1845.24	1072.48	9.85	1063.54	24.78	965.15	269.89	972.23	249.18	-3401.561595
654	17	6	-13.87	0.81	1249.07	1010.77	258.12	2044.65	2060.46	1072.79	8.33	1064.37	21.15	967.38	211.44	970.42	188.02	-3401.560659

Polarizability models:				n*alp	DFT results		AM model		TL model		TE model		RP model		GD model		Etot	
i	n	isomer	Eb	Erel	Aiso	Aaniso	Aiso	Aaniso	Aiso	Aaniso	Aiso	Aaniso	Aiso	Aaniso	Aiso	Aaniso		
655	17	7	-13.83	0.85	1249.07	1047.00	204.94	7577.55	15518.18	1073.01	8.39	1064.79	20.57	989.62	212.01	997.58	198.36	-3401.559621
656	17	8	-13.80	0.88	1249.07	1052.22	341.26	2504.01	2261.00	1074.27	11.58	1066.77	28.65	1005.35	344.27	1012.22	345.95	-3401.558788
657	17	9	-13.75	0.93	1249.07	1027.24	207.56	1879.17	826.35	1072.42	7.71	1063.55	19.03	976.34	189.94	983.71	169.17	-3401.557482
658	17	10	-13.65	1.03	1249.07	996.57	252.91	622.58	7811.71	1071.44	8.78	1061.38	21.71	965.26	207.73	954.22	209.56	-3401.554738
659	17	11	-13.62	1.06	1249.07	1062.51	279.70	2179.19	1404.28	1074.41	10.85	1067.38	26.47	999.83	271.32	1007.72	271.82	-3401.553766
660	17	12	-13.56	1.12	1249.07	1072.60	258.88	-962.36	8709.37	1074.19	10.98	1066.81	26.13	1012.04	258.90	1020.76	259.18	-3401.552315
661	17	13	-13.47	1.21	1249.07	1035.31	252.74	1872.67	2437.23	1072.32	9.39	1063.19	23.17	982.83	248.44	989.80	236.04	-3401.549641
662	17	14	-13.43	1.25	1249.07	1093.69	334.17	792.65	4741.62	1075.48	12.83	1069.25	29.96	1028.59	334.79	1038.98	350.10	-3401.548790
663	17	15	-13.33	1.35	1249.07	1112.16	625.46	5205.59	9670.15	1075.51	18.56	1067.91	44.00	1059.90	618.72	1066.24	606.20	-3401.545950
664	17	16	-13.17	1.51	1249.07	1128.16	602.29	-2229.81	8890.43	1077.28	18.63	1071.76	42.51	1067.70	592.91	1069.30	581.12	-3401.541588
665	17	17	-13.14	1.54	1249.07	1111.08	610.51	663.71	4343.32	1075.63	19.18	1068.09	43.47	1059.36	601.18	1068.01	586.51	-3401.540947
666	17	18	-13.13	1.55	1249.07	1095.12	623.99	-2211.07	10804.42	1075.37	17.89	1067.59	41.03	1055.00	604.79	1053.29	571.65	-3401.540629
667	17	19	-13.10	1.58	1249.07	1110.27	773.00	3974.81	8130.49	1077.94	25.84	1071.34	57.57	1052.47	757.55	1064.12	754.14	-3401.539847
668	17	20	-13.09	1.59	1249.07	1127.37	683.65	-268.21	4477.75	1076.74	17.78	1069.53	38.25	1083.88	628.84	1077.08	618.71	-3401.539602
669	17	21	-13.08	1.60	1249.07	1092.95	539.64	1651.62	3695.32	1075.53	16.87	1068.72	40.77	1030.05	510.67	1038.08	508.00	-3401.539266
670	17	22	-13.01	1.67	1249.07	1115.06	591.00	4808.29	9718.61	1075.74	16.28	1069.12	38.03	1062.52	576.93	1057.55	543.86	-3401.537401
671	17	23	-13.01	1.67	1249.07	1137.56	616.89	10837.95	25680.06	1077.37	18.69	1071.77	43.46	1077.05	604.93	1080.99	592.55	-3401.537228
672	17	24	-12.92	1.76	1249.07	1108.72	632.84	6295.29	14069.17	1076.78	20.69	1070.33	47.71	1052.68	624.60	1054.72	611.76	-3401.534829
673	17	25	-12.85	1.83	1249.07	1143.15	634.39	35110.00	100205.70	1078.01	19.80	1073.10	43.49	1098.86	616.12	1099.25	600.07	-3401.532875
674	17	26	-12.82	1.86	1249.07	1125.24	677.75	12761.23	34136.77	1077.41	22.55	1071.02	51.17	1061.10	678.33	1070.43	680.85	-3401.532148
675	17	27	-12.80	1.88	1249.07	1128.12	525.58	-19937.24	66726.41	1075.82	15.42	1069.41	36.77	1069.41	524.06	1074.64	508.73	-3401.531506
676	17	28	-12.74	1.94	1249.07	1132.09	758.09	2884.38	3511.31	1077.78	23.84	1071.60	54.98	1053.11	736.10	1060.58	739.92	-3401.529931
677	17	29	-12.69	1.99	1249.07	1141.16	660.64	3389.24	4150.76	1077.89	20.57	1072.80	48.35	1089.01	660.68	1088.78	637.14	-3401.528626
678	17	30	-12.56	2.12	1249.07	1183.10	837.12	1406.02	2338.19	1080.03	25.79	1075.35	57.47	1113.43	835.55	1119.19	831.50	-3401.525161
679	17	31	-12.38	2.30	1249.07	1190.88	604.92	1166.28	7398.56	1079.38	18.20	1075.78	40.38	1145.98	609.07	1147.19	592.86	-3401.520313
680	17	32	-12.34	2.34	1249.07	1273.94	1312.08	-66149.39	202723.71	1086.20	39.75	1082.31	77.00	1223.60	1302.54	1211.99	1238.27	-3401.519025
681	17	33	-11.83	2.85	1249.07	1362.81	1239.87	22729.52	62461.80	1086.66	33.33	1084.13	61.80	1316.03	1246.18	1309.16	1204.34	-3401.505416
682	17	34	-11.52	3.16	1249.07	1520.90	1771.11	-72.63	4738.78	1092.30	41.70	1090.07	74.31	1452.78	1753.96	1442.11	1706.58	-3401.497030
683	17	35	-11.31	3.37	1249.07	1567.66	1791.79	-2618.69	8001.20	1096.00	41.80	1093.37	65.48	1508.67	1739.28	1472.73	1610.32	-3401.491364
684	18	1*	-15.01	0.00	1322.55	1010.85	143.93	3721.01	4256.29	1124.78	4.90	1114.48	12.01	990.39	123.06	977.11	107.88	-3601.685070
685	18	2	-14.96	0.05	1322.55	995.04	157.97	1288.94	436.62	1124.54	6.28	1113.95	15.82	971.69	140.61	953.98	121.25	-3601.683618
686	18	3	-14.93	0.08	1322.55	1030.31	224.20	1819.74	1309.27	1125.51	8.26	1115.66	20.45	995.75	208.90	991.53	212.55	-3601.682770
687	18	4	-14.92	0.09	1322.55	1009.29	198.27	1702.40	1164.39	1124.92	7.18	1114.62	17.87	986.99	169.07	971.88	170.97	-3601.682467
688	18	5	-14.86	0.15	1322.55	1016.28	178.79	2144.35	1622.03	1125.17	6.27	1115.21	15.43	993.52	148.73	979.88	149.58	-3601.680814
689	18	6	-14.82	0.19	1322.55	1015.53	198.43	1799.24	1435.02	1125.09	7.86	1114.98	19.81	975.13	191.59	966.24	171.02	-3601.679725
690	18	7	-14.82	0.19	1322.55	989.97	107.90	597.42	2249.38	1124.51	4.49	1114.08	10.96	982.46	70.69	950.02	70.09	-3601.679706
691	18	8	-14.72	0.29	1322.55	1036.78	257.31	3021.45	5129.98	1125.64	8.48	1115.92	21.03	1011.64	236.75	1003.77	240.23	-3601.676804
692	18	9	-14.59	0.42	1322.55	1072.18	251.24	2649.34	2511.71	1127.02	9.04	1118.56	21.78	1035.59	247.85	1037.25	246.20	-3601.673078
693	18	10	-14.11	0.90	1322.55	1082.34	224.61	2049.10	1127.53	1127.59	6.65	1120.07	15.50	1047.31	210.23	1047.77	204.12	-3601.659401
694	18	11	-14.09	0.92	1322.55	1067.48	225.05	2048.27	1555.18	1127.23	8.71	1119.39	21.04	1018.00	218.82	1013.75	235.12	-3601.658836
695	18	12	-13.68	1.33	1322.55	1198.69	669.69	1970.96	1515.12	1132.41	18.36	1126.88	39.09	1135.56	630.35	1136.00	624.51	-3601.647065
696	18	13	-13.67	1.34	1322.55	1150.07	650.32	3618.01	6005.77	1131.29	22.68	1125.09	52.69	1105.98	662.35	1113.25	649.99	-3601.646592
697	18	14	-13.51	1.50	1322.55	1171.31	663.34	1931.47	1811.09	1133.29	24.60	1128.72	55.71	1121.08	666.80	1120.47	645.95	-3601.641979
698	18	15	-13.43	1.58	1322.55	1138.42	656.50	6360.03	16923.75	1131.55	23.22	1125.92	53.13	1066.15	628.11	1073.86	622.79	-3601.639848
699	18	16	-13.43	1.58	1322.55	1145.81	635.26	3745.70	5306.97	1131.79	22.86	1126.30	53.12	1095.46	644.96	1094.07	613.29	-3601.639772
700	18	17	-13.37	1.64	1322.55	1235.09	647.41	-62555.88	171785.60	1133.53	18.20	1129.44	39.95	1188.24	636.89	1187.80	624.17	-3601.638001
701	18	18	-13.23	1.78	1322.55	1188.03	556.48	5591.73	11602.51	1131.45	17.12	1126.60	39.91	1123.76	535.49	1129.46	526.20	-3601.634101
702	18	19	-13.15	1.86	1322.55	1203.69	586.40	3123.35	2697.01	1131.72	18.98	1126.98	43.56	1149.53	591.16	1152.03	586.39	-3601.631658
703	18	20	-13.13	1.88	1322.55	1172.55	516.46	3328.09	3678.26	1130.59	17.36	1124.95	39.62	1123.77	522.33	1123.35	489.52	-3601.631164
704	18	21	-13.09	1.92	1322.55	1172.95	649.79	2875.89	5216.87	1131.92	20.70	1126.64	47.30	1104.37	617.63	1115.55	621.33	-3601.630070
705	18	22	-13.07	1.94	1322.55	1204.34	738.31	12696.99	34083.19	1132.76	23.92	1127.80	54.53	1154.02	734.69	1158.44	720.65	-3601.629585

Polarizability models:					n*alp	DFT results		AM model		TL model		TE model		RP model		GD model		Etot
i	n	isomer	Eb	Erel	Aiso	Aaiso	Aaiso	Aaiso	Aaiso	Aaiso	Aaiso	Aaiso	Aaiso	Aaiso	Aaiso	Aaiso	Aaiso	
706	18	23	-13.06	1.95	1322.55	1203.81	479.06	50648.30	129878.38	1132.65	16.01	1129.11	35.83	1148.43	473.74	1147.27	457.50	-3601.629296
707	19	1*	-15.62	0.00	1396.02	1058.19	163.84	1558.87	1321.84	1178.54	6.16	1168.98	14.69	1022.57	130.11	1007.38	158.63	-3801.797339
708	19	2	-15.52	0.10	1396.02	1088.11	107.22	2110.85	1028.26	1178.87	4.67	1169.66	11.24	1041.10	112.78	1040.23	102.79	-3801.794159
709	19	3	-15.51	0.11	1396.02	1079.98	140.04	4390.93	6460.93	1178.93	5.15	1169.76	12.40	1037.86	121.16	1034.29	131.79	-3801.793940
710	19	4	-15.44	0.18	1396.02	1067.12	167.52	2511.09	2655.90	1178.67	6.47	1169.23	15.78	1023.37	146.65	1016.09	156.67	-3801.791717
711	19	5	-15.42	0.20	1396.02	1067.58	107.43	1880.88	778.57	1178.57	2.70	1169.19	6.44	1038.40	72.30	1023.61	98.27	-3801.791042
712	19	6	-15.37	0.25	1396.02	1082.73	145.37	1813.38	709.38	1178.96	5.33	1169.86	12.82	1040.96	126.44	1035.77	137.87	-3801.789742
713	19	7	-15.08	0.54	1396.02	1095.00	127.29	1954.35	1078.40	1179.64	5.11	1171.28	12.49	1047.75	120.76	1046.28	108.47	-3801.780937
714	19	8	-15.06	0.56	1396.02	1102.33	204.84	613.97	3945.39	1179.65	6.33	1171.17	14.95	1069.80	187.43	1063.62	212.70	-3801.780243
715	19	9	-14.24	1.38	1396.02	1206.16	591.84	56.88	4366.56	1184.14	16.71	1178.13	35.03	1170.49	538.06	1151.27	508.31	-3801.755395
716	19	10	-13.76	1.86	1396.02	1207.11	686.74	1494.87	1186.75	1186.04	25.89	1181.27	57.38	1132.42	653.59	1147.73	658.51	-3801.740949
717	19	11	-13.54	2.08	1396.02	1219.72	811.29	1989.90	3120.38	1188.13	32.69	1183.27	67.82	1149.78	810.60	1163.88	801.14	-3801.734358
718	19	12	-13.49	2.13	1396.02	1242.89	744.72	3163.41	5284.17	1188.89	30.46	1185.41	63.54	1188.91	758.83	1194.75	748.32	-3801.732760
719	19	13	-13.38	2.24	1396.02	1252.18	686.01	37.23	6084.99	1188.02	26.88	1184.71	57.69	1184.49	681.18	1192.54	683.50	-3801.729414
720	19	14	-13.02	2.60	1396.02	1368.12	1138.30	878.33	2046.35	1191.90	35.17	1188.98	70.83	1290.43	1091.94	1298.27	1075.71	-3801.718532
721	19	15	-12.77	2.85	1396.02	1361.77	839.86	-421.82	5972.31	1192.46	31.25	1191.21	62.15	1310.25	873.16	1312.47	859.40	-3801.710890
722	20	1*	-16.23	0.00	1469.50	1137.87	82.48	2492.48	1290.81	1232.11	2.18	1223.91	4.64	1083.05	76.32	1087.09	106.03	-4001.911195
723	20	2	-16.10	0.13	1469.50	1124.23	83.08	2272.76	1132.16	1231.60	2.39	1223.02	5.55	1070.90	76.53	1067.86	103.78	-4001.907113
724	20	3	-16.08	0.15	1469.50	1125.09	47.19	2047.45	619.38	1231.40	0.57	1222.66	1.19	1064.41	42.42	1061.31	58.71	-4001.906578
725	20	4	-15.90	0.33	1469.50	1168.24	57.04	2667.46	631.09	1233.29	1.42	1226.11	2.44	1118.08	72.48	1122.93	72.96	-4001.900667
726	20	5	-15.88	0.35	1469.50	1133.52	79.91	2784.03	2443.99	1232.05	2.80	1223.98	6.19	1075.68	69.74	1076.08	97.36	-4001.900006
727	20	6	-15.87	0.36	1469.50	1150.20	99.67	2833.30	948.88	1232.58	3.32	1224.91	7.99	1098.11	89.40	1104.98	119.54	-4001.899622
728	20	7	-15.68	0.55	1469.50	1136.77	82.14	2313.18	1435.95	1231.95	3.36	1223.80	7.80	1075.76	69.72	1078.06	105.59	-4001.893814
729	20	8	-15.65	0.58	1469.50	1122.35	80.04	2456.85	2128.31	1231.28	3.40	1222.46	8.25	1056.25	53.73	1060.54	91.31	-4001.892691
730	20	9	-15.47	0.76	1469.50	1161.58	81.80	1523.86	1259.83	1232.75	3.23	1225.26	7.20	1100.77	94.73	1107.23	101.20	-4001.887140
731	20	10	-15.45	0.78	1469.50	1151.50	139.46	3086.26	2839.72	1232.59	4.77	1224.88	10.69	1104.27	132.40	1101.83	171.03	-4001.886343
732	20	11	-15.21	1.02	1469.50	1180.77	461.40	2207.68	2410.66	1234.17	13.63	1227.58	30.19	1143.84	437.14	1124.93	448.19	-4001.878604
733	20	12	-15.12	1.11	1469.50	1220.23	465.34	3576.12	6086.76	1236.28	13.35	1230.69	26.55	1172.31	408.92	1149.89	408.40	-4001.875771
734	20	13	-15.10	1.13	1469.50	1190.72	483.31	2469.16	3076.40	1234.68	15.21	1228.24	33.30	1151.09	463.26	1139.78	484.99	-4001.875247
735	20	14	-15.03	1.20	1469.50	1194.67	489.24	4315.44	8281.75	1234.77	15.55	1228.28	34.17	1146.26	462.97	1138.85	476.37	-4001.872824
736	20	15	-15.01	1.22	1469.50	1201.48	427.00	2557.04	2222.86	1234.41	12.50	1228.11	27.94	1157.73	411.50	1146.77	402.18	-4001.872318
737	20	16	-15.00	1.23	1469.50	1186.91	436.94	2214.42	2763.41	1234.18	13.19	1227.61	29.38	1139.81	417.25	1129.82	419.84	-4001.871870
738	20	17	-14.92	1.31	1469.50	1231.05	505.27	2604.00	2885.02	1236.05	14.61	1230.39	30.17	1182.96	469.18	1173.03	471.43	-4001.869593
739	20	18	-14.89	1.34	1469.50	1205.34	395.47	3481.76	3874.62	1235.12	11.40	1229.61	25.25	1161.96	375.60	1158.71	370.17	-4001.868503
740	20	19	-14.85	1.38	1469.50	1161.59	408.07	2118.45	2093.83	1233.54	13.90	1226.32	31.45	1126.74	388.69	1107.48	380.27	-4001.867180
741	20	20	-14.83	1.40	1469.50	1234.75	420.12	31204.87	83889.38	1236.08	12.53	1231.11	27.32	1188.87	398.47	1182.87	396.99	-4001.866647
742	20	21	-14.78	1.45	1469.50	1231.82	424.84	-1426.74	10293.91	1235.98	12.49	1230.89	27.24	1197.87	398.35	1184.57	392.87	-4001.865117
743	20	22	-14.66	1.57	1469.50	1169.38	477.87	2535.03	3345.10	1235.38	18.71	1229.51	42.69	1144.13	470.91	1131.82	458.25	-4001.861063
744	20	23	-14.54	1.69	1469.50	1242.55	480.79	4869.91	7792.19	1236.54	14.76	1231.69	32.24	1197.35	469.48	1195.09	458.68	-4001.857508
745	20	24	-14.54	1.69	1469.50	1179.21	463.47	1864.91	1611.86	1234.90	15.96	1228.78	35.16	1154.26	441.52	1127.00	439.00	-4001.857468
746	20	25	-14.47	1.76	1469.50	1206.13	594.82	3414.49	3588.16	1237.55	22.71	1233.09	51.14	1144.14	553.66	1153.70	567.37	-4001.855002
747	20	26	-14.43	1.80	1469.50	1202.40	621.03	1139.35	2547.26	1237.26	23.54	1232.37	52.98	1144.44	577.65	1152.75	593.48	-4001.853966
748	20	27	-14.30	1.93	1469.50	1222.96	505.26	2206.27	2142.48	1237.69	21.30	1233.80	47.92	1157.81	501.98	1169.61	486.10	-4001.849707
749	20	28	-14.26	1.97	1469.50	1233.87	558.44	3252.27	3974.71	1238.31	21.73	1234.72	47.62	1173.39	532.29	1181.85	539.04	-4001.848398
750	20	29	-14.25	1.98	1469.50	1240.66	576.61	3485.98	6063.50	1239.79	25.72	1236.73	55.02	1179.36	570.57	1191.71	570.08	-4001.848187
751	20	30	-14.11	2.12	1469.50	1277.98	757.95	2545.05	3289.52	1239.26	27.59	1235.06	62.95	1214.39	727.67	1236.67	750.77	-4001.843548
752	20	31	-14.10	2.13	1469.50	1333.50	0.02	-95529.28	396.13	1242.08	0.00	1242.40	0.00	1288.98	0.03	1317.98	0.02	-4001.843275
753	20	32	-14.08	2.15	1469.50	1220.32	489.78	2241.46	3357.60	1237.53	20.81	1233.51	47.40	1168.15	489.79	1173.95	470.46	-4001.842833
754	20	33	-14.03	2.20	1469.50	1266.50	580.75	2813.85	3624.02	1240.72	23.89	1238.67	49.70	1218.86	584.78	1218.50	565.35	-4001.841127
755	20	34	-14.02	2.21	1469.50	1260.47	644.73	-7738.69	28589.11	1240.71	28.99	1237.55	59.12	1219.62	660.48	1222.86	618.62	-4001.840705
756	20	35	-13.95	2.28	1469.50	1306.01	848.32	3258.38	4282.43	1242.29	32.22	1239.80	73.94	1244.51	845.61	1254.24	854.03	-4001.838549

Polarizability models:				n*alp	DFT results		AM model		TL model		TE model		RP model		GD model		Etot	
i	n	isomer	Eb	Erel	Aiso	Aaniso	Aiso	Aaniso	Aiso	Aaniso	Aiso	Aaniso	Aiso	Aaniso	Aiso	Aaniso		
757	20	36	-13.92	2.31	1469.50	1269.30	745.19	7376.36	16094.89	1241.24	32.79	1237.83	67.31	1226.08	757.44	1234.10	737.40	-4001.837671
758	20	37	-13.81	2.42	1469.50	1304.39	730.50	4091.86	5370.67	1242.70	32.09	1240.05	64.81	1261.48	767.94	1263.66	737.97	-4001.834153
759	20	38	-13.80	2.43	1469.50	1279.84	787.44	4959.37	10206.93	1242.22	33.32	1239.59	68.42	1194.55	742.28	1209.81	765.61	-4001.833754
760	20	39	-13.69	2.54	1469.50	1360.04	1150.92	1208.35	886.55	1245.41	42.97	1242.20	84.09	1314.41	1171.01	1324.81	1134.49	-4001.830347
761	20	40	-13.69	2.54	1469.50	1342.89	522.82	-9394.25	35962.67	1240.46	18.52	1238.78	38.25	1294.93	543.22	1301.16	535.78	-4001.830270
762	20	41	-13.64	2.59	1469.50	1306.97	752.72	2464.16	3201.13	1242.77	31.60	1240.86	66.59	1230.69	736.68	1242.70	744.09	-4001.828515
763	20	42	-13.59	2.64	1469.50	1328.79	634.12	-7330.36	40350.39	1242.46	25.86	1241.23	55.71	1287.73	661.00	1292.75	656.23	-4001.827175
764	20	43	-13.28	2.95	1469.50	1360.52	642.03	2278.67	8065.83	1241.90	22.49	1240.82	48.00	1315.93	634.61	1317.59	605.37	-4001.817073
765	20	44	-13.25	2.98	1469.50	1390.92	1227.16	-3481.69	15794.72	1247.52	45.14	1245.76	89.12	1320.74	1209.04	1334.28	1229.90	-4001.816294
766	20	45	-13.25	2.98	1469.50	1497.57	1193.51	1763.65	5238.40	1249.07	36.35	1248.39	72.47	1437.40	1177.92	1440.32	1156.80	-4001.816188
767	20	46	-12.99	3.24	1469.50	1504.92	978.98	-1136.89	6283.24	1251.11	36.56	1251.96	67.93	1460.84	1009.92	1465.98	1004.84	-4001.807850
768	20	47	-12.70	3.53	1469.50	1625.49	1343.73	1910.60	3943.17	1256.88	37.36	1258.36	69.08	1555.21	1296.80	1511.66	1186.18	-4001.798590
769	20	48	-12.22	4.01	1469.50	1676.20	1727.93	1175.98	7798.07	1262.95	58.13	1265.04	98.66	1631.13	1732.48	1623.33	1694.32	-4001.783450
770	20	49	-11.17	5.06	1469.50	2045.73	2846.07	2737.74	3227.86	1292.25	91.34	1288.25	110.53	1952.50	2730.78	1912.76	2602.12	-4001.749968
771	21	1*	-15.83	0.00	1542.97	1260.06	378.66	4635.77	6910.39	1287.27	10.42	1282.29	21.71	1201.90	366.25	1199.82	366.60	-4201.993305
772	21	2	-15.69	0.14	1542.97	1231.08	309.72	2282.79	1065.84	1285.70	7.46	1279.93	16.63	1170.36	301.75	1163.11	293.07	-4201.988802
773	21	3	-15.66	0.17	1542.97	1316.63	508.94	1251.40	3168.85	1290.09	12.44	1285.80	21.25	1252.51	464.78	1244.31	461.23	-4201.987752
774	21	4	-15.60	0.23	1542.97	1263.89	383.24	1180.54	3457.21	1287.63	9.72	1282.81	19.36	1206.51	367.99	1191.20	344.52	-4201.985672
775	21	5	-15.50	0.33	1542.97	1262.16	324.20	-4811.02	23415.61	1287.26	8.90	1282.63	19.66	1206.53	322.14	1208.51	317.24	-4201.982209
776	21	6	-15.41	0.42	1542.97	1247.68	437.18	1741.72	1004.75	1287.06	13.52	1281.85	28.84	1195.35	430.40	1192.79	460.56	-4201.979379
777	21	7	-15.34	0.49	1542.97	1148.41	85.76	1955.72	963.40	1282.59	2.80	1273.86	6.52	1088.14	13.32	1085.67	76.69	-4201.977037
778	21	8	-15.27	0.56	1542.97	1264.77	346.33	2189.01	1514.91	1287.03	10.17	1282.03	21.60	1206.62	332.05	1202.22	321.04	-4201.974772
779	21	9	-15.26	0.57	1542.97	1296.56	414.69164	4836.77492	4105.60	1289.43	12.36	1285.83	24.47	1233.78	387.32	1230.16	387.13	-4201.974282
780	21	10	-15.19	0.64	1542.97	1263.43	280.94	2735.80	6682.61	1287.45	9.58	1283.04	20.39	1204.09	270.05	1197.43	253.07	-4201.971977
781	21	11	-15.10	0.73	1542.97	1296.47	468.02	6668.45	14020.72	1289.13	14.46	1284.97	28.71	1239.64	438.54	1236.62	452.57	-4201.968955
782	21	12	-15.09	0.74	1542.97	1236.70	550.92	2073.97	1821.46	1287.55	21.48	1282.06	47.84	1184.77	545.89	1196.60	565.42	-4201.968532
783	21	13	-15.04	0.79	1542.97	1231.88	419.75	2058.88	1244.77	1287.76	16.89	1283.33	37.79	1193.50	430.81	1182.34	396.25	-4201.966855
784	21	14	-15.00	0.83	1542.97	1224.65	461.68	3096.39	4271.44	1288.20	19.75	1283.79	44.53	1190.98	478.70	1179.89	463.24	-4201.965640
785	21	15	-14.96	0.87	1542.97	1278.67	269.95	8820.54	15731.90	1288.18	8.90	1284.68	19.27	1218.53	266.04	1227.01	259.11	-4201.964283
786	21	16	-14.93	0.90	1542.97	1239.26	493.57	3004.16	3542.10	1288.99	20.02	1285.19	43.47	1194.20	469.36	1192.78	478.80	-4201.963199
787	21	17	-14.91	0.92	1542.97	1219.37	480.98	2451.47	2808.52	1288.32	20.65	1283.86	45.01	1168.95	462.60	1164.99	456.96	-4201.962577
788	21	18	-14.91	0.92	1542.97	1228.43	453.01	2486.08	2483.39	1288.34	19.45	1284.28	43.71	1188.23	466.35	1182.28	452.68	-4201.962552
789	21	19	-14.86	0.97	1542.97	1267.15	402.81	6226.92	11046.87	1289.65	16.67	1286.66	36.35	1231.89	422.47	1224.80	392.56	-4201.961105
790	21	20	-14.80	1.03	1542.97	1230.05	470.50	2461.68	2049.45	1288.16	20.03	1283.68	44.57	1195.73	491.28	1197.08	489.53	-4201.958806
791	21	21	-14.80	1.03	1542.97	1245.27	589.64	5645.32	10687.36	1290.89	24.62	1287.66	49.85	1228.97	556.97	1207.05	525.48	-4201.958787
792	21	22	-14.79	1.04	1542.97	1300.83	664.30	4325.07	7785.80	1293.44	28.77	1291.13	57.85	1271.41	690.30	1266.35	651.47	-4201.958439
793	21	23	-14.78	1.05	1542.97	1268.29	553.07	26.47	5223.97	1288.90	20.49	1284.62	43.69	1221.17	550.55	1226.01	559.62	-4201.958285
794	21	24	-14.75	1.08	1542.97	1226.77	482.62	2208.22	2357.57	1287.04	19.76	1281.51	43.99	1181.16	463.23	1193.62	496.30	-4201.957314
795	21	25	-14.74	1.09	1542.97	1305.43	573.27	4305.78	5799.43	1290.20	19.46	1287.02	41.83	1262.32	560.76	1250.08	558.79	-4201.956783
796	21	26	-14.73	1.10	1542.97	1231.37	512.89	3339.62	4291.12	1288.53	22.03	1284.09	48.66	1173.90	497.00	1184.09	518.49	-4201.956605
797	21	27	-14.68	1.15	1542.97	1245.33	467.00	2649.27	1867.12	1289.08	19.38	1285.45	43.55	1220.31	485.02	1205.94	445.97	-4201.954838
798	21	28	-14.50	1.33	1542.97	1319.86	659.17	38252.68	108492.66	1294.24	28.80	1292.68	57.99	1280.59	676.69	1278.33	639.64	-4201.948791
799	21	29	-14.38	1.45	1542.97	1291.50	631.39	1453.74	2234.54	1292.46	29.82	1290.01	62.64	1236.24	649.31	1251.71	640.62	-4201.944715
800	21	30	-14.36	1.47	1542.97	1294.84	735.69	29475.78	81799.22	1292.85	30.96	1290.70	67.94	1230.77	716.80	1238.98	731.61	-4201.944048
801	21	31	-14.32	1.51	1542.97	1283.58	560.10	3108.47	5259.01	1292.13	27.23	1289.93	57.21	1246.50	593.37	1241.81	570.39	-4201.942982
802	21	32	-14.29	1.54	1542.97	1362.59	836.57	9082.38	16215.01	1296.05	32.64	1295.85	74.04	1304.12	835.93	1311.66	832.01	-4201.941740
803	21	33	-14.12	1.71	1542.97	1345.92	690.68	4224.39	8047.42	1293.40	28.75	1291.72	62.51	1277.26	672.42	1292.28	673.04	-4201.936022
804	21	34	-14.08	1.75	1542.97	1367.39	756.52	-3393.80	14725.85	1297.47	34.83	1297.89	70.09	1313.36	769.07	1314.33	739.98	-4201.934740
805	21	35	-14.02	1.81	1542.97	1360.55	755.06	4319.65	8373.72	1296.15	33.68	1295.71	68.76	1307.33	767.47	1319.04	767.54	-4201.932840
806	21	36	-13.92	1.91	1542.97	1344.70	683.93	12068.14	31087.13	1293.37	26.50	1292.16	55.34	1281.52	681.85	1295.74	708.13	-4201.929553
807	21	37	-13.60	2.23	1542.97	1446.33	1159.53	-3746.43	16286.92	1301.15	46.54	1300.84	88.36	1364.47	1113.45	1379.42	1121.55	-4201.918604

Polarizability models:				n*alp	DFT results		AM model		TL model		TE model		RP model		GD model		Etot	
i	n	isomer	Eb	Erel	Aiso	Aaniso	Aiso	Aaniso	Aiso	Aaniso	Aiso	Aaniso	Aiso	Aaniso	Aiso	Aaniso		
808	21	38	-13.58	2.25	1542.97	1442.58	1136.43	-6006.38	22954.65	1302.11	45.83	1302.03	85.38	1373.26	1117.78	1394.96	1143.63	-4201.918173
809	21	39	-13.33	2.50	1542.97	1445.50	969.37	-6003.06	24391.49	1300.43	38.30	1302.00	75.18	1388.24	964.97	1396.88	941.61	-4201.909859
810	22	1*	-15.82	0.00	1616.45	1287.31	402.98	3095.76	3787.22	1339.20	15.05	1335.75	32.49	1235.60	408.97	1235.35	408.77	-4402.087956
811	22	2	-15.80	0.02	1616.45	1310.72	404.42	4189.53	5727.10	1340.95	15.56	1338.53	32.02	1266.14	438.74	1263.81	423.89	-4402.087345
812	22	3	-15.79	0.03	1616.45	1266.69	365.49	2531.50	2137.44	1338.92	14.32	1335.26	30.54	1216.02	378.22	1206.97	372.47	-4402.086815
813	22	4	-15.77	0.05	1616.45	1290.62	386.76	3276.65	3238.96	1339.19	14.35	1335.85	30.90	1237.59	390.39	1239.57	391.83	-4402.086250
814	22	5	-15.70	0.12	1616.45	1320.59	433.21	3317.02	3596.82	1342.17	17.28	1340.35	34.27	1273.32	452.14	1271.52	446.93	-4402.083745
815	22	6	-15.58	0.24	1616.45	1266.61	403.53	3298.04	5052.71	1338.43	15.83	1334.42	34.69	1211.88	404.46	1213.68	426.11	-4402.079507
816	22	7	-15.56	0.26	1616.45	1298.54	422.40	5427.36	9110.45	1340.19	15.49	1337.46	32.19	1246.25	439.15	1235.83	434.63	-4402.078828
817	22	8	-15.51	0.31	1616.45	1288.24	387.27	2363.46	1378.48	1339.04	15.36	1335.47	32.97	1238.70	401.84	1240.57	403.42	-4402.077009
818	22	9	-15.54	0.28	1616.45	1300.67	438.64	3106.36	3448.63	1339.87	15.60	1336.93	33.23	1238.74	428.70	1246.46	453.93	-4402.078301
819	22	10	-15.49	0.33	1616.45	1269.76	357.32	-4.23	6511.76	1338.35	14.53	1334.39	32.02	1220.77	377.25	1226.76	377.30	-4402.076253
820	22	11	-15.44	0.38	1616.45	1359.32	545.33	57907.24	167560.07	1342.32	18.05	1340.42	34.79	1294.53	531.90	1286.32	528.86	-4402.074804
821	22	12	-15.42	0.40	1616.45	1269.64	344.98	2679.97	2296.18	1339.06	15.40	1335.56	33.49	1214.05	339.32	1216.37	346.01	-4402.074108
822	22	13	-15.38	0.44	1616.45	1279.20	447.63	3624.54	5673.06	1340.31	19.40	1337.42	40.51	1234.89	450.01	1224.54	459.50	-4402.072442
823	22	14	-15.35	0.47	1616.45	1371.64	337.06	7871.61	14043.97	1341.66	10.72	1340.35	21.97	1315.41	337.86	1302.35	315.35	-4402.071630
824	22	15	-15.30	0.52	1616.45	1275.55	319.34	1925.68	3650.15	1338.77	14.08	1335.36	31.23	1224.19	349.52	1229.31	343.58	-4402.069879
825	22	16	-15.26	0.56	1616.45	1298.10	617.25	898.83	1975.07	1342.54	27.96	1340.02	57.10	1267.24	630.42	1254.21	618.20	-4402.068387
826	22	17	-15.11	0.71	1616.45	1293.33	568.83	4458.39	7261.34	1341.74	25.77	1339.34	56.06	1256.95	576.91	1247.97	559.97	-4402.063020
827	22	18	-15.07	0.75	1616.45	1271.39	520.53	3594.15	5290.96	1339.56	23.91	1335.30	51.49	1234.03	543.62	1247.78	534.75	-4402.061796
828	22	19	-15.00	0.82	1616.45	1346.73	507.96	2914.31	2794.67	1341.28	18.24	1339.00	37.33	1273.59	483.40	1284.40	506.88	-4402.059200
829	22	20	-14.88	0.94	1616.45	1330.72	619.95	88673.60	259825.47	1343.17	25.66	1341.87	55.70	1292.03	613.38	1282.44	612.56	-4402.055118
830	22	21	-14.74	1.08	1616.45	1321.46	631.85	-150.69	5788.10	1341.81	24.95	1339.43	53.87	1263.28	618.58	1268.19	623.85	-4402.050093
831	22	22	-14.65	1.17	1616.45	1290.09	644.27	2490.37	2820.66	1342.30	30.50	1339.52	65.52	1249.08	677.42	1253.49	662.51	-4402.046991
832	22	23	-14.59	1.23	1616.45	1370.00	551.95	-21543.00	73173.47	1345.87	28.92	1346.22	58.90	1318.86	570.68	1324.54	539.23	-4402.044991
833	22	24	-14.53	1.29	1616.45	1357.33	690.86	-21808.31	70976.27	1344.89	28.89	1344.61	60.80	1287.28	665.38	1294.42	681.70	-4402.042760
834	22	25	-14.41	1.41	1616.45	1390.61	739.93	4486.61	6022.59	1347.01	30.49	1347.79	68.28	1340.08	753.92	1337.49	737.13	-4402.038587
835	22	26	-14.39	1.43	1616.45	1393.35	671.48	-1111.45	10306.79	1345.16	30.49	1344.53	64.69	1336.03	685.73	1354.80	674.03	-4402.037938
836	22	27	-14.39	1.43	1616.45	1481.12	703.20	1708.55	2235.77	1348.51	22.32	1349.34	38.29	1415.13	687.17	1418.71	683.81	-4402.037712
837	22	28	-14.36	1.46	1616.45	1429.50	487.38	3313.10	3201.19	1344.96	14.72	1346.27	29.16	1349.50	495.49	1359.68	457.34	-4402.036925
838	22	29	-14.28	1.54	1616.45	1438.57	791.92	5894.38	11983.35	1348.44	33.39	1349.72	71.86	1381.05	792.17	1402.48	816.45	-4402.033904
839	22	30	-14.04	1.78	1616.45	1459.96	849.97	-178.89	11946.65	1350.63	36.36	1352.92	76.99	1412.28	856.67	1420.82	865.35	-4402.025428
840	22	31	-13.97	1.85	1616.45	1471.54	1118.46	8002.29	23603.56	1350.34	42.43	1349.99	79.63	1421.65	1098.88	1433.73	1092.88	-4402.023235
841	22	32	-13.79	2.03	1616.45	1496.91	1116.74	-15290.48	51834.29	1354.13	46.76	1356.29	88.50	1429.86	1114.07	1439.32	1105.22	-4402.016849
842	22	33	-13.42	2.40	1616.45	1543.09	1080.97	-6224.00	19989.37	1355.88	42.46	1359.09	78.05	1485.36	1091.53	1483.19	1074.87	-4402.003922
843	22	34	-13.23	2.59	1616.45	1637.12	1245.00	2464.29	12893.26	1361.74	50.16	1366.66	88.91	1588.73	1247.03	1590.77	1224.84	-4401.997161
844	22	35	-12.85	2.97	1616.45	1702.50	1348.57	-1673.14	19875.84	1368.97	60.76	1375.43	98.72	1635.70	1308.77	1642.69	1291.10	-4401.983668
845	23	1*	-15.95	0.00	1689.92	1332.01	446.69	5536.27	10033.07	1391.12	20.05	1389.51	42.26	1278.99	451.03	1282.69	455.82	-4602.187622
846	23	2	-15.82	0.13	1689.92	1284.41	499.14	2815.73	4163.44	1388.94	24.77	1384.55	52.88	1240.72	506.09	1257.88	560.61	-4602.182782
847	23	3	-15.81	0.14	1689.92	1292.87	451.80	-2926.57	14100.17	1389.25	21.36	1385.78	45.76	1243.87	461.95	1253.77	500.54	-4602.182553
848	23	4	-15.79	0.16	1689.92	1287.29	487.26	1796.56	2327.66	1389.26	23.14	1385.53	49.41	1237.27	500.22	1250.08	533.99	-4602.181850
849	23	5	-15.73	0.22	1689.92	1338.21	463.21	1713.66	2574.17	1392.21	22.93	1390.84	47.41	1298.21	500.78	1295.70	474.94	-4602.179565
850	23	6	-15.73	0.22	1689.92	1361.65	469.48	3150.70	3394.08	1392.86	19.18	1392.59	40.07	1311.07	474.26	1307.73	470.23	-4602.179487
851	23	7	-15.73	0.22	1689.92	1323.70	459.48	2741.75	2059.13	1390.69	20.47	1388.70	43.16	1268.53	454.60	1269.63	471.22	-4602.179418
852	23	8	-15.71	0.24	1689.92	1384.66	536.40	4549.67	6910.99	1394.60	24.28	1394.43	47.44	1332.55	549.80	1330.18	541.63	-4602.178732
853	23	9	-15.69	0.26	1689.92	1282.64	463.02	2250.58	2410.05	1389.64	24.08	1386.15	50.98	1260.56	508.59	1256.04	505.09	-4602.178241
854	23	10	-15.67	0.28	1689.92	1365.00	511.37	4898.23	8577.68	1392.20	19.60	1391.42	41.92	1305.13	501.24	1309.75	530.33	-4602.177266
855	23	11	-15.64	0.31	1689.92	1329.57	507.44	2322.08	1639.69	1391.16	21.98	1389.39	45.75	1272.59	515.39	1272.43	532.58	-4602.176338
856	23	12	-15.62	0.33	1689.92	1358.47	530.84	2813.22	3935.97	1392.69	22.41	1391.98	47.46	1309.76	532.28	1307.29	556.11	-4602.175521
857	23	13	-15.61	0.34	1689.92	1362.17	461.88	30653.60	83886.55	1393.24	20.72	1392.84	44.22	1324.45	488.44	1312.35	463.38	-4602.175070
858	23	14	-15.60	0.35	1689.92	1356.14	502.46	3032.14	3253.56	1392.92	22.41	1392.20	45.46	1317.01	523.46	1309.32	528.36	-4602.174711

Polarizability models:					n*alp	DFT results		AM model		TL model		TE model		RP model		GD model		Etot
i	n	isomer	Eb	Erel	Aiso	Aaiso	Aaiso	Aaiso	Aaiso	Aaiso	Aaiso	Aaiso	Aaiso	Aaiso	Aaiso	Aaiso	Aaiso	
859	23	15	-15.58	0.37	1689.92	1299.03	563.80	798.43	3933.40	1391.43	28.33	1388.95	59.91	1285.13	603.07	1269.14	563.12	-4602.174125
860	23	16	-15.55	0.40	1689.92	1406.34	466.38	3871.21	3916.37	1395.66	22.05	1396.68	43.22	1360.66	479.67	1358.04	452.81	-4602.172961
861	23	17	-15.54	0.41	1689.92	1353.52	515.36	2678.25	3047.43	1391.77	20.96	1390.59	44.64	1288.82	500.52	1294.44	529.88	-4602.172633
862	23	18	-15.50	0.45	1689.92	1332.59	446.95	-2798.62	14178.28	1391.71	21.20	1390.57	44.52	1284.95	452.21	1282.86	461.57	-4602.171137
863	23	19	-15.45	0.50	1689.92	1334.38	386.31	2473.30	2066.11	1391.41	18.05	1390.32	38.76	1290.64	411.70	1281.46	400.15	-4602.169299
864	23	20	-15.44	0.51	1689.92	1337.21	421.25	1872.18	1165.53	1391.87	18.73	1391.06	39.88	1285.90	411.17	1275.81	416.69	-4602.169068
865	23	21	-15.43	0.52	1689.92	1352.07	418.92	3128.93	2255.52	1391.58	17.26	1390.72	37.80	1294.48	411.80	1299.21	423.97	-4602.168628
866	23	22	-15.40	0.55	1689.92	1373.03	476.52	3808.73	4760.64	1394.50	21.74	1394.93	42.28	1315.66	488.57	1309.30	464.05	-4602.167657
867	23	23	-15.40	0.55	1689.92	1336.34	553.47	1441.35	1106.85	1393.90	27.74	1393.57	56.80	1309.79	560.70	1294.81	552.57	-4602.167594
868	23	24	-15.35	0.60	1689.92	1323.06	583.01	2617.52	3532.99	1393.00	29.94	1391.58	62.10	1298.01	604.94	1292.56	603.48	-4602.165707
869	23	25	-15.35	0.60	1689.92	1346.96	626.95	2580.44	4073.98	1395.29	31.73	1395.44	65.00	1317.94	658.34	1309.77	612.11	-4602.165529
870	23	26	-15.35	0.60	1689.92	1319.93	634.34	2350.88	2094.78	1393.20	30.71	1391.81	64.84	1286.78	633.42	1282.90	643.09	-4602.165521
871	23	27	-15.34	0.61	1689.92	1369.45	498.06	3396.15	3180.15	1392.33	20.97	1391.67	44.69	1305.84	494.02	1310.20	516.11	-4602.165376
872	23	28	-15.34	0.61	1689.92	1383.29	418.40	2534.87	985.06	1394.60	20.86	1395.37	41.61	1331.91	430.90	1337.17	396.15	-4602.165194
873	23	29	-15.32	0.63	1689.92	1362.97	544.63	3332.63	3965.37	1393.51	26.28	1392.92	54.80	1329.14	573.81	1321.95	570.16	-4602.164401
874	23	30	-15.26	0.69	1689.92	1378.17	429.93	2599.54	1780.57	1393.23	17.29	1393.46	36.86	1320.24	432.28	1322.56	417.84	-4602.162446
875	23	31	-15.24	0.71	1689.92	1428.89	570.54	3422.28	5438.19	1395.68	20.21	1397.04	39.41	1377.64	559.74	1361.08	534.70	-4602.161463
876	23	32	-15.23	0.72	1689.92	1384.93	652.56	976.72	4353.84	1397.63	34.50	1398.91	69.08	1337.02	669.77	1339.58	642.69	-4602.161219
877	23	33	-15.10	0.85	1689.92	1354.17	625.92	-1653.65	13273.42	1394.97	31.60	1394.88	66.32	1313.46	645.19	1316.64	635.41	-4602.156566
878	23	34	-15.08	0.87	1689.92	1341.40	642.55	2273.99	2805.01	1395.10	31.66	1395.32	65.87	1300.37	664.77	1292.49	653.40	-4602.155792
879	23	35	-15.03	0.92	1689.92	1379.78	426.23	1630.29	1659.87	1394.22	22.82	1394.48	46.16	1347.01	475.89	1342.56	436.31	-4602.154048
880	23	36	-15.01	0.94	1689.92	1355.18	585.47	1851.69	708.71	1393.97	29.14	1393.53	60.24	1326.14	617.44	1323.43	593.25	-4602.153228
881	23	37	-14.76	1.19	1689.92	1478.58	824.40	4720.24	7661.04	1400.88	36.16	1403.73	79.87	1413.35	801.72	1430.72	814.12	-4602.143997
882	23	38	-14.66	1.29	1689.92	1463.31	811.98	4516.17	6629.00	1400.38	37.51	1402.68	82.51	1398.21	793.49	1428.89	831.80	-4602.140266
883	23	39	-14.58	1.37	1689.92	1449.54	811.53	3264.64	3347.45	1400.23	37.73	1402.32	83.45	1386.60	802.99	1405.74	810.22	-4602.137385
884	23	40	-14.54	1.41	1689.92	1444.43	778.91	2496.00	4338.83	1399.73	34.34	1402.55	75.38	1393.19	762.10	1397.59	756.40	-4602.135899
885	23	41	-14.51	1.44	1689.92	1422.07	637.68	2617.34	3110.41	1397.34	31.72	1398.97	68.13	1376.31	658.07	1389.47	610.63	-4602.135047
886	23	42	-14.20	1.75	1689.92	1521.63	992.42	1951.82	14004.67	1404.22	44.01	1408.21	83.59	1444.31	950.96	1457.49	940.69	-4602.123350
887	23	43	-14.06	1.89	1689.92	1514.83	1050.74	44.33	4310.96	1408.86	57.90	1411.40	101.43	1474.47	1143.92	1489.32	1113.79	-4602.118420
888	23	44	-13.84	2.11	1689.92	1575.02	1116.11	283.89	6112.36	1411.16	53.52	1417.01	97.22	1549.91	1178.99	1537.24	1137.97	-4602.110301
889	23	45	-13.79	2.16	1689.92	1677.15	1046.11	769.76	3285.81	1411.21	42.21	1417.13	79.47	1614.69	1047.16	1626.29	1057.61	-4602.108510
890	24	1*	-16.21	0.00	1763.40	1314.77	502.54	2518.84	2045.92	1440.66	27.61	1438.80	57.43	1304.17	561.19	1281.22	541.48	-4802.292625
891	24	2	-16.18	0.03	1763.40	1316.77	512.29	4991.31	6680.72	1441.16	28.05	1439.75	58.32	1310.56	568.54	1284.23	542.59	-4802.291734
892	24	3	-16.11	0.10	1763.40	1321.62	456.87	2479.34	2057.34	1440.35	24.00	1438.79	50.28	1294.09	491.96	1288.28	498.52	-4802.289018
893	24	4	-16.05	0.16	1763.40	1351.95	420.81	195.76	5156.12	1442.70	23.36	1443.60	48.25	1293.11	425.31	1294.20	419.20	-4802.286775
894	24	5	-16.05	0.16	1763.40	1334.35	407.75	3851.25	4142.86	1440.18	22.64	1438.52	47.77	1300.78	459.88	1305.67	443.47	-4802.286619
895	24	6	-16.01	0.20	1763.40	1359.19	459.20	2573.17	2014.04	1442.83	23.98	1443.40	49.24	1324.57	486.45	1310.29	473.91	-4802.285157
896	24	7	-16.01	0.20	1763.40	1367.87	500.79	387.91	4622.95	1443.16	26.23	1443.62	53.30	1336.95	552.98	1322.95	531.33	-4802.284871
897	24	8	-15.99	0.22	1763.40	1322.98	445.11	2119.47	1347.89	1440.58	24.35	1439.22	51.14	1293.02	487.84	1290.46	488.45	-4802.284344
898	24	9	-15.99	0.22	1763.40	1340.22	432.70	2672.50	1881.19	1441.25	23.16	1440.72	48.43	1318.99	490.09	1306.43	462.13	-4802.284173
899	24	10	-15.96	0.25	1763.40	1349.73	420.06	2136.17	1744.18	1441.07	22.30	1440.55	46.70	1296.56	447.90	1295.47	435.51	-4802.283252
900	24	11	-15.96	0.25	1763.40	1353.18	615.15	2479.02	3320.91	1443.52	33.05	1443.18	67.92	1335.32	643.61	1318.71	626.25	-4802.283222
901	24	12	-15.91	0.30	1763.40	1345.64	425.73	2100.87	1167.84	1441.31	23.07	1440.81	48.38	1321.54	488.69	1311.98	463.73	-4802.281137
902	24	13	-15.89	0.32	1763.40	1357.62	414.61	2284.91	1065.77	1442.11	22.43	1442.43	46.63	1296.82	422.78	1301.32	418.30	-4802.280521
903	24	14	-15.88	0.33	1763.40	1356.86	422.07	2342.30	1979.29	1442.25	22.39	1442.61	46.31	1319.50	448.50	1308.66	433.26	-4802.279897
904	24	15	-15.87	0.34	1763.40	1339.39	449.08	1697.83	1639.49	1441.09	24.16	1440.16	50.50	1320.79	504.36	1304.36	483.14	-4802.279562
905	24	16	-15.86	0.35	1763.40	1409.09	508.07	111.25	7191.90	1443.64	25.04	1444.64	50.94	1352.21	512.71	1353.59	511.90	-4802.279188
906	24	17	-15.85	0.36	1763.40	1339.78	512.86	2394.59	2234.20	1441.32	26.20	1440.17	54.32	1311.32	514.97	1310.24	556.46	-4802.278859
907	24	18	-15.82	0.39	1763.40	1357.39	512.14	4127.27	6507.91	1442.63	27.93	1442.46	57.04	1333.72	542.27	1326.28	531.97	-4802.277616
908	24	19	-15.80	0.41	1763.40	1363.65	462.68	2547.70	2403.71	1443.52	25.19	1444.72	51.72	1331.98	492.21	1310.99	475.11	-4802.276849
909	24	20	-15.79	0.42	1763.40	1375.81	500.19	3113.83	4313.94	1442.57	24.66	1442.86	51.36	1310.64	491.00	1316.21	513.41	-4802.276634

Polarizability models:					n*alp	DFT results		AM model		TL model		TE model		RP model		GD model		Etot
i	n	isomer	Eb	Erel	Aiso	Aaiso	Aaiso	Aaiso	Aaiso	Aaiso	Aaiso	Aaiso	Aaiso	Aaiso	Aaiso	Aaiso	Aaiso	
910	24	21	-15.78	0.43	1763.40	1343.21	399.64	2251.18	1669.54	1440.93	20.90	1440.45	44.07	1310.36	449.95	1308.25	428.15	-4802.276193
911	24	22	-15.74	0.47	1763.40	1378.54	530.82	3040.38	4104.85	1443.27	26.82	1443.82	55.41	1329.47	528.09	1328.43	552.77	-4802.274714
912	24	23	-15.72	0.49	1763.40	1422.20	497.64	3819.57	3787.03	1444.72	23.83	1446.82	48.55	1372.44	511.63	1368.62	504.23	-4802.273869
913	24	24	-15.66	0.55	1763.40	1388.14	445.21	3164.25	3165.06	1443.18	23.84	1443.80	49.07	1354.94	485.67	1356.61	463.62	-4802.271594
914	24	25	-15.63	0.58	1763.40	1424.84	486.48	2785.50	2329.44	1444.98	23.94	1447.12	48.28	1374.86	502.86	1368.06	481.31	-4802.270582
915	24	26	-15.62	0.59	1763.40	1385.40	524.05	3145.18	4825.92	1443.21	25.52	1444.25	52.18	1302.62	484.08	1309.54	512.78	-4802.270201
916	24	27	-15.61	0.60	1763.40	1385.45	460.89	2692.20	2549.32	1444.51	24.73	1446.51	51.27	1350.64	497.88	1337.70	483.22	-4802.269682
917	24	28	-15.61	0.60	1763.40	1424.64	453.43	2160.48	3266.86	1444.13	20.82	1445.73	44.40	1367.47	475.21	1359.80	448.96	-4802.269638
918	24	29	-15.60	0.61	1763.40	1400.34	561.62	519.66	4512.44	1446.38	31.23	1448.72	61.75	1376.23	598.78	1362.48	563.18	-4802.269554
919	24	30	-15.60	0.61	1763.40	1374.47	584.38	4116.77	6319.78	1445.28	31.10	1446.91	63.26	1331.98	589.82	1325.53	572.87	-4802.269243
920	24	31	-15.58	0.63	1763.40	1399.75	516.23	4377.17	4090.29	1443.97	24.05	1445.57	49.24	1347.99	529.35	1355.93	537.91	-4802.268708
921	24	32	-15.55	0.66	1763.40	1393.53	599.99	3270.04	5601.98	1443.93	27.73	1444.68	56.24	1343.89	615.26	1341.60	609.36	-4802.267399
922	24	33	-15.53	0.68	1763.40	1414.21	531.66	706.63	3959.79	1445.72	28.06	1448.08	56.33	1354.99	528.97	1361.24	522.93	-4802.266801
923	24	34	-15.51	0.70	1763.40	1453.56	673.66	10624.58	26144.45	1446.73	30.54	1448.67	59.23	1406.58	701.83	1407.80	719.49	-4802.266094
924	24	35	-15.50	0.71	1763.40	1401.70	506.61	2531.65	1889.20	1443.41	23.12	1444.61	48.27	1340.89	503.37	1346.49	504.86	-4802.265600
925	24	36	-15.46	0.75	1763.40	1390.15	626.97	1317.82	4112.76	1446.19	33.99	1448.00	68.39	1360.68	644.07	1354.79	643.30	-4802.263943
926	24	37	-15.43	0.78	1763.40	1428.29	621.87	2747.72	2923.87	1445.78	29.75	1447.92	64.32	1388.24	624.65	1380.51	607.70	-4802.262957
927	24	38	-15.40	0.81	1763.40	1403.96	522.68	-358.96	7619.91	1443.93	23.39	1445.67	48.34	1350.86	529.07	1350.19	527.38	-4802.261883
928	24	39	-15.36	0.85	1763.40	1502.79	879.52	-1435.89	8989.95	1449.30	37.86	1451.95	72.46	1437.22	857.81	1449.18	865.31	-4802.260229
929	24	40	-15.35	0.86	1763.40	1502.99	686.51	9299.55	19249.80	1447.50	27.42	1450.02	52.48	1441.02	690.24	1436.96	672.18	-4802.259879
930	24	41	-15.32	0.89	1763.40	1421.79	333.05	2092.01	1932.64	1444.29	13.63	1447.36	28.46	1370.52	330.30	1365.45	339.66	-4802.258771
931	24	42	-15.19	1.02	1763.40	1466.61	414.45	4645.59	7246.41	1445.84	17.38	1449.19	36.44	1407.91	416.44	1409.89	425.42	-4802.253673
932	24	43	-15.14	1.07	1763.40	1431.70	703.63	3187.62	4238.08	1447.83	36.90	1450.29	75.92	1388.27	715.09	1309.28	699.19	-4802.251951
933	24	44	-15.07	1.14	1763.40	1475.98	719.41	7037.01	14986.16	1449.24	34.11	1452.87	65.85	1425.71	705.35	1430.01	725.89	-4802.249024
934	24	45	-15.06	1.15	1763.40	1465.73	514.18	-26124.21	89386.40	1445.77	24.83	1448.61	50.64	1393.45	519.33	1408.45	519.21	-4802.248624
935	24	46	-15.02	1.19	1763.40	1464.67	699.45	1555.87	1652.56	1448.49	33.63	1451.81	68.62	1429.79	721.77	1411.01	690.98	-4802.247209
936	24	47	-15.01	1.20	1763.40	1475.55	700.52	8364.81	14173.28	1447.37	30.75	1450.41	67.75	1425.83	710.98	1431.92	719.13	-4802.246620
937	24	48	-14.92	1.29	1763.40	1495.26	719.47	-2564.97	17480.95	1449.84	33.08	1454.07	71.65	1424.46	704.43	1436.30	703.87	-4802.243557
938	24	49	-14.57	1.64	1763.40	1562.73	1034.37	3520.31	4710.93	1453.96	47.42	1458.20	89.67	1497.16	1016.27	1517.93	1034.28	-4802.229896
939	24	50	-14.33	1.88	1763.40	1645.32	1295.82	-361315.831087911.74	1465.90	1465.90	67.00	1471.72	114.58	1572.46	1320.25	1582.39	1314.72	-4802.220612
940	24	51	-14.31	1.90	1763.40	1616.30	1093.80	2197.94	5666.45	1457.24	50.81	1462.88	93.75	1552.94	1080.33	1559.49	1085.38	-4802.220033
941	24	52	-14.14	2.07	1763.40	1654.83	1094.34	5985.95	21983.12	1458.31	47.80	1464.72	86.56	1599.60	1101.80	1604.20	1091.05	-4802.213658
942	24	53	-13.99	2.22	1763.40	1660.08	1150.51	238.47	6030.26	1464.10	57.88	1471.55	98.51	1588.34	1148.66	1602.63	1159.70	-4802.207816
943	24	54	-13.79	2.42	1763.40	1697.26	1353.56	1647.22	3638.29	1467.94	63.25	1474.54	103.49	1627.06	1341.64	1633.94	1324.00	-4802.200064
944	25	1*	-16.48	0.00	1836.87	1368.82	445.12	4112.94	5076.97	1491.21	25.93	1492.13	53.39	1349.43	508.15	1334.82	483.00	-5002.399141
945	25	2	-16.48	0.00	1836.87	1377.40	503.79	4126.95	6930.70	1491.75	29.01	1492.46	59.04	1358.78	549.35	1339.57	533.20	-5002.398854
946	25	3	-16.47	0.01	1836.87	1362.06	511.25	1368.29	3672.68	1491.22	29.07	1491.57	59.41	1342.98	542.97	1321.17	546.25	-5002.398561
947	25	4	-16.47	0.01	1836.87	1368.38	488.69	2459.12	2336.31	1491.66	27.54	1492.68	56.21	1346.28	524.49	1329.07	515.33	-5002.398513
948	25	5	-16.42	0.06	1836.87	1375.22	535.79	2985.89	3806.32	1491.75	30.05	1492.36	61.20	1346.93	563.16	1335.26	576.02	-5002.396708
949	25	6	-16.42	0.06	1836.87	1369.68	445.45	2694.16	2610.99	1491.46	24.77	1492.88	50.99	1335.32	491.47	1326.57	468.61	-5002.396669
950	25	7	-16.41	0.07	1836.87	1370.31	504.41	2484.33	2880.78	1491.83	29.89	1492.62	61.00	1347.48	566.95	1331.79	533.62	-5002.396168
951	25	8	-16.30	0.18	1836.87	1392.97	530.47	2986.61	5320.78	1492.55	30.26	1493.73	61.41	1359.44	563.25	1356.64	557.60	-5002.392007
952	25	9	-16.30	0.18	1836.87	1384.01	446.57	2438.64	1909.32	1492.27	25.56	1494.20	52.32	1355.43	507.68	1345.75	474.30	-5002.391823
953	25	10	-16.26	0.22	1836.87	1416.44	519.10	2725.01	1866.89	1494.07	29.96	1496.46	59.89	1396.31	569.02	1385.41	568.27	-5002.390372
954	25	11	-16.09	0.39	1836.87	1423.28	585.34	2859.30	4047.03	1494.32	31.95	1496.60	63.52	1390.30	620.96	1382.67	621.32	-5002.383646
955	25	12	-15.84	0.64	1836.87	1458.52	523.71	-6835.65	27389.30	1494.34	25.50	1497.97	53.06	1407.06	538.84	1410.55	557.58	-5002.373640
956	25	13	-15.81	0.67	1836.87	1472.48	753.40	-3249.18	14889.72	1497.07	35.06	1500.71	67.13	1340.55	773.64	1420.42	782.19	-5002.372332
957	25	14	-15.81	0.67	1836.87	1428.36	463.35	3333.78	3285.70	1495.09	26.15	1499.20	53.74	1464.26	455.76	1375.36	473.18	-5002.372271
958	25	15	-15.75	0.73	1836.87	1495.01	664.22	-4027.65	17960.33	1499.32	35.58	1503.99	66.00	1443.90	682.15	1438.80	694.23	-5002.369873
959	25	16	-15.71	0.77	1836.87	1457.04	625.39	3184.92	3857.13	1496.61	33.92	1500.59	69.33	1409.31	634.88	1408.17	621.80	-5002.368247
960	25	17	-15.70	0.78	1836.87	1462.20	795.36	10002.81	24125.34	1496.25	38.51	1498.51	75.09	1423.11	838.96	1422.86	829.93	-5002.367965

Polarizability models:				n*alp	DFT results		AM model		TL model		TE model		RP model		GD model		Etot	
i	n	isomer	Eb	Erel	Aiso	Aaniso	Aiso	Aaniso	Aiso	Aaniso	Aiso	Aaniso	Aiso	Aaniso	Aiso	Aaniso		
961	25	18	-15.66	0.82	1836.87	1500.62	537.29	2625.55	2355.41	1495.72	25.22	1499.91	52.12	1443.81	540.66	1441.65	544.24	-5002.366426
962	25	19	-15.59	0.89	1836.87	1517.85	579.78	5360.68	5830.82	1498.40	28.01	1503.97	56.47	1464.18	583.76	1464.71	584.26	-5002.363472
963	25	20	-15.58	0.90	1836.87	1456.38	488.06	-550823.9416	58502.54	1494.71	25.55	1498.85	51.88	1402.12	514.92	1395.62	500.20	-5002.363319
964	25	21	-15.56	0.92	1836.87	1512.88	532.42	-53142.23	168666.09	1496.49	25.70	1501.19	52.52	1469.69	548.00	1461.40	533.40	-5002.362508
965	25	22	-15.55	0.93	1836.87	1474.11	650.20	2118.64	1896.26	1497.28	34.56	1501.35	69.50	1445.01	669.90	1443.89	652.79	-5002.361793
966	25	23	-15.44	1.04	1836.87	1544.65	861.38	-7257.44	27539.12	1500.07	40.01	1504.95	75.53	1465.47	849.34	1481.82	880.37	-5002.357405
967	25	24	-15.43	1.05	1836.87	1497.46	768.32	7908.07	17796.95	1498.66	39.40	1502.57	75.18	1454.72	796.49	1456.94	801.41	-5002.357306
968	25	25	-15.40	1.08	1836.87	1531.20	853.80	1323.73	9207.07	1499.46	38.51	1504.59	73.84	1480.22	865.01	1472.68	854.66	-5002.356121
969	25	26	-15.36	1.12	1836.87	1499.10	467.82	25553.88	65712.97	1498.52	26.11	1504.63	54.54	1472.18	515.65	1455.05	474.25	-5002.354365
970	25	27	-15.33	1.15	1836.87	1494.18	672.51	4341.72	5786.74	1498.35	34.24	1503.25	69.31	1452.43	684.01	1442.57	659.38	-5002.353068
971	25	28	-15.31	1.17	1836.87	1526.64	525.50	3499.10	3670.67	1497.97	25.96	1503.67	52.53	1475.45	543.77	1471.10	534.72	-5002.352515
972	25	29	-15.29	1.19	1836.87	1583.54	1005.13	1739.11	4948.14	1503.25	45.58	1508.56	82.16	1522.95	997.83	1526.47	1008.55	-5002.351545
973	25	30	-13.48	3.00	1836.87	1978.89	1760.38	-31202.30	90501.33	1531.82	84.53	1542.13	135.43	1913.50	1782.25	1910.67	1770.67	-5002.279388
974	26	1*	-16.52	0.00	1910.35	1450.71	472.51	3225.04	3309.70	1542.92	28.72	1547.22	56.96	1423.13	532.88	1408.31	505.80	-5202.496575
975	26	2	-16.52	0.00	1910.35	1421.98	441.61	2575.31	2098.07	1542.06	26.16	1546.36	53.39	1384.75	498.98	1373.26	470.71	-5202.496422
976	26	3	-16.49	0.03	1910.35	1426.92	466.37	2299.82	2998.18	1542.32	28.79	1546.37	57.80	1394.92	514.93	1377.77	499.06	-5202.495232
977	26	4	-16.48	0.04	1910.35	1444.82	479.43	2038.83	3055.23	1542.27	28.17	1546.23	57.06	1419.05	531.33	1403.25	512.48	-5202.495114
978	26	5	-16.48	0.04	1910.35	1419.20	439.45	2386.06	1917.19	1541.76	26.17	1545.70	53.75	1395.06	501.60	1378.48	470.73	-5202.494940
979	26	6	-16.47	0.05	1910.35	1423.41	447.19	2560.58	1734.54	1541.23	26.79	1544.41	54.44	1384.94	497.85	1376.24	458.63	-5202.494594
980	26	7	-16.46	0.06	1910.35	1416.16	450.40	2465.61	2542.70	1541.82	26.72	1545.86	54.21	1373.20	496.03	1360.12	477.31	-5202.494297
981	26	8	-16.45	0.07	1910.35	1421.28	421.53	15673.52	40776.27	1541.40	24.77	1545.31	50.41	1393.44	476.23	1380.32	455.22	-5202.493628
982	26	9	-16.44	0.08	1910.35	1462.56	596.34	3309.26	5000.42	1543.68	33.75	1547.57	66.47	1417.05	604.03	1414.58	625.87	-5202.493421
983	26	10	-16.42	0.10	1910.35	1433.86	448.56	1993.53	1503.93	1541.79	26.75	1545.64	54.95	1401.36	505.03	1387.75	481.72	-5202.492291
984	26	11	-16.41	0.11	1910.35	1417.12	426.72	996.38	2913.97	1541.34	25.08	1545.18	50.90	1388.52	473.70	1374.20	455.16	-5202.492036
985	26	12	-16.38	0.14	1910.35	1431.87	452.19	2067.17	2109.87	1541.74	25.96	1545.71	53.13	1395.12	498.90	1387.63	491.52	-5202.490941
986	26	13	-16.37	0.15	1910.35	1445.04	460.13	6847.63	14695.27	1542.57	27.98	1546.75	55.84	1411.77	500.88	1399.24	486.72	-5202.490324
987	26	14	-16.35	0.17	1910.35	1418.28	414.65	2484.66	1524.86	1541.07	24.74	1544.70	50.75	1385.75	461.23	1378.62	451.19	-5202.489687
988	26	15	-16.35	0.17	1910.35	1420.89	386.96	18810.67	48908.04	1540.89	23.20	1544.34	47.55	1408.25	460.99	1389.49	416.67	-5202.489446
989	26	16	-16.32	0.20	1910.35	1458.79	607.98	3271.06	4901.18	1543.57	34.15	1547.36	67.40	1409.80	600.85	1405.39	619.46	-5202.488516
990	26	17	-16.32	0.20	1910.35	1435.79	432.38	3001.86	2433.14	1541.68	25.44	1545.55	51.93	1404.94	488.20	1395.69	462.44	-5202.488305
991	26	18	-16.31	0.21	1910.35	1431.92	454.29	2665.33	2195.11	1542.29	27.10	1546.55	55.16	1405.93	507.26	1389.35	489.39	-5202.487735
992	26	19	-16.30	0.22	1910.35	1441.70	416.45	2957.71	2658.15	1542.00	23.77	1546.40	48.75	1402.54	478.57	1396.31	443.21	-5202.487656
993	26	20	-16.29	0.23	1910.35	1464.95	463.63	4075.00	7903.32	1542.49	28.57	1546.37	56.86	1432.85	514.37	1429.57	489.70	-5202.487270
994	26	21	-16.28	0.24	1910.35	1421.45	398.41	2052.73	1229.02	1541.35	23.46	1545.43	47.86	1406.49	459.10	1388.95	422.47	-5202.486776
995	26	22	-16.28	0.24	1910.35	1450.13	438.82	2534.27	2333.57	1542.04	26.09	1546.18	53.29	1418.67	491.72	1408.82	467.28	-5202.486704
996	26	23	-16.28	0.24	1910.35	1451.92	544.25	2564.91	1549.53	1545.97	33.52	1552.33	67.33	1422.23	583.60	1404.64	539.35	-5202.486638
997	26	24	-16.25	0.27	1910.35	1438.23	373.00	2535.77	1198.44	1542.34	22.83	1547.28	45.96	1410.02	444.44	1398.40	408.50	-5202.485284
998	26	25	-16.25	0.27	1910.35	1450.10	433.63	2505.46	1646.91	1542.45	26.07	1546.92	53.10	1416.26	478.84	1409.01	469.99	-5202.485247
999	26	26	-16.22	0.30	1910.35	1413.89	410.97	2469.77	1943.96	1541.46	24.63	1545.64	49.96	1365.18	469.40	1356.21	447.16	-5202.484290
1000	26	27	-16.21	0.31	1910.35	1405.59	427.77	2223.60	1630.68	1540.95	24.84	1544.34	51.19	1372.48	468.09	1366.03	455.17	-5202.483726
1001	26	28	-16.20	0.32	1910.35	1455.56	477.73	2682.00	3224.67	1541.01	27.89	1543.60	57.57	1415.37	509.33	1443.43	509.55	-5202.483432
1002	26	29	-16.19	0.33	1910.35	1425.37	386.37	2164.38	1070.40	1541.65	23.48	1546.04	47.69	1404.78	457.18	1384.24	421.29	-5202.482986
1003	26	30	-16.18	0.34	1910.35	1482.98	456.57	4234.48	5717.67	1544.25	26.08	1550.33	52.67	1430.66	487.20	1427.63	471.61	-5202.482442
1004	26	31	-16.08	0.44	1910.35	1481.55	511.62	2875.80	3373.05	1544.00	27.54	1549.35	54.85	1442.22	546.62	1438.07	545.34	-5202.48205
1005	26	32	-16.04	0.48	1910.35	1405.93	349.02	2227.33	1210.55	1541.37	21.10	1545.97	42.82	1358.45	411.48	1354.82	396.96	-5202.476831
1006	26	33	-15.93	0.59	1910.35	1530.00	574.00	4487.03	6799.20	1547.24	31.80	1554.26	62.01	1482.79	590.00	1480.73	601.13	-5202.472172
1007	26	34	-15.85	0.67	1910.35	1492.45	630.99	1438.91	3789.68	1543.84	34.73	1547.82	68.41	1420.92	582.34	1451.36	654.64	-5202.468864
1008	26	35	-15.83	0.69	1910.35	1576.35	591.63	24922.95	73092.94	1548.85	32.83	1556.39	63.88	1521.91	603.56	1517.51	596.44	-5202.468090
1009	26	36	-15.78	0.74	1910.35	1537.24	527.58	6440.49	16037.07	1546.01	26.51	1553.16	53.52	1480.93	545.62	1488.55	546.76	-5202.465771
1010	26	37	-14.29	2.23	1910.35	1893.08	1865.49	-770.64	5804.86	1580.22	95.14	1588.50	144.73	1841.52	1895.41	1858.74	1933.35	-5202.404278
1011	27	1*	-16.79	0.00	1983.82	1459.27	427.81	2537.96	2011.65	1591.90	27.45	1598.99	54.24	1436.00	487.63	1411.90	464.57	-5402.604423

Polarizability models:					n*alp	DFT results		AM model		TL model		TE model		RP model		GD model		Etot
i	n	isomer	Eb	Erel	Aiso	Aaiso	Aaiso	Aaiso	Aaiso	Aaiso	Aaiso	Aaiso	Aaiso	Aaiso	Aaiso	Aaiso	Aaiso	
1012	27	2	-16.79	0.00	1983.82	1483.48	434.80	23501.32	63888.43	1592.44	26.97	1599.98	53.63	1451.42	478.64	1437.27	469.71	-5402.604262
1013	27	3	-16.78	0.01	1983.82	1484.01	468.44	3585.33	5170.30	1592.15	29.76	1598.90	59.75	1450.01	517.39	1440.70	500.75	-5402.603956
1014	27	4	-16.75	0.04	1983.82	1477.92	472.75	2765.80	2147.99	1592.16	28.09	1599.27	57.01	1444.18	517.48	1435.27	502.42	-5402.602532
1015	27	5	-16.75	0.04	1983.82	1504.78	487.58	3065.83	3416.50	1593.11	29.80	1600.57	58.85	1466.06	532.78	1459.98	521.99	-5402.602454
1016	27	6	-16.74	0.05	1983.82	1457.35	382.49	2398.46	1790.67	1591.34	24.16	1598.50	48.57	1414.91	435.12	1407.48	419.43	-5402.602216
1017	27	7	-16.71	0.08	1983.82	1487.83	470.72	3338.68	3785.15	1592.70	29.75	1599.97	59.29	1447.98	517.58	1437.74	505.83	-5402.600918
1018	27	8	-16.70	0.09	1983.82	1472.50	426.12	3571.73	4855.55	1590.23	25.96	1595.83	53.04	1451.41	468.57	1449.05	455.14	-5402.600376
1019	27	9	-16.69	0.10	1983.82	1501.35	472.92	9542.22	21339.53	1593.03	29.52	1600.46	58.40	1461.11	528.82	1454.79	509.11	-5402.600161
1020	27	10	-16.66	0.13	1983.82	1464.58	463.50	-2983.74	11053.84	1592.62	29.53	1599.98	58.40	1430.20	498.44	1410.70	497.90	-5402.598701
1021	27	11	-16.64	0.15	1983.82	1469.55	419.35	1406.62	3428.21	1592.05	26.92	1599.24	53.55	1440.77	472.72	1422.12	456.08	-5402.597821
1022	27	12	-16.62	0.17	1983.82	1503.27	482.74	2736.22	2143.12	1592.94	28.74	1600.26	57.61	1450.32	497.37	1460.45	519.66	-5402.597032
1023	27	13	-16.61	0.18	1983.82	1503.23	515.64	6700.25	10959.03	1593.07	32.26	1600.10	64.44	1470.70	551.15	1460.50	561.51	-5402.596295
1024	27	14	-16.57	0.22	1983.82	1491.47	457.79	2599.08	1833.04	1590.76	27.27	1596.35	55.83	1467.61	512.80	1466.39	488.19	-5402.594957
1025	27	15	-16.57	0.22	1983.82	1510.25	563.82	7214.54	15258.55	1593.66	33.46	1600.80	64.97	1462.39	525.89	1463.45	592.36	-5402.594825
1026	27	16	-16.52	0.27	1983.82	1501.38	494.51	3335.27	4128.79	1593.13	30.37	1600.54	58.82	1467.66	526.95	1452.17	536.85	-5402.592741
1027	27	17	-16.51	0.28	1983.82	1517.15	471.98	2402.08	3886.37	1593.34	29.36	1600.85	58.38	1464.76	483.77	1474.13	498.44	-5402.592332
1028	27	18	-16.44	0.35	1983.82	1572.20	600.41	4938.91	10300.21	1594.06	30.73	1601.65	59.13	1528.12	502.00	1521.43	600.12	-5402.589285
1029	27	19	-16.43	0.36	1983.82	1556.97	474.95	119145.55	347021.57	1594.79	30.83	1602.74	59.62	1516.17	538.52	1517.11	509.04	-5402.588973
1030	27	20	-16.42	0.37	1983.82	1529.16	520.50	3082.27	3150.66	1594.62	29.57	1602.78	60.17	1503.29	551.97	1488.57	544.81	-5402.588131
1031	27	21	-16.15	0.64	1983.82	1521.51	640.52	-7022.69	26935.10	1594.81	39.76	1601.50	76.66	1469.87	635.81	1484.47	662.00	-5402.576842
1032	27	22	-16.14	0.65	1983.82	1557.58	627.79	3083.99	3355.30	1597.41	37.10	1606.68	76.03	1537.65	663.24	1522.65	639.20	-5402.576343
1033	27	23	-16.13	0.66	1983.82	1578.34	841.44	-2904.12	23183.18	1597.04	44.99	1604.34	84.41	1523.66	808.93	1525.18	836.55	-5402.575680
1034	27	24	-16.07	0.72	1983.82	1558.03	501.37	3151.69	3484.72	1596.44	29.23	1606.06	57.16	1525.34	515.84	1510.47	487.97	-5402.573075
1035	27	25	-16.06	0.73	1983.82	1584.01	545.48	3320.85	4676.15	1597.00	29.82	1607.07	59.93	1529.72	545.07	1527.08	552.10	-5402.572731
1036	27	26	-16.04	0.75	1983.82	1593.06	865.26	5430.49	6067.31	1597.91	46.24	1605.49	85.81	1547.44	908.83	1534.57	859.51	-5402.571851
1037	27	27	-15.94	0.85	1983.82	1568.18	490.44	4439.21	4887.02	1596.53	31.54	1605.46	60.76	1539.03	518.25	1528.86	496.10	-5402.567754
1038	27	28	-15.87	0.92	1983.82	1540.76	648.62	-2726.31	18009.35	1595.82	38.38	1603.82	75.19	1506.60	652.91	1513.03	665.30	-5402.564542
1039	27	29	-15.59	1.20	1983.82	1640.08	494.24	3566.70	2460.34	1599.63	27.11	1611.40	53.68	1579.02	498.54	1591.63	485.16	-5402.552698
1040	27	30	-15.57	1.22	1983.82	1674.90	664.42	5472.62	7408.21	1600.60	31.82	1612.05	63.11	1619.62	680.21	1615.20	682.11	-5402.551631
1041	27	31	-15.43	1.36	1983.82	1660.20	879.66	5895.13	11033.18	1600.95	43.09	1611.58	79.87	1584.56	884.57	1599.74	908.09	-5402.545637
1042	27	32	-15.18	1.61	1983.82	1687.98	826.05	3466.31	6344.24	1604.07	45.74	1615.75	85.60	1638.72	831.16	1650.09	842.56	-5402.534974
1043	27	33	-14.97	1.82	1983.82	1724.20	988.63	-9924.43	34420.29	1609.26	53.13	1622.55	100.05	1665.10	980.30	1665.06	975.91	-5402.525785
1044	27	34	-14.93	1.86	1983.82	1789.95	1265.21	-5549.91	23261.85	1619.28	77.85	1632.25	128.44	1724.44	1274.85	1739.74	1276.45	-5402.524175
1045	27	35	-14.81	1.98	1983.82	1869.48	1326.34	2203.12	8184.61	1614.68	64.18	1626.35	109.59	1787.04	1275.50	1791.12	1238.69	-5402.518881
1046	28	1*	-17.16	0.00	2057.30	1544.98	587.18	5237.19	10083.96	1642.26	36.79	1651.26	69.65	1489.22	516.09	1494.44	590.11	-5602.717408
1047	28	2	-17.08	0.08	2057.30	1524.81	455.39	2489.48	1748.17	1641.45	31.13	1650.99	59.58	1488.47	496.87	1473.09	482.22	-5602.713802
1048	28	3	-17.05	0.11	2057.30	1517.33	442.94	2828.76	2478.63	1641.22	29.75	1650.80	57.72	1479.47	484.45	1465.05	467.02	-5602.712447
1049	28	4	-17.03	0.13	2057.30	1527.32	444.69	4137.72	6823.82	1641.25	30.10	1650.64	58.41	1502.38	501.58	1482.92	464.36	-5602.711481
1050	28	5	-17.03	0.13	2057.30	1532.93	450.75	1799.76	1323.53	1641.68	31.22	1651.36	59.80	1495.81	486.74	1480.69	472.69	-5602.711432
1051	28	6	-16.94	0.22	2057.30	1526.88	420.56	2618.77	1823.98	1640.74	29.09	1649.89	56.26	1516.13	506.81	1486.42	446.70	-5602.707398
1052	28	7	-16.92	0.24	2057.30	1540.01	462.01	2883.25	2787.68	1641.96	31.21	1651.81	59.75	1506.11	495.28	1494.97	493.24	-5602.706535
1053	28	8	-16.86	0.30	2057.30	1538.27	534.38	4200.27	6043.24	1642.38	32.11	1652.62	61.76	1483.64	554.43	1481.57	560.38	-5602.703993
1054	28	9	-16.85	0.31	2057.30	1558.53	480.55	4074.63	5531.41	1642.18	31.82	1652.01	61.47	1517.76	539.52	1504.48	513.15	-5602.703374
1055	28	10	-16.81	0.35	2057.30	1512.74	331.77	2772.66	1199.61	1639.39	32.82	1648.41	46.86	1505.26	440.03	1477.45	352.02	-5602.701695
1056	28	11	-16.77	0.39	2057.30	1535.42	456.58	2467.71	1725.16	1641.78	31.38	1651.32	60.77	1505.21	507.52	1483.05	475.81	-5602.700023
1057	28	12	-16.77	0.39	2057.30	1544.22	430.62	3430.30	3921.34	1641.73	27.47	1652.07	53.47	1504.82	480.86	1494.41	465.74	-5602.699789
1058	28	13	-16.75	0.41	2057.30	1528.35	448.65	2540.05	2016.13	1639.89	26.78	1648.85	55.36	1511.49	497.57	1503.41	485.88	-5602.698879
1059	28	14	-16.70	0.46	2057.30	1547.15	437.17	4646.34	7431.25	1641.66	29.23	1651.56	56.50	1521.88	484.11	1504.87	453.30	-5602.696783
1060	28	15	-16.68	0.48	2057.30	1582.40	573.06	3991.25	5805.71	1643.43	34.72	1653.69	66.90	1530.19	579.60	1536.05	624.99	-5602.695908
1061	28	16	-16.66	0.50	2057.30	1532.77	381.90	2481.08	2055.42	1641.65	27.35	1651.96	53.06	1521.94	463.28	1486.08	396.54	-5602.694845
1062	28	17	-16.61	0.55	2057.30	1541.04	476.06	4123.69	3629.69	1640.87	28.23	1650.40	54.72	1492.92	497.82	1492.48	511.65	-5602.692613

Polarizability models:					n*alp	DFT results		AM model		TL model		TE model		RP model		GD model		Etot
i	n	isomer	Eb	Erel	Aiso	Aaiso	Aaiso	Aaiso	Aaiso	Aaiso	Aaiso	Aaiso	Aaiso	Aaiso	Aaiso	Aaiso	Aaiso	
1063	28	18	-16.41	0.75	2057.30	1620.64	956.89	3912.97	6098.92	1648.83	54.70	1659.06	100.05	1585.92	989.55	1571.96	958.71	-5602.683786
1064	28	19	-16.33	0.83	2057.30	1606.68	524.50	2514.70	4536.71	1645.21	29.70	1657.01	59.96	1575.02	567.63	1559.16	546.19	-5602.680400
1065	28	20	-16.32	0.84	2057.30	1606.42	469.13	113878.83	336137.44	1644.99	31.84	1656.34	62.71	1595.32	510.08	1560.60	475.28	-5602.679598
1066	28	21	-16.28	0.88	2057.30	1582.61	365.43	1861.35	1773.81	1642.25	25.87	1652.75	50.16	1556.34	402.26	1545.42	370.78	-5602.678163
1067	28	22	-16.20	0.96	2057.30	1668.66	825.86	2889.10	2259.82	1649.14	48.05	1660.48	87.27	1621.35	854.07	1616.65	842.62	-5602.674344
1068	28	23	-16.12	1.04	2057.30	1683.38	1187.00	5932.59	13405.35	1653.88	69.01	1663.43	121.01	1617.55	1181.94	1630.73	1224.94	-5602.670737
1069	28	24	-16.10	1.06	2057.30	1567.83	547.39	1952.20	1352.15	1642.94	33.21	1653.14	69.21	1548.41	568.20	1553.00	525.86	-5602.669727
1070	28	25	-16.09	1.07	2057.30	1627.53	950.00	1467.78	2353.15	1650.28	56.17	1660.83	104.64	1597.97	966.31	1596.95	949.71	-5602.669401
1071	28	26	-16.09	1.07	2057.30	1626.16	744.42	2735.78	7186.81	1647.19	44.05	1658.11	82.85	1581.39	783.13	1580.14	782.14	-5602.669258
1072	28	27	-16.07	1.09	2057.30	1658.44	1002.52	-26750.17	87010.40	1649.92	55.69	1660.70	100.69	1589.91	998.45	1598.74	1004.64	-5602.668771
1073	28	28	-16.04	1.12	2057.30	1733.69	1120.87	373.36	4407.41	1652.56	51.97	1663.57	87.17	1672.77	1071.64	1669.91	1099.09	-5602.667217
1074	28	29	-16.01	1.15	2057.30	1728.80	1089.73	16338.48	41972.25	1655.20	61.05	1666.91	104.97	1691.96	1125.70	1691.11	1124.40	-5602.666117
1075	28	30	-15.99	1.17	2057.30	1580.64	451.66	2694.92	2929.06	1643.14	27.76	1654.30	54.57	1548.72	489.35	1540.11	448.52	-5602.664993
1076	28	31	-15.86	1.30	2057.30	1788.67	1166.49	1363.32	2241.22	1653.96	50.31	1665.22	82.22	1738.19	1147.32	1732.44	1166.75	-5602.659152
1077	28	32	-15.65	1.51	2057.30	1704.16	426.69	2905.60	3759.10	1648.09	27.89	1661.99	55.05	1645.03	440.99	1653.46	431.57	-5602.649985
1078	28	33	-15.61	1.55	2057.30	1745.38	745.35	-6305.25	27190.04	1654.89	47.85	1670.12	83.54	1688.38	751.95	1680.18	735.37	-5602.647896
1079	28	34	-15.46	1.70	2057.30	1648.82	596.05	11098.88	26312.51	1646.89	36.61	1659.07	69.97	1576.40	592.27	1602.76	644.39	-5602.641241
1080	28	35	-15.43	1.73	2057.30	1756.74	1096.13	2636.38	2471.32	1657.64	61.52	1670.84	105.21	1699.57	1106.29	1701.45	1102.89	-5602.640055
1081	28	36	-15.40	1.76	2057.30	1758.95	1002.12	4876.02	14402.26	1658.35	57.21	1673.77	110.30	1709.43	1035.24	1708.35	1001.53	-5602.638738
1082	28	37	-15.39	1.77	2057.30	1730.88	1022.54	-3469.59	14978.09	1654.86	57.77	1667.81	103.00	1659.91	994.84	1670.97	1044.96	-5602.638341
1083	28	38	-15.15	2.01	2057.30	1822.08	1296.30	-343.51	11972.92	1664.70	71.90	1679.77	124.17	1747.48	1292.27	1765.03	1304.30	-5602.627346
1084	28	39	-15.02	2.14	2057.30	1771.33	871.22	4201.24	3479.75	1653.87	44.46	1669.55	82.21	1708.83	886.12	1724.01	887.16	-5602.621652
1085	28	40	-14.70	2.46	2057.30	1946.31	1540.29	2703.49	5217.39	1670.40	79.74	1684.32	126.58	1880.24	1523.78	1892.64	1552.33	-5602.607458
1086	28	41	-14.50	2.66	2057.30	1896.93	888.24	-3289.87	39244.02	1662.04	44.90	1680.31	81.57	1822.78	899.74	1832.25	897.05	-5602.598455
1087	28	42	-14.30	2.86	2057.30	1920.09	1300.23	23092.38	61128.55	1676.88	84.10	1694.24	125.48	1828.77	1294.32	1864.31	1379.10	-5602.589723
1088	29	1*	-17.28	0.00	2130.77	1542.13	441.77	2376.27	1296.62	1687.10	27.25	1697.61	56.54	1555.31	512.27	1534.90	490.49	-5802.819727
1089	29	2	-17.21	0.07	2130.77	1544.95	433.37	2393.64	1191.00	1687.54	26.38	1698.82	54.70	1544.84	501.66	1525.77	475.22	-5802.816564
1090	29	3	-17.04	0.24	2130.77	1584.33	506.39	2987.43	2223.49	1689.25	30.65	1700.62	62.74	1571.78	560.17	1566.80	542.74	-5802.808935
1091	29	4	-16.93	0.35	2130.77	1645.98	554.67	7284.39	13022.15	1691.62	36.48	1703.90	68.47	1583.47	485.57	1594.68	567.64	-5802.803626
1092	29	5	-16.92	0.36	2130.77	1651.48	483.02	4211.84	5997.92	1691.66	30.11	1704.95	56.86	1599.91	525.41	1596.46	507.85	-5802.803029
1093	29	6	-16.89	0.39	2130.77	1671.58	611.28	34583.83	95683.73	1693.60	38.76	1706.53	71.39	1609.59	542.05	1615.80	625.29	-5802.801602
1094	29	7	-16.86	0.42	2130.77	1609.80	450.36	2569.33	2181.52	1690.32	30.35	1702.86	58.05	1562.16	500.13	1551.55	479.16	-5802.800507
1095	29	8	-16.79	0.49	2130.77	1613.14	433.19	3170.84	2615.95	1691.25	29.74	1704.52	56.82	1581.41	478.19	1558.23	444.23	-5802.797264
1096	29	9	-16.78	0.50	2130.77	1583.41	347.01	2666.07	1698.82	1688.95	22.14	1701.80	43.41	1542.59	387.59	1539.31	364.77	-5802.796897
1097	29	10	-16.77	0.51	2130.77	1655.77	494.94	3571.79	2751.87	1692.82	30.44	1706.67	60.69	1624.79	517.59	1613.04	519.53	-5802.796049
1098	29	11	-16.75	0.53	2130.77	1614.35	496.45	3762.44	3400.57	1691.40	32.30	1704.45	61.29	1568.12	532.19	1555.06	518.58	-5802.795166
1099	29	12	-16.74	0.54	2130.77	1642.43	467.76	6949.29	11087.07	1691.43	29.52	1704.80	56.57	1590.85	504.54	1591.46	498.31	-5802.794868
1100	29	13	-16.71	0.57	2130.77	1594.93	426.19	-410.41	8174.61	1689.93	28.65	1702.52	56.04	1586.87	503.75	1562.31	456.26	-5802.793616
1101	29	14	-16.67	0.61	2130.77	1588.02	385.64	3011.50	1548.80	1688.66	25.95	1700.62	51.90	1576.45	443.60	1555.45	405.32	-5802.791606
1102	29	15	-16.66	0.62	2130.77	1642.39	408.54	5578.95	9693.31	1692.66	30.98	1706.67	57.74	1605.65	485.13	1600.57	443.06	-5802.791207
1103	29	16	-16.64	0.64	2130.77	1619.79	442.83	2985.59	2532.66	1690.99	28.88	1703.92	56.84	1587.81	485.75	1581.88	458.38	-5802.790130
1104	29	17	-16.62	0.66	2130.77	1697.89	1081.53	5835.70	10701.63	1701.16	67.07	1713.75	117.78	1645.89	1091.40	1654.06	1098.35	-5802.789324
1105	29	18	-16.62	0.66	2130.77	1637.00	485.91	3240.86	1955.58	1691.76	29.59	1705.30	58.98	1605.01	523.86	1593.37	503.08	-5802.789323
1106	29	19	-16.39	0.89	2130.77	1670.80	803.07	6784.97	13448.91	1696.31	47.93	1709.96	86.40	1612.80	820.30	1615.20	818.15	-5802.778519
1107	29	20	-16.30	0.98	2130.77	1691.67	941.41	5343.33	8607.68	1697.43	55.45	1710.43	100.32	1639.86	946.49	1650.02	985.12	-5802.774381
1108	29	21	-16.22	1.06	2130.77	1712.67	1144.78	1177.66	7160.60	1702.60	72.93	1714.56	126.48	1680.94	1202.64	1702.92	1252.32	-5802.770890
1109	29	22	-16.20	1.08	2130.77	1718.08	1079.31	6245.38	13636.20	1702.47	68.68	1715.73	119.53	1674.09	1104.54	1708.85	1193.63	-5802.769734
1110	29	23	-16.20	1.08	2130.77	1641.76	367.73	3057.92	1940.97	1690.88	27.30	1704.16	51.38	1589.50	386.01	1600.06	355.34	-5802.769678
1111	29	24	-16.13	1.15	2130.77	1645.58	481.78	-3929.90	16741.72	1692.50	30.69	1706.91	58.60	1598.95	474.03	1604.02	499.10	-5802.766757
1112	29	25	-16.11	1.17	2130.77	1710.60	888.21	4600.24	5870.76	1698.96	52.46	1713.64	101.14	1689.68	930.44	1670.55	904.70	-5802.765626
1113	29	26	-16.08	1.20	2130.77	1725.08	1135.16	10667.82	25984.95	1702.40	68.22	1715.65	119.70	1642.89	1090.94	1669.46	1169.90	-5802.764349

Polarizability models:					n*alp	DFT results		AM model		TL model		TE model		RP model		GD model		Etot
i	n	isomer	Eb	Erel	Aiso	Aaiso	Aaiso	Aaiso	Aaiso	Aaiso	Aaiso	Aaiso	Aaiso	Aaiso	Aaiso	Aaiso	Aaiso	
1114	29	27	-15.97	1.31	2130.77	1720.68	759.66	7790.85	14464.16	1699.03	47.81	1713.73	88.16	1665.56	762.24	1675.96	783.88	-5802.759251
1115	29	28	-15.96	1.32	2130.77	1736.26	979.81	3314.26	4553.11	1699.50	57.29	1713.26	104.44	1694.43	1048.25	1701.30	1032.00	-5802.758669
1116	29	29	-15.84	1.44	2130.77	1819.28	1035.98	34485.43	97379.59	1705.85	57.56	1722.43	103.27	1779.76	1092.94	1773.41	1085.16	-5802.753038
1117	29	30	-15.73	1.55	2130.77	1830.39	1277.78	499.19	5904.54	1710.77	76.63	1725.61	125.90	1782.02	1321.34	1821.92	1344.07	-5802.748146
1118	29	31	-15.67	1.61	2130.77	1820.36	1061.40	582.24	3841.35	1713.87	75.84	1730.43	121.15	1783.40	1162.78	1785.19	1143.22	-5802.745616
1119	29	32	-15.54	1.74	2130.77	1859.54	1139.24	-3137.46	13548.81	1713.41	76.42	1730.15	123.86	1819.41	1204.66	1822.89	1180.42	-5802.739179
1120	29	33	-15.45	1.83	2130.77	1863.67	1186.74	7720.47	18227.79	1713.68	73.56	1730.83	130.91	1811.58	1229.62	1830.49	1223.69	-5802.735053
1121	29	34	-15.34	1.94	2130.77	1790.74	776.87	2952.83	8385.64	1699.36	43.83	1715.82	81.34	1724.43	795.54	1746.54	836.62	-5802.730264
1122	29	35	-14.76	2.52	2130.77	1975.80	1502.86	5786.90	14437.91	1725.49	95.30	1742.69	146.64	1922.03	1551.34	1927.45	1530.25	-5802.703339
1123	30	1*	-17.45	0.00	2204.25	1598.35	416.47	3022.98	1905.51	1735.82	27.21	1749.78	54.99	1597.53	480.40	1586.57	479.36	-6002.925318
1124	30	2	-17.43	0.02	2204.25	1585.53	388.43	-571.17	9314.24	1735.55	24.84	1749.90	50.11	1578.72	462.06	1560.54	430.94	-6002.924048
1125	30	3	-17.37	0.08	2204.25	1599.86	407.98	3149.43	2613.66	1735.87	24.92	1750.27	49.92	1580.80	449.82	1574.09	450.49	-6002.921530
1126	30	4	-17.29	0.16	2204.25	1625.18	480.58	2972.52	2012.14	1737.71	31.06	1752.08	62.01	1621.01	527.35	1601.40	506.09	-6002.917483
1127	30	5	-17.24	0.21	2204.25	1617.74	398.63	2836.84	1382.47	1736.88	27.16	1751.54	53.81	1618.26	454.93	1599.86	426.77	-6002.915117
1128	30	6	-17.08	0.37	2204.25	1634.45	383.27	3001.50	1632.81	1737.15	27.83	1751.73	54.31	1645.03	458.66	1609.28	407.76	-6002.907495
1129	30	7	-17.04	0.41	2204.25	1677.35	358.13	2064.37	3214.36	1739.77	27.68	1756.39	51.53	1625.15	441.74	1617.64	386.91	-6002.905436
1130	30	8	-17.04	0.41	2204.25	1635.84	396.56	3260.34	2444.39	1736.55	25.92	1751.27	52.49	1614.25	431.07	1610.71	416.84	-6002.905422
1131	30	9	-17.04	0.41	2204.25	1644.18	430.91	2650.39	1378.61	1737.89	26.53	1753.38	52.86	1624.79	465.53	1614.87	450.87	-6002.905371
1132	30	10	-16.97	0.48	2204.25	1660.98	484.35	3063.82	2567.71	1740.24	32.79	1756.47	63.29	1635.72	510.39	1619.10	515.72	-6002.902279
1133	30	11	-16.90	0.55	2204.25	1680.38	462.34	3227.02	2178.08	1740.68	30.93	1757.63	60.46	1635.68	467.95	1626.83	484.99	-6002.898747
1134	30	12	-16.85	0.60	2204.25	1670.04	444.52	1164.50	1980.49	1738.51	28.24	1754.00	56.12	1646.75	483.54	1645.80	467.55	-6002.896354
1135	30	13	-16.78	0.67	2204.25	1677.02	911.45	5040.80	7166.72	1744.07	60.57	1758.14	108.14	1650.53	914.17	1667.18	1006.60	-6002.892973
1136	30	14	-16.75	0.70	2204.25	1709.37	426.11	5446.07	7757.22	1741.49	30.39	1758.87	58.18	1669.34	465.92	1660.72	457.64	-6002.891706
1137	30	15	-16.71	0.74	2204.25	1671.80	874.30	2904.50	4343.64	1742.55	57.65	1756.27	104.58	1639.47	881.16	1658.59	970.22	-6002.889867
1138	30	16	-16.67	0.78	2204.25	1650.21	359.77	3062.34	2162.12	1737.19	23.04	1752.90	45.47	1614.26	381.93	1615.48	344.08	-6002.887779
1139	30	17	-16.63	0.82	2204.25	1726.15	1098.77	3463.71	5476.04	1749.42	73.64	1763.74	127.69	1718.25	1213.64	1717.07	1201.99	-6002.886171
1140	30	18	-16.63	0.82	2204.25	1743.87	990.66	7684.27	11145.50	1749.05	61.53	1766.29	109.51	1709.48	1051.82	1695.39	1032.28	-6002.885756
1141	30	19	-16.62	0.83	2204.25	1746.05	739.95	4393.41	5603.83	1743.64	43.66	1760.70	79.16	1692.95	752.69	1691.96	749.44	-6002.885403
1142	30	20	-16.61	0.84	2204.25	1741.81	718.26	3659.72	5704.04	1744.40	46.03	1761.17	81.82	1705.41	767.18	1693.12	775.82	-6002.884954
1143	30	21	-16.59	0.86	2204.25	1691.23	456.42	3471.46	2935.18	1740.54	30.48	1757.23	58.71	1642.08	481.06	1637.82	476.22	-6002.884068
1144	30	22	-16.55	0.90	2204.25	1729.39	875.62	6320.99	11837.08	1746.02	54.18	1762.94	96.24	1667.56	853.48	1667.54	882.65	-6002.882314
1145	30	23	-16.53	0.92	2204.25	1741.70	766.82	3547.27	4181.33	1745.90	52.70	1762.24	92.74	1708.07	821.31	1727.70	875.19	-6002.881354
1146	30	24	-16.52	0.93	2204.25	1752.93	1113.10	3947.93	5820.11	1750.16	70.53	1765.88	122.50	1718.76	1160.31	1713.33	1158.18	-6002.880621
1147	30	25	-16.51	0.94	2204.25	1747.35	1114.28	4222.46	7369.83	1751.92	75.94	1766.98	131.00	1751.52	1239.89	1728.34	1163.92	-6002.880273
1148	30	26	-16.47	0.98	2204.25	1750.60	1064.01	17035.89	27043.34	1750.43	73.18	1765.08	125.58	1743.67	1191.47	1778.68	1144.67	-6002.878540
1149	30	27	-16.43	1.02	2204.25	1717.29	844.61	3032.29	2796.23	1746.85	53.06	1764.55	104.79	1697.01	854.15	1682.82	821.73	-6002.876543
1150	30	28	-16.33	1.12	2204.25	1798.72	951.68	4746.59	7358.85	1751.31	62.12	1768.71	105.24	1780.91	1048.34	1775.06	1041.65	-6002.871432
1151	30	29	-16.33	1.12	2204.25	1834.64	1405.74	3208.97	4822.86	1756.93	85.23	1772.98	142.13	1797.49	1447.92	1792.54	1416.47	-6002.871389
1152	30	30	-16.30	1.15	2204.25	1850.22	1491.84	55678.12	161223.22	1757.66	84.58	1773.28	139.14	1815.94	1542.58	1803.00	1520.46	-6002.870013
1153	30	31	-16.28	1.17	2204.25	1819.20	1105.16	-261967.66	792398.38	1755.32	72.76	1773.07	121.33	1783.84	1167.19	1782.62	1141.05	-6002.869157
1154	30	32	-16.26	1.19	2204.25	1751.79	969.38	580.63	6338.16	1748.67	58.81	1766.05	103.81	1699.37	985.57	1696.69	976.37	-6002.868481
1155	30	33	-16.25	1.20	2204.25	1789.96	818.86	2811.70	2176.92	1748.59	50.57	1766.84	87.50	1752.00	846.93	1747.40	861.09	-6002.867980
1156	30	34	-16.21	1.24	2204.25	1819.17	977.08	2117.29	582.08	1754.33	70.23	1771.51	117.59	1787.03	1070.18	1806.68	1055.29	-6002.866008
1157	30	35	-15.98	1.47	2204.25	1890.29	1210.52	-6857.01	26475.92	1762.50	81.76	1780.69	128.44	1842.63	1267.51	1839.16	1236.65	-6002.864883
1158	30	36	-15.82	1.63	2204.25	1866.92	406.85	5109.16	13992.11	1752.95	29.75	1775.86	55.31	1808.89	416.08	1795.76	406.76	-6002.847352
1159	30	37	-15.63	1.82	2204.25	1871.01	1046.34	7077.14	12122.09	1758.72	67.68	1779.08	117.14	1843.36	1079.91	1840.21	1090.34	-6002.838061
1160	30	38	-15.10	2.35	2204.25	2030.60	1759.53	17774.82	47727.50	1774.92	110.22	1792.58	169.10	1959.75	1753.48	1988.49	1795.27	-6002.813045
1161	30	39	-14.97	2.48	2204.25	2069.63	1811.18	2838.30	2460.89	1775.59	108.20	1793.77	162.84	2032.82	1894.73	2022.21	1821.47	-6002.806706
1162	30	40	-14.89	2.56	2204.25	2099.06	1838.12	692.44	8077.50	1787.45	122.05	1803.99	176.39	2043.02	1901.82	2076.94	1950.92	-6002.802573
1163	31	1*	-17.72	0.00	2277.72	1690.58	441.38	3782.34	3095.56	1786.31	31.01	1804.22	60.11	1689.14	501.20	1664.18	482.50	-6203.036228
1164	31	2	-17.65	0.07	2277.72	1643.32	387.93	3283.70	1235.37	1783.61	26.58	1800.81	52.18	1643.26	455.81	1608.09	423.72	-6203.032421

Polarizability models:					n*alp	DFT results		AM model		TL model		TE model		RP model		GD model		Etot
i	n	isomer	Eb	Erel	Aiso	Aaiso	Aaiso	Aaiso	Aaiso	Aaiso	Aaiso	Aaiso	Aaiso	Aaiso	Aaiso	Aaiso	Aaiso	
1165	31	3	-17.64	0.08	2277.72	1647.45	382.19	3047.29	1756.08	1783.81	26.67	1801.19	52.44	1638.20	439.07	1607.44	410.46	-6203.032281
1166	31	4	-17.64	0.08	2277.72	1657.75	405.79	2848.96	1731.63	1784.37	28.87	1801.56	56.72	1666.24	496.11	1622.47	442.17	-6203.032240
1167	31	5	-17.64	0.08	2277.72	1661.03	390.94	3248.20	2030.18	1784.26	28.07	1801.58	55.10	1661.18	453.85	1621.47	418.13	-6203.031901
1168	31	6	-17.62	0.10	2277.72	1669.54	429.62	3033.60	1899.89	1784.85	29.57	1802.41	57.96	1661.97	485.31	1636.18	474.84	-6203.031292
1169	31	7	-17.61	0.11	2277.72	1676.25	409.50	3446.62	2505.03	1785.38	28.95	1802.98	56.45	1674.51	466.03	1646.18	433.48	-6203.030465
1170	31	8	-17.60	0.12	2277.72	1668.54	424.56	3447.05	2660.07	1784.13	28.33	1801.19	55.90	1655.52	477.00	1637.98	463.43	-6203.030266
1171	31	9	-17.60	0.12	2277.72	1666.96	365.35	2944.68	1534.46	1784.46	26.14	1802.26	51.14	1670.10	447.87	1633.78	402.31	-6203.030063
1172	31	10	-17.60	0.12	2277.72	1648.53	391.11	2853.11	1591.35	1783.70	26.81	1800.88	52.93	1652.93	465.38	1620.64	420.30	-6203.029869
1173	31	11	-17.58	0.14	2277.72	1664.49	396.83	2795.75	1744.75	1784.94	29.26	1802.45	57.73	1688.58	488.25	1632.62	429.07	-6203.028964
1174	31	12	-17.58	0.14	2277.72	1686.35	434.53	4601.00	4503.89	1785.86	29.03	1803.78	56.65	1671.90	468.66	1656.72	476.02	-6203.028904
1175	31	13	-17.54	0.18	2277.72	1669.60	401.53	3118.41	2055.20	1784.44	26.64	1802.09	51.95	1671.23	452.59	1639.91	436.74	-6203.027110
1176	31	14	-17.52	0.20	2277.72	1648.27	368.32	2137.39	508.75	1783.60	25.12	1801.12	49.39	1636.06	442.04	1607.15	396.98	-6203.026355
1177	31	15	-17.51	0.21	2277.72	1651.11	388.76	1293.93	12396.36	1784.11	27.59	1801.49	54.31	1658.82	465.06	1616.15	419.87	-6203.025887
1178	31	16	-17.51	0.21	2277.72	1653.08	426.62	3905.45	3792.40	1784.69	29.99	1802.09	59.34	1661.45	501.97	1668.05	535.50	-6203.025884
1179	31	17	-17.51	0.21	2277.72	1656.83	388.10	2680.20	1328.76	1783.91	27.47	1801.34	54.18	1654.53	466.22	1615.57	444.97	-6203.025806
1180	31	18	-17.50	0.22	2277.72	1645.83	346.05	-4011.30	18375.15	1783.21	23.64	1800.63	45.96	1642.68	409.67	1617.32	376.67	-6203.025239
1181	31	19	-17.50	0.22	2277.72	1645.10	321.52	2895.42	1894.68	1783.73	21.93	1801.83	42.23	1625.45	400.70	1604.09	353.69	-6203.025066
1182	31	20	-17.49	0.23	2277.72	1693.17	453.30	3565.67	2837.53	1786.57	31.23	1804.67	60.96	1678.23	503.03	1659.55	499.01	-6203.024455
1183	31	21	-17.48	0.24	2277.72	1661.09	410.83	3261.88	2936.30	1784.27	27.14	1802.02	53.54	1640.12	455.21	1617.38	440.32	-6203.024211
1184	31	22	-17.48	0.24	2277.72	1667.66	409.96	2730.89	4283.37	1784.85	26.40	1802.79	51.11	1651.75	456.63	1634.89	440.01	-6203.024195
1185	31	23	-17.48	0.24	2277.72	1659.20	365.35	2687.90	1293.28	1784.70	25.76	1802.69	50.04	1646.03	444.73	1576.48	354.09	-6203.023971
1186	31	24	-17.48	0.24	2277.72	1662.23	369.45	2756.80	1210.33	1783.00	25.49	1799.81	50.39	1654.94	422.93	1635.26	393.53	-6203.023933
1187	31	25	-17.45	0.27	2277.72	1645.46	284.24	1717.24	3235.24	1782.04	19.59	1798.88	38.35	1652.64	369.17	1629.28	301.43	-6203.022486
1188	31	26	-17.40	0.32	2277.72	1635.96	240.98	68810.00	199406.95	1781.12	16.93	1797.68	33.14	1635.67	325.12	1640.06	216.38	-6203.020354
1189	31	27	-17.38	0.34	2277.72	1684.38	383.01	3448.70	3216.58	1785.18	26.43	1803.32	51.75	1660.07	434.77	1648.20	415.74	-6203.018991
1190	31	28	-17.35	0.37	2277.72	1666.12	375.47	3753.39	3660.94	1783.74	24.43	1801.20	47.52	1659.03	422.46	1643.41	399.93	-6203.017712
1191	31	29	-17.35	0.37	2277.72	1659.10	396.93	2404.75	1463.20	1784.18	26.88	1801.92	52.89	1661.12	484.42	1613.67	430.98	-6203.017494
1192	31	30	-17.29	0.43	2277.72	1702.11	368.09	3517.76	2870.79	1785.70	25.64	1804.32	49.75	1690.80	428.57	1671.00	395.86	-6203.014932
1193	31	31	-16.97	0.75	2277.72	1724.95	902.61	2856.81	2758.53	1791.87	63.03	1809.07	111.97	1719.86	994.82	1709.33	958.09	-6202.998982
1194	31	32	-16.95	0.77	2277.72	1710.47	357.75	1624.28	4277.93	1785.22	25.07	1803.92	48.96	1681.53	393.12	1663.95	363.03	-6202.997952
1195	31	33	-16.71	1.01	2277.72	1754.66	756.86	3951.00	4393.62	1793.43	49.17	1814.65	96.76	1715.75	791.55	1706.88	788.37	-6202.986189
1196	31	34	-16.41	1.31	2277.72	1854.77	1024.68	8130.91	17625.34	1800.62	66.06	1820.89	110.73	1817.04	1060.32	1827.68	1045.23	-6202.971330
1197	31	35	-16.19	1.53	2277.72	1798.39	843.47	4261.17	5486.51	1795.58	59.82	1815.86	109.14	1765.94	900.53	1759.77	896.59	-6202.960587
1198	31	36	-15.95	1.77	2277.72	1970.32	1209.90	203697.88	610506.28	1808.29	76.26	1829.71	124.74	1918.06	1246.16	1929.77	1252.41	-6202.948608
1199	31	37	-15.79	1.93	2277.72	1886.40	1025.05	3852.61	5022.30	1804.63	71.15	1827.07	117.16	1807.66	1012.89	1828.69	1054.77	-6202.940633
1200	31	38	-15.70	2.02	2277.72	1828.60	498.84	2676.46	1545.31	1791.84	32.77	1814.21	60.56	1776.82	504.03	1794.89	560.24	-6202.936445
1201	31	39	-15.69	2.03	2277.72	1924.72	1159.53	-3127.97	16902.52	1808.52	80.27	1830.63	130.24	1868.00	1160.40	1888.03	1210.55	-6202.935763
1202	31	40	-14.85	2.87	2277.72	2322.55	2479.67	159.89	7974.83	1854.23	154.97	1870.08	208.51	2228.87	2481.71	2269.30	2549.98	-6202.894190
1203	32	1*	-17.88	0.00	2351.20	1692.45	355.37	3693.82	5622.20	1831.01	25.38	1851.76	49.14	1676.40	433.27	1643.25	390.72	-6403.141877
1204	32	2	-17.84	0.04	2351.20	1701.42	357.39	5697.22	8833.09	1831.73	26.77	1852.56	51.56	1689.62	411.77	1673.72	418.28	-6403.140134
1205	32	3	-17.83	0.05	2351.20	1685.28	248.42	2732.34	331.31	1828.14	16.56	1847.39	32.66	1718.15	335.29	1689.07	218.37	-6403.139312
1206	32	4	-17.81	0.07	2351.20	1713.01	362.43	3261.91	2148.08	1831.95	25.28	1853.16	48.41	1684.70	422.45	1670.16	401.30	-6403.138468
1207	32	5	-17.80	0.08	2351.20	1699.77	347.72	3069.15	1684.13	1831.26	25.80	1852.02	49.76	1693.73	420.90	1656.08	382.43	-6403.138020
1208	32	6	-17.79	0.09	2351.20	1693.43	312.28	2795.87	1185.06	1829.94	22.06	1850.29	42.68	1686.27	385.24	1661.72	345.82	-6403.137447
1209	32	7	-17.79	0.09	2351.20	1728.23	375.27	3498.18	2359.52	1833.10	28.62	1854.22	54.64	1725.09	444.59	1685.94	409.96	-6403.137303
1210	32	8	-17.78	0.10	2351.20	1722.09	407.01	2807.65	1763.53	1832.38	27.95	1853.38	53.87	1698.34	439.12	1678.29	451.82	-6403.137034
1211	32	9	-17.78	0.10	2351.20	1722.29	436.36	3682.29	6516.92	1832.81	29.37	1853.89	56.20	1686.81	460.32	1678.22	479.35	-6403.136916
1212	32	10	-17.77	0.11	2351.20	1705.28	367.92	1187.48	4362.81	1831.72	27.65	1852.50	53.08	1700.19	439.60	1659.22	397.85	-6403.136539
1213	32	11	-17.76	0.12	2351.20	1713.97	403.44	2737.96	2159.19	1832.55	28.19	1853.60	54.01	1692.85	450.59	1669.89	447.14	-6403.135866
1214	32	12	-17.74	0.14	2351.20	1709.07	345.32	2375.16	1551.23	1832.18	25.82	1853.31	49.41	1711.78	409.96	1653.45	394.87	-6403.135132
1215	32	13	-17.74	0.14	2351.20	1713.01	287.39	2542.12	675.17	1830.64	21.93	1851.14	41.99	1708.35	361.78	1678.51	320.39	-6403.135098

Polarizability models:				n*alp	DFT results		AM model		TL model		TE model		RP model		GD model		Etot	
i	n	isomer	Eb	Erel	Aiso	Aaiso	Aiso	Aaiso	Aiso	Aaiso	Aiso	Aaiso	Aiso	Aaiso	Aiso	Aaiso		
1216	32	14	-17.74	0.14	2351.20	1715.17	431.42	2892.97	2147.68	1832.82	30.32	1853.91	58.51	1699.16	480.60	1663.97	478.34	-6403.134976
1217	32	15	-17.73	0.15	2351.20	1711.18	338.20	3196.94	1896.02	1831.32	23.54	1852.14	45.31	1715.86	403.92	1670.20	394.03	-6403.134531
1218	32	16	-17.72	0.16	2351.20	1717.72	415.15	3002.80	1820.92	1832.60	28.58	1853.66	54.46	1700.27	464.10	1646.03	440.23	-6403.134081
1219	32	17	-17.72	0.16	2351.20	1713.36	409.99	-22643.90	74146.38	1832.58	29.26	1853.64	56.28	1707.93	475.78	1671.67	449.27	-6403.134011
1220	32	18	-17.72	0.16	2351.20	1727.52	386.37	3828.95	3317.79	1832.22	26.59	1853.13	50.83	1712.61	424.50	1693.05	422.74	-6403.133889
1221	32	19	-17.72	0.16	2351.20	1698.64	352.97	2560.86	887.74	1830.81	25.44	1851.28	49.61	1693.12	424.85	1657.47	381.93	-6403.133762
1222	32	20	-17.68	0.20	2351.20	1699.09	287.60	31345.65	85728.62	1829.67	20.94	1849.82	40.63	1698.49	338.14	1681.02	286.52	-6403.131684
1223	32	21	-17.67	0.21	2351.20	1719.32	367.96	4196.62	3914.63	1832.44	25.82	1853.63	49.37	1709.02	414.78	1680.15	405.75	-6403.131641
1224	32	22	-17.63	0.25	2351.20	1750.64	286.64	3662.89	2542.73	1832.95	24.84	1854.41	46.61	1740.30	352.34	1715.68	322.32	-6403.129309
1225	32	23	-17.62	0.26	2351.20	1712.22	377.09	3896.30	5286.02	1831.84	26.74	1852.87	51.18	1695.71	427.57	1676.36	412.50	-6403.128717
1226	32	24	-17.58	0.30	2351.20	1735.23	337.09	8301.98	15384.12	1832.68	25.97	1854.02	49.79	1724.03	394.07	1702.62	366.98	-6403.126744
1227	32	25	-17.56	0.32	2351.20	1757.10	424.69	3579.49	2878.02	1832.99	27.08	1854.53	52.25	1727.31	441.31	1730.27	466.55	-6403.125758
1228	32	26	-17.44	0.44	2351.20	1728.28	231.47	2549.97	761.19	1830.85	17.41	1851.62	32.13	1736.78	246.44	1754.16	178.49	-6403.119814
1229	32	27	-17.41	0.47	2351.20	1727.10	261.55	3377.09	2450.93	1830.97	19.81	1851.78	36.75	1719.41	307.64	1712.10	263.07	-6403.118235
1230	32	28	-17.16	0.72	2351.20	1773.06	396.09	2234.91	3032.32	1832.96	25.76	1854.89	49.95	1726.70	408.25	1725.91	409.57	-6403.105166
1231	32	29	-17.10	0.78	2351.20	1831.86	920.54	4863.95	7153.06	1844.40	65.77	1867.35	113.16	1793.93	961.81	1785.44	925.35	-6403.102406
1232	32	30	-16.65	1.23	2351.20	1860.65	1041.79	3697.46	4279.93	1845.39	71.70	1866.96	121.98	1841.09	1132.64	1830.07	1077.84	-6403.079481
1233	32	31	-16.61	1.27	2351.20	1902.87	1058.05	-1167.98	10674.64	1849.32	68.54	1873.37	114.30	1863.70	1105.81	1852.49	1100.69	-6403.077442
1234	32	32	-16.58	1.30	2351.20	1831.77	407.56	3739.69	2903.24	1837.49	27.88	1861.88	52.25	1778.17	431.64	1782.03	448.37	-6403.075753
1235	32	33	-16.17	1.71	2351.20	1942.04	935.76	8411.39	20236.71	1850.04	59.12	1875.73	98.53	1916.06	1008.24	1900.09	997.64	-6403.054873
1236	32	34	-15.86	2.02	2351.20	1946.17	913.76	-5079.06	23914.77	1846.57	54.43	1872.65	100.91	1897.13	929.81	1897.49	913.42	-6403.038870
1237	32	35	-15.52	2.36	2351.20	2082.42	1017.05	1437.01	11121.40	1856.36	58.98	1884.52	105.35	2035.24	1027.13	2025.12	1014.01	-6403.021653

Table S2. The BP86/6-31G(d) optimized Cartesian coordinates and energies of the 1237 cluster isomers Mg₂-Mg₃₂ considered in the study. All coordinates in Å, E_{tot} in Hartree, E_b in kcal/mol.

@mg02-isomer01 bp86/6-31G(d) Etot=-400.142698 Eb=-1.03				
Mg1	1.780662	0.000000	0.000000	
Mg2	-1.780662	0.000000	0.000000	
@mg03-isomer01 bp86/6-31G(d) Etot=-600.224345 Eb=-3.18				
Mg1	0.000000	1.902376	0.000000	
Mg2	1.647506	-0.951188	0.000000	
Mg3	-1.647506	-0.951188	0.000000	
@mg04-isomer01 bp86/6-31G(d) Etot=-800.323396 Eb=-6.99				
Mg1	-1.096804	1.096804	-1.096804	
Mg2	1.096804	1.096804	1.096804	
Mg3	-1.096804	-1.096804	1.096804	
Mg4	1.096804	-1.096804	-1.096804	
@mg04-isomer02 bp86/6-31G(d) Etot=-800.300209 Eb=-3.35				
Mg1	-2.249527	-1.632649	0.000056	
Mg2	3.930773	0.000002	0.000093	
Mg3	-2.247226	1.633987	0.000055	
Mg4	0.565980	-0.001340	-0.000204	
@mg05-isomer01 bp86/6-31G(d) Etot=-1000.404667 Eb=-7.04				
Mg1	2.836517	-0.000081	0.000116	
Mg2	0.000950	1.740961	-0.061305	
Mg3	-2.836797	0.000708	0.000092	
Mg4	-0.000331	-0.817760	1.538392	
Mg5	-0.000339	-0.923828	-1.477295	
@mg05-isomer02 bp86/6-31G(d) Etot=-1000.400777 Eb=-6.56				
Mg1	-4.136871	-0.000023	0.000006	
Mg2	-0.863485	0.000020	0.000307	
Mg3	1.667083	-0.572978	1.685889	
Mg4	1.666577	-1.173642	-1.339309	
Mg5	1.666695	1.746623	-0.346893	
@mg05-isomer03 bp86/6-31G(d) Etot=-1000.380032 Eb=-3.95				
Mg1	1.341641	2.385274	0.000001	
Mg2	2.683736	-0.538866	-0.000002	
Mg3	-1.854239	2.013030	0.000001	
Mg4	0.316729	-2.718088	0.000003	
Mg5	-2.487868	-1.141350	-0.000003	
@mg05-isomer04 bp86/6-31G(d) Etot=-1000.376405 Eb=-3.50				
Mg1	-4.622874	1.430906	-0.001440	
Mg2	-1.604091	-0.018902	0.003906	
Mg3	4.622883	1.430898	0.001082	
Mg4	-0.000064	-2.823903	-0.000185	
Mg5	1.604146	-0.018999	-0.003363	
@mg05-isomer05 bp86/6-31G(d) Etot=-1000.375797 Eb=-3.42				
Mg1	3.674906	-1.624342	-0.002562	
Mg2	3.670783	1.628293	-0.002538	
Mg3	-5.809367	0.003484	-0.002828	
Mg4	0.867596	-0.001662	0.006528	
Mg5	-2.403918	-0.005773	0.001399	
@mg06-isomer01 bp86/6-31G(d) Etot=-1200.488831 Eb=-7.38				
Mg1	-1.889693	1.738591	-0.000021	
Mg2	1.889700	1.738593	-0.000002	
Mg3	0.000009	-0.405637	-1.469603	

Mg4	-2.802135	-1.332971	0.000006	
Mg5	-0.000014	-0.405597	1.469615	
Mg6	2.802132	-1.332979	0.000005	
@mg06-isomer02 bp86/6-31G(d) Etot=-1200.487224 Eb=-7.21				
Mg1	1.705210	1.644287	-0.000001	
Mg2	3.466324	-1.070474	0.000000	
Mg3	0.276803	-1.263339	-0.000011	
Mg4	-2.897758	-1.316386	0.000000	
Mg5	-1.275297	1.002964	-1.492371	
Mg6	-1.275281	1.002948	1.492383	
@mg06-isomer03 bp86/6-31G(d) Etot=-1200.482144 Eb=-6.68				
Mg1	-1.718019	0.000020	1.498576	
Mg2	-1.718023	0.000020	-1.498573	
Mg3	-0.829918	-2.819375	-0.000001	
Mg4	-0.829832	2.819389	-0.000001	
Mg5	4.182200	-0.000034	0.000000	
Mg6	0.913592	-0.000019	-0.000002	
@mg06-isomer04 bp86/6-31G(d) Etot=-1200.481561 Eb=-6.62				
Mg1	-3.884322	-0.000250	0.000065	
Mg2	-0.994868	-1.736163	-0.027112	
Mg3	1.770386	0.000298	-0.000065	
Mg4	5.099019	-0.000185	0.000043	
Mg5	-0.995070	0.844683	1.517121	
Mg6	-0.995145	0.891617	-1.490053	
@mg06-isomer05 bp86/6-31G(d) Etot=-1200.478280 Eb=-6.28				
Mg1	-0.000203	-2.025753	-1.534227	
Mg2	1.542358	0.151258	-0.000145	
Mg3	4.317685	1.874020	0.000005	
Mg4	-4.317699	1.874006	0.000006	
Mg5	-1.541945	0.151844	-0.000140	
Mg6	-0.000196	-2.025375	1.534502	
@mg06-isomer06 bp86/6-31G(d) Etot=-1200.476980 Eb=-6.14				
Mg1	2.832548	0.000067	0.000005	
Mg2	6.202165	-0.000039	-0.000004	
Mg3	-2.892318	-1.559823	-0.849027	
Mg4	-2.892338	1.515165	-0.926341	
Mg5	-2.892379	0.044627	1.775329	
Mg6	-0.357679	0.000004	0.000038	
@mg06-isomer07 bp86/6-31G(d) Etot=-1200.464364 Eb=-4.82				
Mg1	0.393721	-2.018765	-1.359688	
Mg2	1.637459	-0.799556	1.660961	
Mg3	1.801074	1.168213	-1.212846	
Mg4	-1.637463	0.799554	-1.660953	
Mg5	-1.801093	-1.168211	1.212842	
Mg6	-0.393698	2.018765	1.359683	
@mg06-isomer08 bp86/6-31G(d) Etot=-1200.459470 Eb=-4.31				
Mg1	4.389200	1.155680	-1.155249	
Mg2	1.598551	-0.000040	-0.000045	
Mg3	-1.598553	-0.000034	0.000026	
Mg4	-4.389211	-1.156654	-1.154250	
Mg5	-4.389192	1.156691	1.154249	
Mg6	4.389205	-1.155643	1.155269	
@mg06-isomer09 bp86/6-31G(d) Etot=-1200.457757 Eb=-4.13				
Mg1	-3.245675	1.601869	0.000032	
Mg2	-0.172046	2.490803	-0.000031	
Mg3	5.047188	-0.000555	0.000062	

Mg4	1.783382	0.002043	-0.000064
Mg5	-0.168950	-2.489212	-0.000031
Mg6	-3.243899	-1.604947	0.000032
@mg06-isomer10 bp86/6-31G(d) Etot=-1200.452844 Eb=-3.62			
Mg1	-2.722223	-4.404174	0.000078
Mg2	-0.967637	-1.567699	-0.000400
Mg3	1.841767	-0.054290	0.000276
Mg4	5.175491	-0.154936	-0.000162
Mg5	-2.453862	4.559080	-0.000215
Mg6	-0.873536	1.622018	0.000423
@mg07-isomer01 bp86/6-31G(d) Etot=-1400.583646 Eb=-8.58			
Mg1	-0.495079	-2.792633	0.000064
Mg2	-1.240265	2.550878	-0.000013
Mg3	-2.809557	-0.391881	-0.000227
Mg4	2.503007	-1.334190	-0.000224
Mg5	2.042639	1.967879	0.000030
Mg6	-0.000415	-0.000108	1.450759
Mg7	-0.000331	0.000055	-1.450389
@mg07-isomer02 bp86/6-31G(d) Etot=-1400.580557 Eb=-8.30			
Mg1	3.043445	0.745202	-1.206559
Mg2	-1.337400	-1.089216	1.385999
Mg3	-3.043451	-0.745692	-1.206206
Mg4	-2.140686	1.740657	0.456616
Mg5	2.140534	-1.740513	0.457130
Mg6	-0.000098	-0.000144	-1.272649
Mg7	1.337656	1.089705	1.385668
@mg07-isomer03 bp86/6-31G(d) Etot=-1400.579466 Eb=-8.20			
Mg1	3.693897	0.000261	-0.000076
Mg2	-1.749321	2.793138	-0.000040
Mg3	-1.250963	-0.000063	-1.449735
Mg4	-1.748936	-2.793321	-0.000067
Mg5	-1.251110	-0.000083	1.449696
Mg6	1.153083	1.757622	0.000099
Mg7	1.153350	-1.757553	0.000125
@mg07-isomer04 bp86/6-31G(d) Etot=-1400.577931 Eb=-8.07			
Mg1	1.427252	1.475880	-0.837356
Mg2	-2.274701	-2.344662	0.368894
Mg3	-0.002149	0.002354	1.403815
Mg4	3.169959	-0.792001	0.367748
Mg5	-0.898251	3.139759	0.370429
Mg6	0.564913	-1.979824	-0.831171
Mg7	-1.987024	0.498494	-0.842360
@mg07-isomer05 bp86/6-31G(d) Etot=-1400.573298 Eb=-7.65			
Mg1	-0.000244	-2.007203	1.469646
Mg2	-2.590365	-0.835461	-0.000408
Mg3	2.590337	-0.835488	0.000265
Mg4	2.676725	2.413128	-0.000188
Mg5	-2.676712	2.413127	0.000196
Mg6	0.000244	-2.008231	-1.469030
Mg7	0.000014	0.860128	-0.000481
@mg07-isomer06 bp86/6-31G(d) Etot=-1400.569708 Eb=-7.33			
Mg1	0.975000	0.325965	-1.262665
Mg2	2.173429	-0.427973	1.534520
Mg3	-2.173574	-0.428920	-1.534310
Mg4	-3.978259	1.242948	0.528519
Mg5	3.978375	1.242582	-0.529090
Mg6	0.000335	-2.280508	0.000342

Mg7	-0.975306	0.325906	1.262685	
@mg07-isomer07 bp86/6-31G(d) Etot=-1400.566380 Eb=-7.03				
Mg1	-3.036991	2.131168	0.000036	
Mg2	0.183347	-2.409901	-0.000104	
Mg3	5.393493	0.707847	-0.000787	
Mg4	-0.714637	0.284136	-1.463097	
Mg5	-3.285114	-1.038449	-0.001002	
Mg6	2.175439	0.041766	0.001289	
Mg7	-0.715537	0.283434	1.463665	
@mg07-isomer08 bp86/6-31G(d) Etot=-1400.565617 Eb=-6.96				
Mg1	0.000000	-1.465241	1.485593	
Mg2	0.000651	-1.464642	-1.485599	
Mg3	5.422009	0.790572	-0.000513	
Mg4	-3.853630	1.915323	-0.000063	
Mg5	-3.034623	-1.164055	-0.000652	
Mg6	2.222964	0.206087	0.000826	
Mg7	-0.757371	1.181956	0.000407	
@mg07-isomer09 bp86/6-31G(d) Etot=-1400.565055 Eb=-6.91				
Mg1	2.571146	0.492002	-0.008452	
Mg2	0.480549	-1.893782	-0.001820	
Mg3	-2.375870	-0.861291	1.493962	
Mg4	-3.631108	1.631394	0.001579	
Mg5	5.834588	0.344322	0.005737	
Mg6	-2.388167	-0.872234	-1.482339	
Mg7	-0.491138	1.159590	-0.008666	
@mg07-isomer10 bp86/6-31G(d) Etot=-1400.558857 Eb=-6.36				
Mg1	-0.000090	-0.038257	1.731931	
Mg2	-2.802696	-0.027466	0.000446	
Mg3	2.802684	0.026664	0.001969	
Mg4	-0.012048	1.517204	-0.831262	
Mg5	-6.124277	0.010506	-0.002918	
Mg6	6.124295	-0.008349	-0.003449	
Mg7	0.012133	-1.480302	-0.896718	
@mg07-isomer11 bp86/6-31G(d) Etot=-1400.558521 Eb=-6.33				
Mg1	-3.050880	-0.002465	-0.000543	
Mg2	2.778600	0.001050	1.492626	
Mg3	2.775038	0.001083	-1.494716	
Mg4	-6.409930	0.000508	0.000318	
Mg5	1.884276	2.810381	0.000167	
Mg6	1.888339	-2.809665	0.000149	
Mg7	0.134556	-0.000892	0.002000	
@mg07-isomer12 bp86/6-31G(d) Etot=-1400.557669 Eb=-6.25				
Mg1	0.578433	0.003985	0.001298	
Mg2	7.196361	-0.009613	-0.000419	
Mg3	-2.165388	-1.037685	-1.388587	
Mg4	-5.078792	-0.004763	-0.001205	
Mg5	-2.170483	1.720689	-0.203557	
Mg6	3.807023	0.012180	-0.000231	
Mg7	-2.167154	-0.684793	1.592701	
@mg07-isomer13 bp86/6-31G(d) Etot=-1400.555887 Eb=-6.09				
Mg1	-0.001793	-1.772751	0.032776	
Mg2	0.000500	0.004618	2.527611	
Mg3	-4.246818	2.455844	-0.872292	
Mg4	4.252835	2.445505	-0.872266	
Mg5	-0.005898	-4.905099	-0.871095	
Mg6	-1.534374	0.887232	0.028036	
Mg7	1.535549	0.884653	0.027230	

@mg07-isomer14 bp86/6-31G(d) Etot=-1400.554529 Eb=-5.97
Mg1 -2.537624 0.452041 0.000966
Mg2 0.409435 -0.451398 -0.014161
Mg3 6.798180 0.981213 0.021384
Mg4 -1.700385 -2.066584 1.543613
Mg5 -4.744089 2.857047 0.001096
Mg6 3.496875 0.315932 -0.034848
Mg7 -1.722391 -2.088253 -1.518050

@mg07-isomer15 bp86/6-31G(d) Etot=-1400.552983 Eb=-5.83
Mg1 1.476119 -0.003192 -0.000628
Mg2 8.131501 0.007000 0.000660
Mg3 -4.224017 -1.164607 -1.335356
Mg4 -4.221989 1.741117 -0.341727
Mg5 -4.223007 -0.572264 1.677875
Mg6 4.745777 -0.007900 -0.000542
Mg7 -1.684386 -0.000154 -0.000282

@mg07-isomer16 bp86/6-31G(d) Etot=-1400.536001 Eb=-4.31
Mg1 -3.648531 -0.194139 -0.009306
Mg2 5.352656 -0.504393 1.630131
Mg3 5.350623 -0.494051 -1.633826
Mg4 -2.653447 2.885020 0.004181
Mg5 -6.448204 -2.002857 0.000885
Mg6 2.584657 -0.146571 0.001144
Mg7 -0.537755 0.456991 0.006792

@mg07-isomer17 bp86/6-31G(d) Etot=-1400.535679 Eb=-4.28
Mg1 -1.597525 -2.650084 0.000832
Mg2 -0.000073 1.879883 -0.004007
Mg3 -5.775874 1.417110 0.003243
Mg4 5.775890 1.417082 0.004320
Mg5 1.597637 -2.649990 -0.000104
Mg6 -2.722847 0.292919 -0.001275
Mg7 2.722792 0.293080 -0.003010

@mg07-isomer18 bp86/6-31G(d) Etot=-1400.535580 Eb=-4.27
Mg1 6.001936 -1.255238 -1.035370
Mg2 -6.002053 -1.255138 1.035370
Mg3 0.000000 0.000269 0.000138
Mg4 6.002703 1.255118 1.034853
Mg5 -6.002586 1.255217 -1.034853
Mg6 3.210340 0.000026 0.000688
Mg7 -3.210340 -0.000255 -0.000826

@mg07-isomer19 bp86/6-31G(d) Etot=-1400.534056 Eb=-4.13
Mg1 -4.503229 -1.593846 -0.002590
Mg2 3.859949 -0.006218 0.001376
Mg3 -1.384245 2.365060 0.001660
Mg4 -1.393194 -2.366119 0.001631
Mg5 7.233601 0.003965 -0.003728
Mg6 -4.496649 1.601582 -0.002593
Mg7 0.683767 -0.004424 0.004244

@mg07-isomer20 bp86/6-31G(d) Etot=-1400.533191 Eb=-4.06
Mg1 -3.446168 -1.287146 0.000003
Mg2 2.021932 -3.071906 -0.000002
Mg3 2.545840 2.654353 0.000002
Mg4 -3.154848 1.890433 -0.000001
Mg5 -1.141117 -3.493869 -0.000001
Mg6 3.662476 -0.334948 0.000001
Mg7 -0.488115 3.643084 -0.000002

@mg07-isomer21 bp86/6-31G(d) Etot=-1400.528727 Eb=-3.66

Mg1	-2.082392	1.593965	-0.000572
Mg2	3.901581	-0.015120	-0.001477
Mg3	-3.858355	-4.411885	0.000781
Mg4	-3.826885	4.430105	0.000718
Mg5	7.295055	-0.001597	0.001200
Mg6	-2.093317	-1.588565	-0.000729
Mg7	0.664313	-0.006902	0.000080

@mg07-isomer22 bp86/6-31G(d) Etot=-1400.528069 Eb=-3.60

Mg1	1.584117	0.351333	-0.007948
Mg2	-4.610737	-0.809861	-0.003730
Mg3	7.987750	-1.120032	0.000237
Mg4	-0.002128	3.150019	0.002133
Mg5	-7.987067	-1.116922	0.003160
Mg6	4.612216	-0.803431	0.004597
Mg7	-1.584152	0.348894	0.001551

@mg08-isomer01 bp86/6-31G(d) Etot=-1600.675118 Eb=-9.21

Mg1	-1.271712	2.686706	-0.048605
Mg2	-1.255483	0.000031	1.574132
Mg3	1.683922	1.587102	0.978671
Mg4	1.684037	-1.587015	0.978805
Mg5	0.139175	-0.000108	-1.242876
Mg6	-1.271705	-2.686728	-0.048590
Mg7	-2.929237	-0.000007	-0.941145
Mg8	3.221003	0.000019	-1.250392

@mg08-isomer02 bp86/6-31G(d) Etot=-1600.674015 Eb=-9.13

Mg1	-0.835019	-1.692685	-0.337508
Mg2	2.005602	2.774632	0.088482
Mg3	1.305141	0.000006	1.489236
Mg4	-0.835040	1.692668	-0.337553
Mg5	-3.195103	-0.000029	-1.313195
Mg6	2.010921	0.000008	-1.400631
Mg7	-2.462141	0.000013	1.722691
Mg8	2.005638	-2.774614	0.088478

@mg08-isomer03 bp86/6-31G(d) Etot=-1600.670429 Eb=-8.85

Mg1	0.000017	1.789556	0.000035
Mg2	-1.786010	-0.619094	1.506582
Mg3	-1.785986	-0.619108	-1.506576
Mg4	1.785969	-0.619137	1.506544
Mg5	1.785989	-0.619074	-1.506623
Mg6	-3.017768	1.781269	-0.000028
Mg7	-0.000005	-2.875649	0.000022
Mg8	3.017794	1.781236	0.000044

@mg08-isomer04 bp86/6-31G(d) Etot=-1600.669471 Eb=-8.77

Mg1	0.901899	-0.481358	1.302324
Mg2	-1.740013	1.610775	0.739442
Mg3	2.403968	-1.309019	-1.297740
Mg4	-0.901924	-0.483618	-1.301611
Mg5	-4.088202	0.179610	-0.791916
Mg6	1.740026	1.609556	-0.742182
Mg7	4.088162	0.180912	0.791730
Mg8	-2.403916	-1.306858	1.299952

@mg08-isomer05 bp86/6-31G(d) Etot=-1600.669410 Eb=-8.77

Mg1	-2.480301	0.000032	1.480200
Mg2	0.736315	-0.000005	1.616006
Mg3	-0.769978	-2.451884	0.000113
Mg4	2.514323	1.792989	-0.000220
Mg5	0.735859	-0.000028	-1.615881

Mg6	-0.770016	2.451842	0.000083	
Mg7	-2.480629	-0.000049	-1.480129	
Mg8	2.514428	-1.792897	-0.000173	
@mg08-isomer06 bp86/6-31G(d)	Etot=-1600.667789		Eb=-8.64	
Mg1	-3.511450	-1.543603	-0.425879	
Mg2	1.226345	-0.000040	1.473613	
Mg3	-2.105161	-0.000069	1.808781	
Mg4	2.167872	-1.513974	-1.005382	
Mg5	4.384408	-0.000014	0.581455	
Mg6	-0.818440	0.000030	-1.001516	
Mg7	2.167872	1.514029	-1.005304	
Mg8	-3.511447	1.543640	-0.425767	
@mg08-isomer07 bp86/6-31G(d)	Etot=-1600.665545		Eb=-8.46	
Mg1	-1.153106	-0.000057	1.154201	
Mg2	1.153097	-0.000119	-1.154182	
Mg3	-3.754468	-1.543348	0.309907	
Mg4	2.092761	-0.000122	1.747384	
Mg5	-3.754085	1.543666	0.309595	
Mg6	-2.092713	-0.000259	-1.747348	
Mg7	3.754092	1.543631	-0.309730	
Mg8	3.754422	-1.543393	-0.309826	
@mg08-isomer08 bp86/6-31G(d)	Etot=-1600.661642		Eb=-8.16	
Mg1	0.729999	-0.000005	-1.445112	
Mg2	3.065734	1.642216	0.000001	
Mg3	-0.098116	2.695867	-0.000003	
Mg4	-2.070014	0.000000	-0.000006	
Mg5	0.729997	0.000000	1.445112	
Mg6	-5.325218	0.000001	0.000005	
Mg7	-0.098118	-2.695864	-0.000002	
Mg8	3.065735	-1.642214	0.000004	
@mg08-isomer09 bp86/6-31G(d)	Etot=-1600.659801		Eb=-8.01	
Mg1	0.546027	0.738920	-0.929098	
Mg2	-0.897758	-2.164213	-0.626546	
Mg3	2.490995	-1.478446	0.296507	
Mg4	2.760562	1.378702	1.383338	
Mg5	3.627764	0.738509	-1.529065	
Mg6	-5.660489	0.736984	-0.177443	
Mg7	-0.391689	-0.410037	1.846201	
Mg8	-2.475412	0.459581	-0.263895	
@mg08-isomer10 bp86/6-31G(d)	Etot=-1600.659626		Eb=-8.00	
Mg1	-4.086845	1.669431	-0.642173	
Mg2	-4.087246	-1.390821	-1.124541	
Mg3	-4.086752	-0.278422	1.766965	
Mg4	4.087082	0.252912	-1.770644	
Mg5	-1.560547	-0.000169	-0.000257	
Mg6	4.086771	1.407142	1.104379	
Mg7	1.560534	-0.000141	-0.000150	
Mg8	4.087003	-1.659932	0.666421	
@mg08-isomer11 bp86/6-31G(d)	Etot=-1600.657976		Eb=-7.87	
Mg1	-5.691862	0.272659	0.000004	
Mg2	-2.451356	0.260019	0.000000	
Mg3	0.048730	-1.020013	-1.443336	
Mg4	2.916142	-0.190270	0.000016	
Mg5	3.045573	2.885487	0.000000	
Mg6	0.110827	1.933259	0.000000	
Mg7	1.973219	-3.121103	-0.000009	
Mg8	0.048726	-1.020039	1.443326	

@mg08-isomer12 bp86/6-31G(d) Etot=-1600.657728 Eb=-7.85

Mg1	2.163295	0.000000	1.447246
Mg2	-0.290854	1.704426	-0.000019
Mg3	-0.290840	-1.704424	-0.000002
Mg4	-2.833178	-0.000010	-0.000067
Mg5	2.163264	0.000011	-1.447237
Mg6	2.585825	-2.802917	0.000005
Mg7	-6.083313	-0.000005	0.000054
Mg8	2.585802	2.802920	0.000021

@mg08-isomer13 bp86/6-31G(d) Etot=-1600.656142 Eb=-7.73

Mg1	-2.453530	-0.000224	-0.270342
Mg2	0.503831	-0.000037	1.306330
Mg3	2.324694	2.847749	0.555833
Mg4	-0.051374	1.734546	-1.097401
Mg5	2.324724	-2.847714	0.555895
Mg6	3.019537	0.000012	-0.434496
Mg7	-5.616872	-0.000014	0.481816
Mg8	-0.051010	-1.734318	-1.097635

@mg08-isomer14 bp86/6-31G(d) Etot=-1600.651542 Eb=-7.36

Mg1	-0.291164	0.639028	-0.000020
Mg2	-2.086562	-1.632977	1.466701
Mg3	-2.086606	-1.633000	-1.466665
Mg4	-1.502244	3.481936	-0.000007
Mg5	2.721894	0.151291	-0.000022
Mg6	5.966429	0.434742	0.000019
Mg7	-3.389140	0.848479	0.000014
Mg8	0.667393	-2.289500	-0.000019

@mg08-isomer15 bp86/6-31G(d) Etot=-1600.644026 Eb=-6.77

Mg1	-0.000328	0.252219	1.457256
Mg2	2.814571	-0.508504	0.000872
Mg3	0.000287	0.251893	-1.457112
Mg4	-2.814642	-0.508378	-0.000475
Mg5	5.618652	-2.207777	-0.000519
Mg6	1.831669	2.464161	0.000303
Mg7	-5.618604	-2.207851	0.000299
Mg8	-1.831604	2.464237	-0.000625

@mg08-isomer16 bp86/6-31G(d) Etot=-1600.643629 Eb=-6.74

Mg1	0.095982	-0.754919	-0.000041
Mg2	-5.916172	-1.915513	0.000065
Mg3	1.755302	2.009826	0.000084
Mg4	-1.262344	1.669865	-1.481124
Mg5	3.221221	-0.759025	0.000025
Mg6	6.396167	-1.479237	-0.000014
Mg7	-3.027709	-0.440747	-0.000139
Mg8	-1.262447	1.669750	1.481143

@mg08-isomer17 bp86/6-31G(d) Etot=-1600.642793 Eb=-6.68

Mg1	-1.749722	-0.303445	1.459814
Mg2	7.618928	-0.466356	-0.000036
Mg3	-1.749665	-0.303502	-1.459777
Mg4	1.094486	0.199545	0.000074
Mg5	-4.424294	0.830087	-0.000066
Mg6	-3.957836	-2.300524	0.000001
Mg7	-1.101507	2.451740	-0.000019
Mg8	4.269609	-0.107546	0.000009

@mg08-isomer18 bp86/6-31G(d) Etot=-1600.642410 Eb=-6.65

Mg1	1.236852	1.536460	-1.482454
Mg2	-1.150877	0.136258	0.000784
Mg3	1.688096	-1.178997	0.000509

Mg4	-4.297423	-0.137495	0.001700
Mg5	1.237662	1.537538	1.481612
Mg6	4.216815	0.905851	-0.000667
Mg7	-7.621775	-0.573818	-0.001378
Mg8	4.690649	-2.225799	-0.000106

@mg08-isomer19 bp86/6-31G(d) Etot=-1600.641804 Eb=-6.60

Mg1	-2.895550	0.657784	1.605258
Mg2	3.010238	-0.000703	0.000927
Mg3	-0.152191	-0.004321	-0.001315
Mg4	-2.900090	-1.720472	-0.233265
Mg5	5.800714	1.628794	-0.000082
Mg6	-2.896296	1.061807	-1.372392
Mg7	-5.769861	0.003335	0.000933
Mg8	5.803036	-1.626224	-0.000063

@mg08-isomer20 bp86/6-31G(d) Etot=-1600.641643 Eb=-6.59

Mg1	1.455638	-0.346871	-0.000013
Mg2	-1.561187	-1.137271	-0.000009
Mg3	-3.545080	0.811031	-1.486296
Mg4	4.624575	-0.176919	0.000001
Mg5	-4.686731	-1.723326	0.000001
Mg6	7.981261	-0.172779	0.000005
Mg7	-3.545066	0.811016	1.486313
Mg8	-0.723411	1.935118	-0.000002

@mg08-isomer21 bp86/6-31G(d) Etot=-1600.637626 Eb=-6.27

Mg1	2.462718	-1.999753	1.636438
Mg2	3.207103	0.481530	-0.025079
Mg3	0.295308	-0.520582	0.021570
Mg4	-2.780182	0.112726	-0.010630
Mg5	-5.490938	0.792278	1.612174
Mg6	2.466753	-2.154543	-1.430984
Mg7	5.386633	2.904187	-0.147065
Mg8	-5.547395	0.384157	-1.656424

@mg08-isomer22 bp86/6-31G(d) Etot=-1600.636667 Eb=-6.20

Mg1	-4.363107	-1.160937	-1.611244
Mg2	-2.018607	0.061219	0.003587
Mg3	1.089460	0.468222	0.002967
Mg4	3.228929	2.885556	-0.000917
Mg5	-4.840122	1.322229	0.150389
Mg6	4.176897	-0.237997	-0.000857
Mg7	-4.320091	-1.420681	1.456182
Mg8	7.046642	-1.917610	-0.000106

@mg08-isomer23 bp86/6-31G(d) Etot=-1600.635252 Eb=-6.09

Mg1	-1.150213	-0.079189	1.726172
Mg2	-3.966681	-0.000054	-0.000400
Mg3	-1.150005	1.534223	-0.795003
Mg4	-7.282369	0.000761	0.000670
Mg5	1.627561	-0.000495	0.000019
Mg6	-1.150219	-1.455917	-0.931649
Mg7	4.844538	0.000215	-0.000385
Mg8	8.227388	0.000455	0.000576

@mg08-isomer24 bp86/6-31G(d) Etot=-1600.630553 Eb=-5.72

Mg1	8.855230	0.688725	0.000132
Mg2	-5.768689	3.130276	0.000067
Mg3	-3.733828	0.579871	-0.000091
Mg4	-3.116312	-2.004389	-1.528425
Mg5	-0.867217	-0.552401	-0.000059
Mg6	2.248212	-0.081982	-0.002104
Mg7	5.498747	0.243549	0.001127

Mg8	-3.116144	-2.003648	1.529353	
@mg08-isomer25 bp86/6-31G(d) Etot=-1600.628965 Eb=-5.59				
Mg1	5.627984	-1.577157	-0.675623	
Mg2	-0.104259	-0.060782	-0.000086	
Mg3	-9.786148	0.459965	-0.000570	
Mg4	5.574286	0.293376	1.755966	
Mg5	-6.560760	-0.555425	0.000395	
Mg6	5.541657	1.463059	-1.080099	
Mg7	3.041115	-0.014553	-0.000511	
Mg8	-3.333875	-0.008482	0.000528	
@mg09-isomer01 bp86/6-31G(d) Etot=-1800.784275 Eb=-10.94				
Mg1	1.764832	0.562731	-1.576453	
Mg2	2.242046	-2.041018	-0.000018	
Mg3	-0.395129	-1.809835	1.576582	
Mg4	-0.395059	-1.809809	-1.576530	
Mg5	-1.369804	1.246990	1.576552	
Mg6	-2.888661	-0.921045	-0.000029	
Mg7	0.646583	2.962175	0.000036	
Mg8	1.764980	0.562766	1.576390	
Mg9	-1.369788	1.247045	-1.576528	
@mg09-isomer02 bp86/6-31G(d) Etot=-1800.774042 Eb=-10.23				
Mg1	-2.086162	-0.372009	-1.558801	
Mg2	1.103298	2.686537	1.149008	
Mg3	2.807929	-1.869686	-1.087184	
Mg4	-1.103841	2.686365	-1.149022	
Mg5	2.086304	-0.371641	1.558887	
Mg6	-1.164214	0.667014	1.260887	
Mg7	-2.807502	-1.870360	1.087099	
Mg8	0.000249	-2.223403	-0.000026	
Mg9	1.163939	0.667184	-1.260847	
@mg09-isomer03 bp86/6-31G(d) Etot=-1800.770778 Eb=-10.00				
Mg1	0.041255	-2.002166	-0.775043	
Mg2	-0.071726	3.491180	-0.944351	
Mg3	-1.755188	0.965757	-0.775556	
Mg4	1.714082	1.037117	-0.774891	
Mg5	-2.987445	-1.808030	-0.944650	
Mg6	3.059348	-1.683517	-0.944694	
Mg7	-1.634208	-0.988490	1.719777	
Mg8	1.673282	-0.920781	1.719677	
Mg9	-0.039400	1.908931	1.719732	
@mg09-isomer04 bp86/6-31G(d) Etot=-1800.769753 Eb=-9.93				
Mg1	1.619828	0.000456	-1.532787	
Mg2	2.135839	2.707541	0.000685	
Mg3	2.136092	-2.707394	-0.000760	
Mg4	-0.738975	-1.720927	-0.000478	
Mg5	-3.177122	-0.000146	0.000062	
Mg6	-1.428160	-0.000813	2.647748	
Mg7	1.619872	-0.000372	1.532847	
Mg8	-1.428216	0.000785	-2.647762	
Mg9	-0.739158	1.720869	0.000445	
@mg09-isomer05 bp86/6-31G(d) Etot=-1800.762794 Eb=-9.44				
Mg1	0.652368	-0.000027	1.284836	
Mg2	1.503369	0.000005	-1.604377	
Mg3	1.774078	2.659463	-0.017188	
Mg4	3.754988	0.000051	0.432312	
Mg5	-2.606637	0.000010	1.811659	
Mg6	1.774184	-2.659459	-0.017174	
Mg7	-1.324208	1.571598	-0.557684	

Mg8	-1.324182	-1.571604	-0.557688	
Mg9	-4.203960	-0.000036	-0.774695	
@mg09-isomer06 bp86/6-31G(d) Etot=-1800.761993 Eb=-9.39				
Mg1	-0.000111	2.976732	-0.000013	
Mg2	-0.915529	0.181867	-1.292138	
Mg3	2.276558	0.949781	-1.313390	
Mg4	-1.533429	-2.061357	0.686847	
Mg5	1.533359	-2.061214	-0.686884	
Mg6	0.915669	0.182044	1.292259	
Mg7	4.047896	-0.558798	0.706528	
Mg8	-2.276586	0.949606	1.313455	
Mg9	-4.047828	-0.558661	-0.706663	
@mg09-isomer07 bp86/6-31G(d) Etot=-1800.758576 Eb=-9.15				
Mg1	0.536351	0.657082	-0.000667	
Mg2	3.271268	2.257094	0.000027	
Mg3	3.060391	-0.472858	-1.486161	
Mg4	1.116195	-2.592427	-0.000056	
Mg5	3.059276	-0.472476	1.486822	
Mg6	-1.779130	-1.543654	0.000407	
Mg7	-2.301780	1.144933	-1.506047	
Mg8	-4.661323	-0.123655	0.000408	
Mg9	-2.301249	1.145961	1.505268	
@mg09-isomer08 bp86/6-31G(d) Etot=-1800.758383 Eb=-9.14				
Mg1	0.662260	0.764454	-0.747617	
Mg2	-2.327435	2.053495	-0.434854	
Mg3	3.415671	2.077458	0.009686	
Mg4	-4.479243	0.012701	0.398895	
Mg5	3.384272	-0.908425	-0.962416	
Mg6	2.205323	-0.297405	1.701935	
Mg7	0.561584	-2.466326	-0.077714	
Mg8	-2.058408	-0.955522	-1.349366	
Mg9	-1.364024	-0.280430	1.461451	
@mg09-isomer09 bp86/6-31G(d) Etot=-1800.758190 Eb=-9.12				
Mg1	0.165763	1.632915	0.001239	
Mg2	-2.381329	0.000362	1.457658	
Mg3	2.319605	-0.000837	1.509800	
Mg4	2.318138	-0.000907	-1.509621	
Mg5	5.127574	0.000438	-0.000797	
Mg6	0.164722	-1.633372	0.001332	
Mg7	-2.667088	2.786173	-0.000559	
Mg8	-2.378623	0.000376	-1.458468	
Mg9	-2.668762	-2.785148	-0.000584	
@mg09-isomer10 bp86/6-31G(d) Etot=-1800.757765 Eb=-9.09				
Mg1	1.718729	-0.385136	1.504158	
Mg2	0.546306	1.880533	-0.336962	
Mg3	-0.940403	-1.167216	-0.395753	
Mg4	3.645258	1.793100	0.247902	
Mg5	-1.892524	0.977450	1.551598	
Mg6	1.258706	-3.268093	0.008733	
Mg7	-4.379236	-0.560867	0.193639	
Mg8	-2.394415	1.298038	-1.419004	
Mg9	2.437579	-0.567809	-1.354311	
@mg09-isomer11 bp86/6-31G(d) Etot=-1800.757748 Eb=-9.09				
Mg1	1.338660	-3.265778	-0.000015	
Mg2	0.493016	1.863347	-0.000081	
Mg3	2.147326	-0.465642	-1.470287	
Mg4	-2.209095	1.113000	-1.515831	
Mg5	3.634794	1.859510	0.000027	

Mg6	2.147238	-0.465581	1.470335
Mg7	-4.441273	-0.574003	0.000012
Mg8	-0.901584	-1.177885	0.000029
Mg9	-2.209081	1.113032	1.515811

@mg09-isomer12 bp86/6-31G(d) Etot=-1800.757416 Eb=-9.07

Mg1	0.914554	1.069409	-1.264282
Mg2	-1.743212	-1.223903	-0.619673
Mg3	-2.301039	1.632222	-1.415849
Mg4	2.301210	1.632049	1.416001
Mg5	-0.914526	1.069323	1.264405
Mg6	1.743250	-1.224019	0.619539
Mg7	4.095870	0.401675	-0.776960
Mg8	-0.000119	-3.758465	0.000021
Mg9	-4.095988	0.401709	0.776799

@mg09-isomer13 bp86/6-31G(d) Etot=-1800.754982 Eb=-8.90

Mg1	-0.000064	2.046203	0.000147
Mg2	2.045466	0.030085	1.691369
Mg3	-2.045672	0.030238	-1.691508
Mg4	1.221183	-0.696829	-1.112341
Mg5	3.546111	1.372726	-0.571163
Mg6	-4.086107	-1.728895	0.018673
Mg7	-3.545793	1.372733	0.571377
Mg8	-1.221034	-0.697205	1.112046
Mg9	4.085910	-1.729056	-0.018600

@mg09-isomer14 bp86/6-31G(d) Etot=-1800.754898 Eb=-8.89

Mg1	0.637402	0.000018	-1.210041
Mg2	2.488901	-1.578713	0.798425
Mg3	-2.340541	0.000258	-0.462971
Mg4	-0.571971	-2.676688	0.162131
Mg5	2.489206	1.578474	0.798316
Mg6	-5.512270	-0.000164	-0.427070
Mg7	3.707516	-0.000335	-1.585658
Mg8	-0.571499	2.676974	0.161961
Mg9	-0.326743	0.000176	1.764907

@mg09-isomer15 bp86/6-31G(d) Etot=-1800.754427 Eb=-8.86

Mg1	0.711604	0.823747	-0.001704
Mg2	-1.464689	-1.410826	-0.000875
Mg3	-2.176005	1.220279	-1.517618
Mg4	1.316590	-1.933263	1.501191
Mg5	1.317514	-1.936571	-1.499322
Mg6	-2.174402	1.219337	1.517724
Mg7	3.326299	2.647271	0.000061
Mg8	3.647489	-0.477489	-0.000136
Mg9	-4.504400	-0.152485	0.000678

@mg09-isomer16 bp86/6-31G(d) Etot=-1800.753438 Eb=-8.79

Mg1	2.263321	-0.000117	1.280086
Mg2	-1.213147	0.000744	2.262996
Mg3	-0.172833	-1.657795	-0.178482
Mg4	2.693836	2.774445	-0.204268
Mg5	2.692615	-2.775286	-0.203646
Mg6	-2.711549	0.000742	-0.428456
Mg7	2.511719	-0.000545	-1.680043
Mg8	-0.172112	1.658203	-0.178944
Mg9	-5.891851	-0.000390	-0.669243

@mg09-isomer17 bp86/6-31G(d) Etot=-1800.753114 Eb=-8.77

Mg1	-0.849769	-2.596004	0.883975
Mg2	0.103573	-1.168168	-1.593541
Mg3	-2.275243	0.186392	-0.121375

Mg4	2.335686	-2.543240	0.162190
Mg5	0.635948	0.079798	1.220848
Mg6	2.972874	0.495121	-0.863436
Mg7	0.263177	2.144102	-1.070571
Mg8	2.292460	2.680534	1.274527
Mg9	-5.478707	0.721464	0.107383

@mg09-isomer18 bp86/6-31G(d) Etot=-1800.752934 Eb=-8.76

Mg1	0.220719	-1.690311	0.436691
Mg2	2.519562	0.808364	0.232728
Mg3	2.459198	-1.584556	-1.754481
Mg4	-0.693190	1.450261	1.455521
Mg5	-2.613873	-0.605964	0.109159
Mg6	-5.819384	-0.774029	-0.123147
Mg7	3.165097	-1.997141	1.245717
Mg8	1.074815	3.492067	-0.169130
Mg9	-0.312944	0.901311	-1.433058

@mg09-isomer19 bp86/6-31G(d) Etot=-1800.751812 Eb=-8.68

Mg1	-1.605489	-1.359008	0.000118
Mg2	-0.000012	1.448747	0.000092
Mg3	-2.963201	0.960608	1.498900
Mg4	1.605454	-1.358972	0.000670
Mg5	4.781869	-1.286455	0.000004
Mg6	2.962815	0.960038	-1.499320
Mg7	-4.781883	-1.286429	-0.000046
Mg8	2.963476	0.961014	1.498587
Mg9	-2.963029	0.960457	-1.499007

@mg09-isomer20 bp86/6-31G(d) Etot=-1800.750247 Eb=-8.57

Mg1	1.783304	-2.741444	0.000062
Mg2	-0.697243	-1.260117	1.500942
Mg3	2.644696	-0.016219	-1.498146
Mg4	-5.903373	0.561306	0.000080
Mg5	2.644663	-0.016086	1.498289
Mg6	2.885662	2.677853	-0.000093
Mg7	-0.697143	-1.260151	-1.501039
Mg8	-2.729216	0.478114	-0.000140
Mg9	0.068651	1.576744	0.000045

@mg09-isomer21 bp86/6-31G(d) Etot=-1800.749330 Eb=-8.50

Mg1	-3.185607	0.915739	1.495772
Mg2	-1.584005	-1.226695	-0.000561
Mg3	-3.186150	0.916574	-1.495160
Mg4	2.918245	1.655091	0.001243
Mg5	-0.337658	1.762909	0.000051
Mg6	1.601072	-1.099984	-0.000495
Mg7	4.262799	-0.690645	-1.538459
Mg8	4.263049	-0.692819	1.537683
Mg9	-4.751746	-1.540170	-0.000075

@mg09-isomer22 bp86/6-31G(d) Etot=-1800.748505 Eb=-8.45

Mg1	1.108611	1.717068	1.504900
Mg2	-1.879682	1.262397	0.000000
Mg3	3.381966	0.323162	-0.000013
Mg4	0.375551	-0.887568	-0.000040
Mg5	1.108611	1.717142	-1.504853
Mg6	-2.601815	-1.323628	1.513026
Mg7	-4.928616	0.010630	0.000018
Mg8	6.037219	-1.495587	0.000002
Mg9	-2.601845	-1.323617	-1.513040

@mg09-isomer23 bp86/6-31G(d) Etot=-1800.739871 Eb=-7.84

Mg1	-0.000005	-0.377244	-1.440649
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Mg2	-1.665207	-2.677359	-0.000017
Mg3	-0.000021	-0.377242	1.440679
Mg4	2.691506	0.449114	0.000020
Mg5	-2.691512	0.449109	0.000001
Mg6	-5.798961	1.392454	-0.000018
Mg7	5.798958	1.392452	-0.000029
Mg8	0.000011	2.426054	0.000011
Mg9	1.665231	-2.677339	0.000003

@mg09-isomer24 bp86/6-31G(d) Etot=-1800.739090 Eb=-7.79

Mg1	-1.734674	0.956177	-2.094039
Mg2	3.107643	-0.694858	-0.098432
Mg3	-6.151258	-1.642300	0.336541
Mg4	-1.500846	1.806926	0.836088
Mg5	1.500295	1.806010	-0.839150
Mg6	0.000335	-0.853009	0.001119
Mg7	1.734486	0.961179	2.092612
Mg8	-3.107012	-0.696205	0.100274
Mg9	6.151031	-1.643920	-0.335013

@mg09-isomer25 bp86/6-31G(d) Etot=-1800.738193 Eb=-7.73

Mg1	-1.662087	0.000000	1.441855
Mg2	-0.854868	-2.695072	0.000057
Mg3	-1.661927	-0.000010	-1.441827
Mg4	-0.856725	2.695588	0.000053
Mg5	1.128796	0.000953	0.000163
Mg6	-4.017739	1.630699	-0.000120
Mg7	4.290896	0.000655	0.000082
Mg8	-4.016562	-1.632382	-0.000117
Mg9	7.650216	-0.000431	-0.000146

@mg09-isomer26 bp86/6-31G(d) Etot=-1800.736913 Eb=-7.64

Mg1	-0.676038	0.654462	1.827452
Mg2	1.531368	-0.154281	-0.169319
Mg3	-1.429558	-0.789288	-0.851017
Mg4	-3.656725	-1.434185	1.455960
Mg5	-3.599135	1.337878	0.152902
Mg6	-0.290716	2.251103	-0.762410
Mg7	4.641338	-0.296671	-0.092752
Mg8	7.969291	-0.472913	-0.051885
Mg9	-4.489825	-1.096104	-1.508930

@mg09-isomer27 bp86/6-31G(d) Etot=-1800.736492 Eb=-7.61

Mg1	1.757245	1.956936	-0.000027
Mg2	2.774094	-0.925698	0.000272
Mg3	-1.757439	1.956641	0.000047
Mg4	0.000096	-0.431593	-1.437122
Mg5	-2.773777	-0.926199	0.000362
Mg6	5.389423	-2.839188	-0.000376
Mg7	-0.000314	4.479614	-0.000433
Mg8	-5.389455	-2.839221	-0.000439
Mg9	0.000127	-0.431293	1.437716

@mg09-isomer28 bp86/6-31G(d) Etot=-1800.736289 Eb=-7.59

Mg1	-1.673319	1.769658	0.000085
Mg2	-3.272179	-0.830136	0.000067
Mg3	1.264669	1.208105	1.441343
Mg4	-0.258023	-1.339229	0.000155
Mg5	2.791648	-1.146782	-0.000014
Mg6	5.634836	-2.696033	-0.000053
Mg7	0.498213	3.949485	-0.000099
Mg8	-6.250295	-2.123017	-0.000087
Mg9	1.264449	1.207949	-1.441397

@mg09-isomer29 bp86/6-31G(d) Etot=-1800.734760 Eb=-7.49

Mg1	-1.064079	-1.026991	-1.440102
Mg2	1.473177	0.166938	-0.000433
Mg3	4.623671	0.104913	-0.000167
Mg4	-3.054224	-3.074301	0.000156
Mg5	-1.036121	1.913492	-0.000196
Mg6	-1.063767	-1.026930	1.439925
Mg7	7.972424	0.107106	0.000358
Mg8	-3.910845	-0.118972	0.000236
Mg9	-3.940236	2.954745	0.000224

@mg09-isomer30 bp86/6-31G(d) Etot=-1800.734463 Eb=-7.47

Mg1	-0.736733	1.681921	-0.000059
Mg2	-3.212671	0.000160	1.445892
Mg3	1.813245	-0.000433	-0.000030
Mg4	4.973734	-0.000320	0.000035
Mg5	8.321828	0.000260	-0.000002
Mg6	-3.605107	-2.805093	-0.000006
Mg7	-0.737134	-1.682190	-0.000031
Mg8	-3.604408	2.805531	0.000013
Mg9	-3.212754	0.000164	-1.445812

@mg09-isomer31 bp86/6-31G(d) Etot=-1800.732834 Eb=-7.35

Mg1	1.000969	-1.715967	1.152758
Mg2	4.038620	0.000048	0.241401
Mg3	-1.452563	-0.000095	0.470675
Mg4	-4.574145	-0.000031	-0.021463
Mg5	-7.902394	0.000010	-0.416167
Mg6	1.378931	0.000022	-1.285630
Mg7	3.254800	2.853243	-0.647161
Mg8	3.254944	-2.853171	-0.647195
Mg9	1.000838	1.715943	1.152783

@mg09-isomer32 bp86/6-31G(d) Etot=-1800.729710 Eb=-7.14

Mg1	0.584314	-1.920955	0.977258
Mg2	0.417134	0.921830	-0.174192
Mg3	-2.266049	-0.965555	-0.092268
Mg4	-1.275709	0.203795	2.418095
Mg5	0.064446	3.868711	-1.028290
Mg6	3.133960	-0.460926	-0.234872
Mg7	-4.578562	-2.697176	-1.558988
Mg8	6.302594	-1.133277	-0.539906
Mg9	-2.382128	2.183553	0.233165

@mg09-isomer33 bp86/6-31G(d) Etot=-1800.726133 Eb=-6.89

Mg1	2.346392	1.152477	0.000095
Mg2	2.003568	-1.578904	-1.484238
Mg3	-0.444695	-0.275831	-0.000179
Mg4	4.925872	-0.824941	-0.000006
Mg5	5.308094	2.331366	0.000348
Mg6	2.003436	-1.579242	1.483807
Mg7	-3.544239	0.025894	-0.000202
Mg8	-6.299390	0.374984	-1.638356
Mg9	-6.299036	0.374197	1.638731

@mg09-isomer34 bp86/6-31G(d) Etot=-1800.720265 Eb=-6.48

Mg1	-2.539145	1.651407	1.479497
Mg2	-2.539501	1.651847	-1.479101
Mg3	0.413375	2.337072	-0.000038
Mg4	2.206706	-0.216547	-0.000181
Mg5	-4.025163	-0.651189	0.000014
Mg6	5.346862	-0.584222	-0.000022
Mg7	-0.881167	-0.590672	-0.000275
Mg8	8.669061	-1.047412	0.000100

Mg9	-6.651027	-2.550284	0.000006
@mg09-isomer35 bp86/6-31G(d) Etot=-1800.718134 Eb=-6.33			
Mg1	4.287271	-0.656909	1.602962
Mg2	1.553834	0.002173	-0.000146
Mg3	-1.611943	0.000536	0.000663
Mg4	-4.802780	-0.000159	0.000497
Mg5	-7.595259	-1.622463	-0.000345
Mg6	7.188664	-0.002067	-0.000054
Mg7	4.286966	-1.059696	-1.370609
Mg8	4.288879	1.717064	-0.232628
Mg9	-7.595634	1.621523	-0.000340
@mg09-isomer36 bp86/6-31G(d) Etot=-1800.717925 Eb=-6.31			
Mg1	-2.778373	-1.129269	-0.001591
Mg2	-4.776146	0.808998	1.486176
Mg3	0.229736	-0.329100	-0.001332
Mg4	-4.778477	0.810808	-1.484104
Mg5	3.366057	-0.200982	-0.000510
Mg6	-1.957734	1.934602	-0.000162
Mg7	-5.907461	-1.721600	0.000392
Mg8	6.617324	-0.208459	0.001557
Mg9	9.985072	0.035003	-0.000427
@mg09-isomer37 bp86/6-31G(d) Etot=-1800.708469 Eb=-5.66			
Mg1	-1.533571	-0.024320	-0.322742
Mg2	0.000300	1.237578	-2.650622
Mg3	1.533583	-0.024297	-0.322364
Mg4	-0.000053	2.597604	0.080244
Mg5	4.244459	-1.565946	0.246166
Mg6	7.209197	-3.109909	0.653083
Mg7	-4.244180	-1.566387	0.245757
Mg8	-0.001043	5.566373	1.417335
Mg9	-7.208692	-3.110696	0.653142
@mg10-isomer01 bp86/6-31G(d) Etot=-2000.892523 Eb=-12.26			
Mg1	1.911802	-0.861051	1.590869
Mg2	0.399550	-3.035216	0.083732
Mg3	1.911363	-0.947363	-1.541456
Mg4	1.911412	1.808446	-0.050046
Mg5	0.399927	1.590080	2.586599
Mg6	-1.141307	-0.879634	1.625789
Mg7	-1.141504	-0.968023	-1.574517
Mg8	0.399383	1.445076	-2.670332
Mg9	-1.141783	1.847946	-0.050860
Mg10	-3.508843	-0.000260	0.000221
@mg10-isomer02 bp86/6-31G(d) Etot=-2000.875833 Eb=-11.22			
Mg1	1.955937	1.138720	0.512644
Mg2	-1.099450	2.021969	-0.296551
Mg3	-0.592214	0.007075	2.243721
Mg4	1.331624	2.898866	-1.863869
Mg5	2.264197	-0.805376	2.806303
Mg6	1.099440	-2.022007	0.296579
Mg7	-3.352918	0.818402	1.318651
Mg8	0.592259	-0.007084	-2.243695
Mg9	-1.955944	-1.138696	-0.512681
Mg10	-0.242933	-2.911870	-2.261102
@mg10-isomer03 bp86/6-31G(d) Etot=-2000.863680 Eb=-10.45			
Mg1	-5.600711	0.000013	0.000027
Mg2	-2.420909	-0.000004	0.000007
Mg3	-0.301779	-1.594664	-1.574647
Mg4	-0.301798	1.594488	-1.574703

Mg5	-0.301764	-1.594493	1.574692
Mg6	2.475452	-0.000075	-1.580057
Mg7	2.138904	2.623849	-0.000117
Mg8	2.138881	-2.623852	0.000100
Mg9	2.475453	0.000069	1.580081
Mg10	-0.301728	1.594668	1.574617
@mg10-isomer04 bp86/6-31G(d) Etot=-2000.862955 Eb=-10.41			
Mg1	-1.611750	-0.201269	1.510660
Mg2	-0.366497	2.648955	1.132812
Mg3	1.611879	0.201234	1.510720
Mg4	-4.145121	0.250835	-0.222275
Mg5	0.366506	-2.648963	1.132794
Mg6	4.145104	-0.250880	-0.222398
Mg7	1.715193	1.903030	-1.038931
Mg8	-1.715226	-1.903003	-1.038967
Mg9	-1.318594	1.196625	-1.382205
Mg10	1.318506	-1.196564	-1.382210
@mg10-isomer05 bp86/6-31G(d) Etot=-2000.862692 Eb=-10.39			
Mg1	1.633844	0.828240	1.345407
Mg2	-1.633824	0.828398	-1.345445
Mg3	1.392416	-0.617096	-1.590825
Mg4	1.270265	-2.240709	0.931777
Mg5	0.965412	2.507957	-1.183729
Mg6	-4.106439	-0.478693	0.005857
Mg7	4.106477	-0.478737	-0.005879
Mg8	-1.270498	-2.240577	-0.931725
Mg9	-0.965211	2.508102	1.183720
Mg10	-1.392441	-0.616886	1.590842
@mg10-isomer06 bp86/6-31G(d) Etot=-2000.860211 Eb=-10.24			
Mg1	-1.421557	-1.048813	1.610563
Mg2	-3.817456	0.017364	-0.188607
Mg3	1.195219	-2.061322	0.126846
Mg4	-1.736198	-2.596610	-1.046833
Mg5	4.093162	-0.772964	0.782385
Mg6	1.243331	0.842401	1.283764
Mg7	0.467910	2.956098	-0.963446
Mg8	-0.774083	0.237992	-1.268976
Mg9	-1.671294	2.058655	1.201528
Mg10	2.420966	0.367200	-1.537223
@mg10-isomer07 bp86/6-31G(d) Etot=-2000.858469 Eb=-10.13			
Mg1	-3.200155	-1.603609	-0.762265
Mg2	-0.578363	-0.000081	-1.183286
Mg3	-3.200018	1.603705	-0.762270
Mg4	-2.038874	0.000061	1.607353
Mg5	2.097522	1.626468	-1.045137
Mg6	2.097544	-1.626474	-1.045084
Mg7	1.227392	-0.000046	1.453654
Mg8	4.490875	0.000021	0.221187
Mg9	-0.447930	2.586649	0.757936
Mg10	-0.447992	-2.586693	0.757913
@mg10-isomer08 bp86/6-31G(d) Etot=-2000.858427 Eb=-10.13			
Mg1	-1.002077	0.575282	-1.007321
Mg2	-0.015064	2.043218	1.684463
Mg3	3.954466	-1.154384	0.474299
Mg4	0.155916	3.380654	-1.109015
Mg5	-1.417440	-2.358785	-0.510559
Mg6	2.213475	1.163507	-0.420622
Mg7	0.902135	-1.182295	1.333048
Mg8	-4.168675	-0.396268	-0.626232

Mg9	-2.179952	-0.365481	1.759579	
Mg10	1.557217	-1.705447	-1.577639	
@mg10-isomer09 bp86/6-31G(d) Etot=-2000.858417 Eb=-10.12				
Mg1	-1.117119	-0.463016	1.510254	
Mg2	1.117128	-1.510258	-0.463015	
Mg3	-3.883489	-0.000020	-0.000003	
Mg4	1.117123	1.510263	0.463017	
Mg5	-1.117119	0.463010	-1.510256	
Mg6	-1.940959	2.490033	0.763501	
Mg7	-1.940963	-2.490001	-0.763501	
Mg8	1.940944	0.763502	-2.490014	
Mg9	3.883517	-0.000008	-0.000002	
Mg10	1.940936	-0.763505	2.490019	
@mg10-isomer10 bp86/6-31G(d) Etot=-2000.857750 Eb=-10.08				
Mg1	3.636797	-0.743285	0.581181	
Mg2	-1.341761	-1.388910	-1.198744	
Mg3	1.462022	0.487451	-1.345780	
Mg4	1.708127	-2.526106	-1.280221	
Mg5	1.689474	1.845916	1.450006	
Mg6	0.601728	-1.261816	1.276189	
Mg7	-1.323635	1.316413	0.466345	
Mg8	-2.529388	-1.194926	1.643612	
Mg9	-4.299773	0.121623	-0.558012	
Mg10	0.396409	3.343639	-1.034576	
@mg10-isomer11 bp86/6-31G(d) Etot=-2000.856888 Eb=-10.03				
Mg1	0.876532	-2.128484	1.510534	
Mg2	-0.082870	1.121213	1.219646	
Mg3	2.468031	-2.778737	-1.116563	
Mg4	-0.082790	-1.121339	-1.219659	
Mg5	2.831125	0.000128	-0.000106	
Mg6	-2.183304	-1.109059	1.131892	
Mg7	-4.987423	-0.000013	0.000009	
Mg8	-2.183353	1.108817	-1.131916	
Mg9	2.467769	2.778872	1.116650	
Mg10	0.876283	2.128602	-1.510487	
@mg10-isomer12 bp86/6-31G(d) Etot=-2000.856661 Eb=-10.01				
Mg1	1.922763	-2.984272	-1.250900	
Mg2	-0.458016	-1.915348	0.312702	
Mg3	1.610543	0.030548	-1.368819	
Mg4	0.605664	2.904283	-1.147044	
Mg5	-2.637175	-0.279690	1.680028	
Mg6	2.993341	1.875450	0.750205	
Mg7	-4.904175	-0.183968	-0.472598	
Mg8	2.527400	-1.253701	1.287890	
Mg9	-1.732234	0.644288	-1.133443	
Mg10	0.071888	1.162409	1.341980	
@mg10-isomer13 bp86/6-31G(d) Etot=-2000.855433 Eb=-9.94				
Mg1	-1.457569	1.131263	1.336573	
Mg2	-2.423063	1.399295	-1.583251	
Mg3	0.539441	-1.597257	1.682517	
Mg4	-1.841247	-1.460842	-0.357483	
Mg5	0.909126	-2.847977	-1.073548	
Mg6	3.208521	-0.828117	0.110217	
Mg7	1.800500	1.518321	1.640545	
Mg8	0.553846	0.438840	-1.040506	
Mg9	3.200475	2.024247	-1.094834	
Mg10	-4.490031	0.222228	0.379770	
@mg10-isomer14 bp86/6-31G(d) Etot=-2000.854863 Eb=-9.90				

Mg1	3.818746	0.000242	0.875776
Mg2	1.511927	-0.000269	-1.285478
Mg3	1.072948	3.022891	-1.388835
Mg4	0.941254	1.599558	1.349690
Mg5	0.941353	-1.599637	1.349832
Mg6	1.072406	-3.023406	-1.388559
Mg7	-1.570038	1.603390	-0.654791
Mg8	-1.570047	-1.603068	-0.654664
Mg9	-1.885798	0.000169	1.948360
Mg10	-4.332750	0.000129	-0.151329

@mg10-isomer15 bp86/6-31G(d) Etot=-2000.853941 Eb=-9.84

Mg1	-0.195795	-1.138399	1.110455
Mg2	-2.860854	0.061031	0.364878
Mg3	1.985530	1.428221	1.739297
Mg4	-0.495389	1.848745	-0.229261
Mg5	1.341546	-2.888222	-1.034951
Mg6	-0.958979	-0.814258	-1.906500
Mg7	2.243673	0.014369	-1.047832
Mg8	2.771800	-1.698031	1.515701
Mg9	2.203863	3.038140	-0.932687
Mg10	-6.035394	0.148404	0.420899

@mg10-isomer16 bp86/6-31G(d) Etot=-2000.853440 Eb=-9.81

Mg1	2.560388	1.062003	0.336774
Mg2	2.210632	-1.615087	-1.353570
Mg3	1.135552	3.382505	-1.013402
Mg4	-0.264254	0.735993	-1.475867
Mg5	-0.312383	1.996956	1.389194
Mg6	3.339292	-1.604046	1.530977
Mg7	-2.439130	-0.296445	0.510680
Mg8	-0.949192	-2.220926	-1.527900
Mg9	-5.621415	-0.141632	0.425736
Mg10	0.340509	-1.299322	1.177378

@mg10-isomer17 bp86/6-31G(d) Etot=-2000.853428 Eb=-9.81

Mg1	-2.048802	0.507835	1.714947
Mg2	-2.169377	2.068449	-0.946626
Mg3	-4.570954	0.119009	-0.161119
Mg4	0.617052	1.614557	0.456728
Mg5	0.565056	-1.571489	1.592521
Mg6	3.314331	0.451409	1.450236
Mg7	3.152016	2.005258	-1.236485
Mg8	-1.313255	-0.889936	-0.930192
Mg9	2.102551	-0.861885	-1.089097
Mg10	0.351382	-3.443207	-0.850911

@mg10-isomer18 bp86/6-31G(d) Etot=-2000.853379 Eb=-9.81

Mg1	-0.266204	-1.722643	-0.973997
Mg2	-0.266444	1.722733	-0.973969
Mg3	2.477577	-3.014634	-0.650530
Mg4	-1.680713	-0.000095	1.241780
Mg5	2.652495	0.000079	-0.443120
Mg6	2.477364	3.014745	-0.650482
Mg7	1.142272	1.674580	1.789977
Mg8	-2.709837	-0.000099	-1.653606
Mg9	-4.968889	-0.000073	0.523978
Mg10	1.142380	-1.674592	1.789968

@mg10-isomer19 bp86/6-31G(d) Etot=-2000.852884 Eb=-9.78

Mg1	1.594700	3.351359	-0.763615
Mg2	0.893122	1.498753	1.587056
Mg3	-2.166751	0.307536	1.373607
Mg4	-5.115866	-0.211738	0.175765

Mg5	0.047944	-1.606997	0.402613
Mg6	-2.495283	-1.173208	-1.309144
Mg7	2.563410	0.434369	-0.869161
Mg8	2.808623	-1.295526	1.686314
Mg9	-0.642871	1.314015	-1.147007
Mg10	2.512972	-2.618562	-1.136428
@mg10-isomer20	bp86/6-31G(d)	Etot=-2000.852493	Eb=-9.75
Mg1	-1.949439	1.610102	-0.584986
Mg2	-1.949081	-1.609479	-0.586232
Mg3	-2.571052	-0.000753	1.943890
Mg4	0.930748	2.714076	-0.972426
Mg5	0.417973	-0.000019	0.803062
Mg6	3.176345	1.597504	1.057575
Mg7	3.176573	-1.597253	1.057610
Mg8	2.472985	0.000023	-1.494560
Mg9	-4.636121	-0.000063	-0.251661
Mg10	0.931067	-2.714139	-0.972272
@mg10-isomer21	bp86/6-31G(d)	Etot=-2000.852151	Eb=-9.73
Mg1	-1.750370	1.051530	1.039229
Mg2	1.183987	2.013022	1.467662
Mg3	-2.157870	-0.328333	-1.695076
Mg4	-0.069777	2.283698	-1.378798
Mg5	-4.644731	-0.170229	0.146219
Mg6	0.524091	-0.935612	0.001123
Mg7	2.873965	0.925313	-0.975305
Mg8	-2.313392	-2.064597	0.837837
Mg9	3.185433	-2.114547	-1.080256
Mg10	3.168666	-0.660244	1.637365
@mg10-isomer22	bp86/6-31G(d)	Etot=-2000.851385	Eb=-9.68
Mg1	-0.132154	1.667264	-0.268171
Mg2	-2.456897	0.001381	-1.250814
Mg3	-4.970594	-0.000720	0.667735
Mg4	2.585429	2.726786	0.629545
Mg5	1.529241	-0.002168	1.947784
Mg6	-1.833393	-0.002035	1.820008
Mg7	2.693561	0.000922	-0.856453
Mg8	-0.132184	-1.666650	-0.271865
Mg9	0.131613	0.003416	-3.041372
Mg10	2.585378	-2.728196	0.623604
@mg10-isomer23	bp86/6-31G(d)	Etot=-2000.851347	Eb=-9.68
Mg1	3.535290	1.518217	0.714788
Mg2	3.535226	-1.518114	0.714614
Mg3	1.082272	2.716313	-0.734205
Mg4	0.646379	-0.000156	-2.033510
Mg5	1.082167	-2.716482	-0.734008
Mg6	0.640637	0.000016	0.969214
Mg7	-1.800558	1.713930	-0.352641
Mg8	-1.800664	-1.714041	-0.352107
Mg9	-2.549292	0.000294	2.120064
Mg10	-4.371459	0.000024	-0.312210
@mg10-isomer24	bp86/6-31G(d)	Etot=-2000.851184	Eb=-9.67
Mg1	1.127080	1.175567	0.654909
Mg2	-1.592004	2.807108	0.222468
Mg3	-4.012995	0.846804	-0.386225
Mg4	-1.052604	0.036166	-1.303021
Mg5	-1.806847	-0.045985	1.560971
Mg6	2.308731	-0.616431	-1.661164
Mg7	4.172546	1.505090	-0.250583
Mg8	3.494773	-1.289585	0.982116

Mg9	-2.968218	-2.305578	-0.274118	
Mg10	0.329539	-2.113156	0.454646	
@mg10-isomer25 bp86/6-31G(d) Etot=-2000.850757 Eb=-9.64				
Mg1	-0.432480	1.690838	-0.612236	
Mg2	-0.942531	-0.000151	2.003137	
Mg3	1.878211	1.656271	1.596663	
Mg4	1.878518	-1.656123	1.596620	
Mg5	-6.102640	-0.000012	-0.350303	
Mg6	-2.929818	-0.000301	-0.328663	
Mg7	2.247645	3.020868	-1.148343	
Mg8	2.587129	0.000165	-0.996191	
Mg9	2.248140	-3.020576	-1.148441	
Mg10	-0.432175	-1.690978	-0.612242	
@mg10-isomer26 bp86/6-31G(d) Etot=-2000.850217 Eb=-9.61				
Mg1	-0.786151	-2.990258	-0.651120	
Mg2	1.852973	-1.137525	-1.032515	
Mg3	0.066401	-1.021969	1.514850	
Mg4	3.542795	-0.276899	1.431540	
Mg5	-1.131245	0.108306	-1.234177	
Mg6	-3.216130	-0.958669	0.745348	
Mg7	1.357890	1.693335	0.331830	
Mg8	-3.942757	1.532635	-1.051368	
Mg9	4.030265	1.206226	-1.285645	
Mg10	-1.774042	1.844818	1.231258	
@mg10-isomer27 bp86/6-31G(d) Etot=-2000.849783 Eb=-9.58				
Mg1	2.764926	2.712321	-0.000434	
Mg2	-0.106074	1.689373	-0.000360	
Mg3	-0.783076	-0.000669	-2.638850	
Mg4	-2.567905	-0.000259	-0.000107	
Mg5	2.272581	0.000390	1.527839	
Mg6	-0.783244	0.000423	2.638768	
Mg7	-5.729421	0.000097	0.000041	
Mg8	2.765327	-2.712037	0.000529	
Mg9	2.272677	-0.000183	-1.527744	
Mg10	-0.105791	-1.689455	0.000317	
@mg10-isomer28 bp86/6-31G(d) Etot=-2000.849196 Eb=-9.55				
Mg1	-2.719246	-0.627292	0.000224	
Mg2	-5.919958	-0.670723	0.000099	
Mg3	0.107570	-1.706901	0.000244	
Mg4	-0.592030	1.076670	1.529470	
Mg5	3.097441	-1.940729	0.000057	
Mg6	-0.592262	1.076315	-1.529490	
Mg7	1.774638	-0.825943	2.637970	
Mg8	0.720930	3.510915	-0.000458	
Mg9	1.774138	-0.826713	-2.637929	
Mg10	2.348780	0.934401	-0.000186	
@mg10-isomer29 bp86/6-31G(d) Etot=-2000.848016 Eb=-9.47				
Mg1	-2.221168	-1.316575	1.282685	
Mg2	-0.994111	-3.139535	-1.044298	
Mg3	-4.239404	0.992115	0.499660	
Mg4	-1.170905	1.843784	0.893223	
Mg5	-1.861457	-0.011091	-1.462684	
Mg6	0.770777	-0.914837	0.040946	
Mg7	3.466464	-1.268975	1.514559	
Mg8	2.041485	1.583760	1.159038	
Mg9	0.663623	1.992265	-1.674464	
Mg10	3.544696	0.239089	-1.208664	
@mg10-isomer30 bp86/6-31G(d) Etot=-2000.847129 Eb=-9.42				

Mg1	-1.127359	0.072885	-1.203195
Mg2	-2.083078	-0.978783	1.597609
Mg3	1.127356	0.072914	1.203205
Mg4	-3.999973	0.784624	0.067842
Mg5	-1.135470	2.231014	1.103701
Mg6	-3.407760	-2.109701	-1.025927
Mg7	3.999960	0.784596	-0.067800
Mg8	1.135541	2.230978	-1.103743
Mg9	2.083073	-0.978784	-1.597606
Mg10	3.407709	-2.109742	1.025914

@mg10-isomer31 bp86/6-31G(d) Etot=-2000.846816 Eb=-9.40

Mg1	3.537136	2.502113	-0.332106
Mg2	3.175724	-0.282588	1.160352
Mg3	1.978598	-0.109115	-1.505906
Mg4	0.625993	1.858757	0.585639
Mg5	2.536824	-3.011359	-0.242053
Mg6	-1.565676	0.476205	-1.348180
Mg7	-2.205438	0.666658	1.551086
Mg8	-3.485819	-1.782158	-0.059624
Mg9	-0.010044	-1.467871	0.588600
Mg10	-4.587298	1.149358	-0.397806

@mg10-isomer32 bp86/6-31G(d) Etot=-2000.846810 Eb=-9.40

Mg1	0.943319	0.944486	0.088622
Mg2	3.608297	0.165645	1.650353
Mg3	-2.090420	1.503328	-1.019200
Mg4	1.077231	-2.061877	1.186782
Mg5	3.795326	2.008764	-0.804784
Mg6	-3.997901	-0.818751	-0.960357
Mg7	-4.156500	1.426082	1.293790
Mg8	3.018018	-0.979755	-1.143811
Mg9	-0.466656	-1.522386	-1.508785
Mg10	-1.730715	-0.665536	1.217389

@mg10-isomer33 bp86/6-31G(d) Etot=-2000.846260 Eb=-9.36

Mg1	3.374274	0.578156	-0.208611
Mg2	2.391988	3.467361	-0.117586
Mg3	0.016667	1.520809	0.287528
Mg4	3.552476	-2.531287	-0.270936
Mg5	-2.251954	0.222089	-1.707314
Mg6	-4.525917	-1.249503	-0.118670
Mg7	0.842491	-1.226323	-1.210544
Mg8	1.574116	-1.182349	1.661629
Mg9	-3.429122	1.549185	0.760116
Mg10	-1.545021	-1.148138	0.924389

@mg10-isomer34 bp86/6-31G(d) Etot=-2000.846072 Eb=-9.35

Mg1	-4.890309	1.073242	-0.000026
Mg2	-3.064184	-0.957996	1.494672
Mg3	-3.064240	-0.958139	-1.494577
Mg4	-1.855879	1.623316	-0.000063
Mg5	-0.119141	-1.018430	0.000021
Mg6	2.147549	-3.122243	0.000019
Mg7	2.742208	-0.413179	1.453872
Mg8	1.144533	2.088247	0.000037
Mg9	2.742125	-0.413174	-1.453950
Mg10	4.217339	2.098357	-0.000006

@mg10-isomer35 bp86/6-31G(d) Etot=-2000.845689 Eb=-9.33

Mg1	-2.035836	1.454395	-1.060343
Mg2	0.708302	1.785423	0.680580
Mg3	-4.637410	0.794892	0.460130
Mg4	-1.689257	-0.254690	1.429702

Mg5	-3.190117	-1.481993	-1.075197
Mg6	0.199695	-1.024878	-0.943868
Mg7	3.324899	3.068598	-0.448086
Mg8	3.306056	-0.047888	-0.368776
Mg9	1.436037	-1.272568	1.788600
Mg10	2.577631	-3.021292	-0.462741
@mg10-isomer36 bp86/6-31G(d)	Etot=-2000.845638	Eb=-9.32	
Mg1	-4.443849	0.787074	0.000499
Mg2	3.276123	0.700364	-1.478854
Mg3	3.271908	0.699836	1.481197
Mg4	1.264619	2.758131	-0.000859
Mg5	-0.145757	-2.974316	-0.000102
Mg6	3.004582	-2.011289	0.000334
Mg7	-2.418471	-1.044949	-1.464010
Mg8	-1.810318	2.199702	-0.000353
Mg9	-2.416116	-1.042917	1.464876
Mg10	0.417279	-0.071637	-0.002728
@mg10-isomer37 bp86/6-31G(d)	Etot=-2000.842865	Eb=-9.15	
Mg1	-3.017611	1.973178	-0.693400
Mg2	-3.000620	-1.069537	-1.162945
Mg3	-0.000011	0.414721	-1.308139
Mg4	-1.635031	-0.116745	1.354930
Mg5	-4.771172	0.244846	1.254963
Mg6	0.000029	-2.478260	-0.198978
Mg7	3.017683	1.973188	-0.693422
Mg8	3.000569	-1.069548	-1.162896
Mg9	1.635005	-0.116622	1.354939
Mg10	4.771159	0.244779	1.254950
@mg10-isomer38 bp86/6-31G(d)	Etot=-2000.842383	Eb=-9.12	
Mg1	1.598743	-0.317761	1.200834
Mg2	-1.598716	0.317908	1.200776
Mg3	-3.738447	-1.790993	0.221326
Mg4	0.461308	1.475821	-1.184919
Mg5	3.738332	1.791059	0.220995
Mg6	2.925408	-0.712450	-1.459050
Mg7	-0.461327	-1.476089	-1.184646
Mg8	4.690872	-1.019807	1.222020
Mg9	-2.925364	0.712183	-1.459171
Mg10	-4.690809	1.020129	1.221834
@mg10-isomer39 bp86/6-31G(d)	Etot=-2000.841926	Eb=-9.09	
Mg1	-0.733032	-1.571723	-0.068075
Mg2	-0.733024	1.571730	-0.068195
Mg3	-3.529929	0.000061	0.406010
Mg4	1.762985	-0.000046	-1.758900
Mg5	4.422259	-0.000052	-0.324868
Mg6	-1.407470	0.000111	2.529846
Mg7	-6.187526	-0.000083	-1.413742
Mg8	2.398139	-2.649371	-0.278368
Mg9	2.398209	2.649335	-0.278515
Mg10	1.609390	0.000038	1.254808
@mg10-isomer40 bp86/6-31G(d)	Etot=-2000.841488	Eb=-9.06	
Mg1	2.065018	-1.557332	-0.462907
Mg2	2.939586	-0.000004	2.090066
Mg3	2.064999	1.557361	-0.462905
Mg4	-0.582958	-0.000004	-1.941011
Mg5	-1.070325	-2.657197	-0.422080
Mg6	-0.169440	-0.000007	1.051170
Mg7	-3.073217	-0.000008	-0.255327
Mg8	-1.070319	2.657175	-0.422083

Mg9	4.959301	0.000001	-0.169806	
Mg10	-6.062644	0.000015	0.994882	
@mg10-isomer41 bp86/6-31G(d) Etot=-2000.840795 Eb=-9.02				
Mg1	1.806693	2.272904	0.466164	
Mg2	4.714650	1.024550	-0.233407	
Mg3	1.839560	-0.279405	-1.195058	
Mg4	-0.951042	1.587087	-1.331438	
Mg5	-3.394561	-0.065421	-0.097675	
Mg6	-0.387780	-0.221792	1.055666	
Mg7	-1.180252	-1.541389	-1.561718	
Mg8	2.816958	-0.471232	1.663865	
Mg9	1.121890	-2.988179	0.348402	
Mg10	-6.386115	0.682876	0.885199	
@mg10-isomer42 bp86/6-31G(d) Etot=-2000.839170 Eb=-8.92				
Mg1	5.352251	1.160732	-0.000360	
Mg2	0.831478	-1.743496	0.000304	
Mg3	-3.469087	1.076761	-1.486867	
Mg4	-3.469476	1.076412	1.486969	
Mg5	-0.509590	1.131742	0.000477	
Mg6	2.447545	0.575209	-1.455785	
Mg7	4.199781	-1.677509	-0.000175	
Mg8	-5.487314	-0.768438	-0.000443	
Mg9	-2.343532	-1.406613	-0.000072	
Mg10	2.447944	0.575199	1.455951	
@mg10-isomer43 bp86/6-31G(d) Etot=-2000.837479 Eb=-8.81				
Mg1	-6.718616	0.316387	0.818556	
Mg2	-3.706463	-0.257117	-0.186658	
Mg3	-1.200991	0.723221	-1.732552	
Mg4	-0.783924	0.244966	1.167798	
Mg5	1.203531	2.433285	-0.296871	
Mg6	-1.429343	-2.215141	-0.687392	
Mg7	2.691315	0.480332	1.830859	
Mg8	1.528313	-0.801223	-0.716340	
Mg9	4.194917	0.994284	-0.677073	
Mg10	4.221261	-1.918994	0.479673	
@mg10-isomer44 bp86/6-31G(d) Etot=-2000.837312 Eb=-8.80				
Mg1	-2.172136	-2.506531	-0.378963	
Mg2	-4.902539	-1.271689	0.350754	
Mg3	-2.086590	0.065437	1.459575	
Mg4	3.234853	-0.544744	0.052750	
Mg5	1.302327	1.258398	1.704228	
Mg6	-0.992038	2.712306	-0.111575	
Mg7	2.164041	2.176094	-0.981564	
Mg8	6.123183	-1.979753	-0.039101	
Mg9	0.220883	-0.338453	-0.687944	
Mg10	-2.891985	0.428934	-1.368161	
@mg10-isomer45 bp86/6-31G(d) Etot=-2000.837165 Eb=-8.79				
Mg1	5.886349	-2.391881	0.000200	
Mg2	2.913900	-1.157487	-0.000279	
Mg3	1.495341	1.229498	-1.453092	
Mg4	-0.123155	-1.293669	-0.000217	
Mg5	-2.762034	-0.674968	-1.506561	
Mg6	-2.761825	-0.675141	1.506590	
Mg7	-5.302756	-1.865500	0.000113	
Mg8	1.495393	1.229260	1.453001	
Mg9	-1.483054	1.693852	0.000060	
Mg10	0.641841	3.906037	0.000185	
@mg10-isomer46 bp86/6-31G(d) Etot=-2000.836672 Eb=-8.76				

Mg1	-2.110113	-1.474966	1.517591
Mg2	-5.017324	-0.867022	0.300329
Mg3	-2.567401	-1.763434	-1.462620
Mg4	0.904478	1.064086	1.451316
Mg5	0.416363	-1.394039	-0.445141
Mg6	-0.607619	3.677591	0.143635
Mg7	3.307496	-0.322352	-0.006683
Mg8	1.326972	1.571544	-1.406339
Mg9	6.317437	-1.462982	0.195563
Mg10	-1.970290	0.971573	-0.287651

@mg10-isomer47 bp86/6-31G(d) Etot=-2000.836141 Eb=-8.73

Mg1	-3.753673	-0.000487	0.992088
Mg2	-0.719768	-1.626692	0.548509
Mg3	-3.398539	-2.782342	-0.384806
Mg4	1.571697	0.001225	1.845708
Mg5	-3.400193	2.781075	-0.385718
Mg6	-2.460866	-0.000555	-1.637344
Mg7	7.368133	-0.000879	-0.608579
Mg8	4.198152	0.000693	0.227377
Mg9	1.315655	0.000494	-1.145012
Mg10	-0.720598	1.627469	0.547777

@mg10-isomer48 bp86/6-31G(d) Etot=-2000.835966 Eb=-8.72

Mg1	6.466224	-1.086055	-0.000172
Mg2	3.440771	-0.026355	0.000287
Mg3	1.140728	1.363986	1.484123
Mg4	1.140974	1.363856	-1.484153
Mg5	0.633090	-1.407447	0.000084
Mg6	-2.282067	-2.574477	0.000053
Mg7	-2.122425	0.097645	1.480566
Mg8	-1.408943	2.887541	-0.000105
Mg9	-2.122166	0.097599	-1.480474
Mg10	-4.886187	-0.716295	-0.000208

@mg10-isomer49 bp86/6-31G(d) Etot=-2000.832335 Eb=-8.49

Mg1	-1.438961	-1.769416	-0.189860
Mg2	-0.181029	1.314850	-0.113592
Mg3	1.434907	-1.130688	1.280345
Mg4	-3.157268	0.720696	-0.394350
Mg5	1.678328	-1.131324	-1.671838
Mg6	2.875251	1.291850	-0.115879
Mg7	-1.795350	0.087439	2.285100
Mg8	5.839637	2.540474	-0.055265
Mg9	0.839862	-3.839975	-0.296650
Mg10	-6.095376	1.916093	-0.728010

@mg10-isomer50 bp86/6-31G(d) Etot=-2000.831004 Eb=-8.40

Mg1	-2.214427	-1.424282	0.000231
Mg2	-0.957312	1.494635	0.000023
Mg3	0.947774	-1.127880	0.000209
Mg4	-5.354964	-1.663688	0.000009
Mg5	2.027606	1.369528	1.492490
Mg6	2.027522	1.369221	-1.492642
Mg7	4.015359	-0.631372	0.000071
Mg8	-3.857259	0.767991	1.492402
Mg9	7.222671	-0.921797	-0.000072
Mg10	-3.856970	0.767644	-1.492721

@mg10-isomer51 bp86/6-31G(d) Etot=-2000.830639 Eb=-8.38

Mg1	-0.716923	1.643602	0.128261
Mg2	-3.574313	2.774007	0.342401
Mg3	0.095825	-0.000024	-2.402284
Mg4	-3.315065	-0.000042	1.804618

Mg5	1.842630	0.000051	0.127515
Mg6	-3.256669	-0.000012	-1.163308
Mg7	4.946001	0.000043	0.271639
Mg8	-3.574268	-2.774054	0.342335
Mg9	-0.716909	-1.643517	0.128365
Mg10	8.269692	-0.000053	0.420457
@mg10-isomer52 bp86/6-31G(d)	Etot=-2000.827924	Eb=-8.21	
Mg1	1.210010	-0.965088	0.000027
Mg2	-1.210141	0.964880	0.000024
Mg3	4.084941	0.530153	0.000032
Mg4	6.916353	-0.976473	-0.000098
Mg5	-4.085074	-0.530402	0.000029
Mg6	-6.915862	0.977346	-0.000097
Mg7	1.701409	1.691951	1.501625
Mg8	-1.701518	-1.692152	1.501633
Mg9	-1.701529	-1.692151	-1.501586
Mg10	1.701412	1.691936	-1.501590
@mg10-isomer53 bp86/6-31G(d)	Etot=-2000.826493	Eb=-8.12	
Mg1	-0.098590	-0.382877	0.000707
Mg2	-2.589423	-1.621481	-1.487123
Mg3	2.959822	0.035756	-0.000351
Mg4	5.550047	-0.373073	1.652281
Mg5	5.301779	2.043635	-0.250568
Mg6	-2.590062	-1.622512	1.486488
Mg7	-2.867619	1.117056	0.000557
Mg8	-5.457852	-0.787446	-0.000589
Mg9	-5.803101	2.395558	0.000188
Mg10	5.595000	-0.804615	-1.401589
@mg10-isomer54 bp86/6-31G(d)	Etot=-2000.825526	Eb=-8.06	
Mg1	4.931249	0.659186	-1.493120
Mg2	2.753294	-1.024154	-0.000008
Mg3	2.304415	2.146913	-0.000020
Mg4	-3.240273	-0.127260	0.000023
Mg5	-5.786987	0.732593	-1.542711
Mg6	-0.154233	0.178226	-0.000001
Mg7	5.787596	-2.016756	0.000013
Mg8	4.931243	0.659225	1.493126
Mg9	-5.739267	-1.941979	0.000811
Mg10	-5.787037	0.734006	1.541886
@mg10-isomer55 bp86/6-31G(d)	Etot=-2000.823953	Eb=-7.96	
Mg1	3.317990	-2.130926	0.002483
Mg2	5.262218	-0.375193	-1.541886
Mg3	0.233164	-0.906248	0.001589
Mg4	-2.538620	0.720103	0.000492
Mg5	5.264107	-0.371497	1.540259
Mg6	-5.500475	-0.310252	0.000494
Mg7	-8.762580	-1.018789	-0.000281
Mg8	-0.051376	1.737780	-1.497190
Mg9	2.826307	0.914112	-0.000895
Mg10	-0.050736	1.740910	1.494934
@mg10-isomer56 bp86/6-31G(d)	Etot=-2000.820529	Eb=-7.75	
Mg1	1.398306	-0.153684	-0.000009
Mg2	4.351966	-1.513287	-0.006388
Mg3	-3.935426	-2.038585	1.531295
Mg4	4.008822	1.067435	1.508460
Mg5	4.007378	1.078387	-1.502095
Mg6	-4.536311	0.553279	0.000017
Mg7	6.927101	0.571570	0.000025
Mg8	-6.609829	3.070485	-0.000003

Mg9	-3.935291	-2.038480	-1.531387	
Mg10	-1.676716	-0.597120	0.000087	
@mg10-isomer57 bp86/6-31G(d) Etot=-2000.820091 Eb=-7.72				
Mg1	4.360379	1.207778	0.045379	
Mg2	-0.872508	0.165813	-0.098654	
Mg3	1.148617	2.360573	-0.884431	
Mg4	1.445492	0.911159	1.802793	
Mg5	-3.941028	-0.193788	-0.044225	
Mg6	-6.830293	1.245339	-0.052815	
Mg7	5.024352	-1.399185	-1.474664	
Mg8	-6.570417	-2.044615	-0.026242	
Mg9	4.217644	-1.484472	1.522374	
Mg10	2.017763	-0.768602	-0.789515	
@mg10-isomer58 bp86/6-31G(d) Etot=-2000.816297 Eb=-7.48				
Mg1	-0.784874	-0.000089	-0.515464	
Mg2	-3.872755	0.000093	-0.093093	
Mg3	2.039494	-0.000269	1.278316	
Mg4	1.671753	1.730017	-1.162220	
Mg5	4.671842	-0.000264	-0.279876	
Mg6	3.917324	2.851094	0.657457	
Mg7	3.916474	-2.851215	0.658131	
Mg8	1.672151	-1.729436	-1.162729	
Mg9	-6.851648	-0.000584	-1.317295	
Mg10	-6.379759	0.000652	1.936773	
@mg10-isomer59 bp86/6-31G(d) Etot=-2000.816186 Eb=-7.47				
Mg1	-8.560249	1.308147	0.182156	
Mg2	2.744437	-0.717666	2.176112	
Mg3	6.776342	2.361787	-0.396071	
Mg4	0.815680	0.688750	-0.064552	
Mg5	-2.236309	0.091315	-0.044189	
Mg6	-5.288358	0.679347	0.067270	
Mg7	-0.314496	-2.080895	0.930520	
Mg8	3.922662	0.951571	-0.108323	
Mg9	-0.558016	-1.494967	-2.057352	
Mg10	2.698308	-1.787390	-0.685571	
@mg10-isomer60 bp86/6-31G(d) Etot=-2000.814879 Eb=-7.39				
Mg1	-1.252998	-0.000253	1.436118	
Mg2	1.183013	1.709251	0.000243	
Mg3	-1.673248	-2.783768	0.000051	
Mg4	-3.586214	5.396016	-0.000566	
Mg5	3.707129	0.000735	-0.000030	
Mg6	-1.674253	2.783295	0.000474	
Mg7	-3.583914	-5.397437	-0.000311	
Mg8	6.949995	0.000950	-0.000300	
Mg9	-1.253154	-0.000083	-1.435665	
Mg10	1.183644	-1.708706	-0.000014	
@mg10-isomer61 bp86/6-31G(d) Etot=-2000.813077 Eb=-7.28				
Mg1	-0.811269	-1.182570	-0.000019	
Mg2	-0.029045	1.668073	-1.438416	
Mg3	2.072603	-0.185823	-0.000006	
Mg4	-0.029039	1.668058	1.438442	
Mg5	-3.012330	1.436303	-0.000010	
Mg6	-1.497986	4.113142	0.000019	
Mg7	-3.851392	-1.494102	-0.000078	
Mg8	5.141640	-0.884563	-0.000002	
Mg9	-6.391642	-3.514263	0.000060	
Mg10	8.408461	-1.624255	0.000010	
@mg10-isomer62 bp86/6-31G(d) Etot=-2000.804205 Eb=-6.72				

Mg1	0.894516	2.208873	1.479680
Mg2	-1.321155	0.586966	-0.000108
Mg3	3.873080	1.822761	0.000226
Mg4	0.894575	2.209387	-1.479252
Mg5	-4.304688	-0.279836	-0.000086
Mg6	-6.959014	-1.096676	1.638360
Mg7	1.633186	-0.471820	-0.000239
Mg8	4.676648	-1.200938	-0.000209
Mg9	7.572199	-2.682676	-0.000065
Mg10	-6.959347	-1.096042	-1.638307

@mg10-isomer63 bp86/6-31G(d) Etot=-2000.796665 Eb=-6.25

Mg1	-2.196093	0.398696	1.451568
Mg2	0.693420	0.605555	-0.000047
Mg3	-4.690293	-1.140221	0.000047
Mg4	3.780175	0.009174	-0.000006
Mg5	-6.869513	-3.584061	-0.000026
Mg6	-4.631340	1.965941	0.000032
Mg7	6.983521	-0.588880	-0.000013
Mg8	-1.196359	3.075837	-0.000036
Mg9	10.322613	-1.140702	0.000027
Mg10	-2.196131	0.398661	-1.451546

@mg11-isomer01 bp86/6-31G(d) Etot=-2200.979169 Eb=-12.12

Mg1	1.544175	-0.015014	-1.807974
Mg2	0.000524	-2.631538	-1.490277
Mg3	-4.184842	0.000375	-0.000138
Mg4	0.000646	2.606435	-1.533573
Mg5	-1.543926	-0.014905	-1.808640
Mg6	-0.000948	0.024734	3.023888
Mg7	-1.544561	-1.558900	0.916496
Mg8	1.543822	1.573760	0.891963
Mg9	1.543682	-1.558405	0.917582
Mg10	-1.543714	1.573688	0.890581
Mg11	4.185143	-0.000229	0.000091

@mg11-isomer02 bp86/6-31G(d) Etot=-2200.972785 Eb=-11.75

Mg1	2.522791	-1.694549	0.615443
Mg2	-0.535006	-1.725558	0.627178
Mg3	2.522690	1.380667	1.159272
Mg4	-0.534778	1.405982	1.181014
Mg5	1.012045	2.851961	-1.036689
Mg6	1.011954	-2.323616	-1.951739
Mg7	-2.911506	0.000144	0.000708
Mg8	-0.535360	0.319634	-1.807585
Mg9	1.012794	-0.528514	2.988018
Mg10	-6.087906	-0.000113	-0.000113
Mg11	2.522283	0.313963	-1.775506

@mg11-isomer03 bp86/6-31G(d) Etot=-2200.971643 Eb=-11.69

Mg1	0.273300	1.192764	-1.591504
Mg2	2.514319	-0.194644	-0.000394
Mg3	-2.059442	-0.505823	-2.627744
Mg4	0.461339	-1.840243	-1.555748
Mg5	-0.814258	3.493590	0.000650
Mg6	5.704473	0.039276	-0.000003
Mg7	-2.253927	-2.034159	-0.000037
Mg8	0.461674	-1.840830	1.555532
Mg9	-2.501922	1.004103	0.000136
Mg10	0.273557	1.192196	1.591423
Mg11	-2.059113	-0.506230	2.627687

@mg11-isomer04 bp86/6-31G(d) Etot=-2200.971201 Eb=-11.66

Mg1	1.651459	1.114700	1.372063
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Mg2	1.040762	1.142748	-1.704690
Mg3	0.412253	3.530814	0.018088
Mg4	0.980081	-1.865819	-1.768253
Mg5	-1.369735	-1.871866	0.343824
Mg6	3.575913	-0.435661	-0.617413
Mg7	1.626387	-1.935857	1.258838
Mg8	-1.407921	1.188243	0.470715
Mg9	-0.482593	-0.467697	2.906084
Mg10	-1.639672	-0.298683	-2.208934
Mg11	-4.386933	-0.100921	-0.070324

@mg11-isomer05 bp86/6-31G(d) Etot=-2200.970553 Eb=-11.62

Mg1	4.204375	0.858703	0.388738
Mg2	1.965428	-1.105996	-0.160995
Mg3	-0.000074	-3.300215	-0.000176
Mg4	-1.965483	-1.105946	0.160998
Mg5	0.244908	-1.063812	2.406436
Mg6	1.695756	1.332856	-1.913767
Mg7	-1.695699	1.332773	1.913928
Mg8	1.187963	1.628107	1.126110
Mg9	-1.187878	1.628273	-1.125925
Mg10	-0.245007	-1.063560	-2.406459
Mg11	-4.204289	0.858817	-0.388888

@mg11-isomer06 bp86/6-31G(d) Etot=-2200.966341 Eb=-11.38

Mg1	-1.224769	-0.145272	-1.954697
Mg2	1.063408	-1.842566	-0.614856
Mg3	0.652582	2.040574	1.803478
Mg4	-1.766817	-2.241373	0.253811
Mg5	-0.833670	2.822194	-0.903386
Mg6	-1.892333	0.679472	0.986757
Mg7	3.874415	-0.838351	-1.466386
Mg8	0.143730	-1.000058	2.513552
Mg9	1.557077	1.128224	-1.316880
Mg10	-4.359241	-0.481846	-0.569641
Mg11	2.785618	-0.120998	1.268248

@mg11-isomer07 bp86/6-31G(d) Etot=-2200.966049 Eb=-11.37

Mg1	2.317663	2.690708	0.499653
Mg2	2.733761	-0.000115	-0.652892
Mg3	1.773206	0.000140	2.251767
Mg4	-0.395438	1.666918	0.755305
Mg5	0.622309	1.572714	-2.193726
Mg6	2.317643	-2.690777	0.500010
Mg7	0.622266	-1.572864	-2.193724
Mg8	-0.395351	-1.666669	0.755282
Mg9	-2.592714	0.000036	1.812610
Mg10	-1.897577	0.000022	-1.350124
Mg11	-5.105769	-0.000113	-0.184161

@mg11-isomer08 bp86/6-31G(d) Etot=-2200.965980 Eb=-11.36

Mg1	-0.645690	-0.548314	-3.001067
Mg2	0.352901	1.701299	-1.445873
Mg3	-5.100926	0.000106	-0.000029
Mg4	0.352306	-2.102744	-0.750681
Mg5	-0.646548	2.873012	1.024860
Mg6	2.606684	-1.354184	1.151556
Mg7	2.607275	1.673410	0.598158
Mg8	2.608112	-0.319716	-1.747092
Mg9	0.351296	0.401435	2.196181
Mg10	-1.838151	0.000203	-0.000766
Mg11	-0.647258	-2.324507	1.974755

@mg11-isomer09 bp86/6-31G(d) Etot=-2200.964741 Eb=-11.29

Mg1	-1.939463	2.015935	-1.791128
Mg2	1.046578	1.480416	-1.145337
Mg3	-1.168293	-0.775111	-1.320361
Mg4	-1.046576	1.480349	1.145340
Mg5	-1.738193	-1.396646	1.918900
Mg6	0.000059	-3.200455	-0.000060
Mg7	1.939435	2.015936	1.791155
Mg8	1.738227	-1.396574	-1.919032
Mg9	1.168368	-0.775179	1.320521
Mg10	-3.883594	0.275630	0.124189
Mg11	3.883452	0.275699	-0.124187

@mg11-isomer10 bp86/6-31G(d) Etot=-2200.962744 Eb=-11.18

Mg1	1.063830	1.519116	-0.487346
Mg2	-1.063758	-1.519558	-0.486318
Mg3	-2.016934	1.492594	0.507772
Mg4	2.016886	-1.492185	0.509007
Mg5	0.249596	2.985873	1.983224
Mg6	-0.000090	0.000954	2.387462
Mg7	-4.071306	-0.398347	-0.764473
Mg8	-0.249785	-2.984275	1.985572
Mg9	1.415852	-0.687502	-2.434833
Mg10	-1.415748	0.685651	-2.435435
Mg11	4.071456	0.397679	-0.764632

@mg11-isomer11 bp86/6-31G(d) Etot=-2200.962013 Eb=-11.14

Mg1	0.330033	-0.000039	1.054792
Mg2	1.015234	2.531241	-0.967123
Mg3	2.797493	-0.000100	-1.072960
Mg4	1.015239	-2.531460	-0.966519
Mg5	2.851583	-1.568758	1.536303
Mg6	-1.881696	-1.578957	-0.436855
Mg7	-1.881625	1.578790	-0.437374
Mg8	-2.481067	0.000443	2.202737
Mg9	2.851426	1.569221	1.535941
Mg10	0.030113	-0.000351	-2.502407
Mg11	-4.646731	-0.000030	0.053466

@mg11-isomer12 bp86/6-31G(d) Etot=-2200.960516 Eb=-11.05

Mg1	3.220196	1.765244	0.310933
Mg2	1.999156	-0.862380	1.045920
Mg3	0.591837	1.634938	2.179906
Mg4	2.858923	-0.255496	-2.025215
Mg5	0.560734	1.400009	-1.102294
Mg6	-1.208739	-0.669074	1.128973
Mg7	-4.573683	0.051002	-0.066953
Mg8	0.214617	-3.244232	1.484688
Mg9	-1.983101	2.112733	0.372986
Mg10	0.310531	-1.963976	-1.356394
Mg11	-1.990471	0.031233	-1.972550

@mg11-isomer13 bp86/6-31G(d) Etot=-2200.959324 Eb=-10.98

Mg1	2.278225	-1.559513	-1.737890
Mg2	4.544370	-0.022858	-0.158030
Mg3	1.428363	1.203961	-0.876311
Mg4	1.810007	-1.040041	1.293610
Mg5	-0.587129	-1.498387	-0.622872
Mg6	-0.036234	3.578365	0.342502
Mg7	-0.927391	-1.800231	2.533200
Mg8	-0.516652	1.083820	1.921686
Mg9	-3.080917	-0.979700	-2.252320
Mg10	-1.717373	1.520634	-1.204443
Mg11	-3.195270	-0.486050	0.760867

@mg11-isomer14 bp86/6-31G(d) Etot=-2200.958725 Eb=-10.95

Mg1	1.089197	0.000043	2.452550
Mg2	-0.029698	2.562493	1.078823
Mg3	2.810990	-1.555305	0.217798
Mg4	-0.029746	-2.562453	1.078902
Mg5	2.811021	1.555324	0.217701
Mg6	-4.620554	-0.000029	-0.311830
Mg7	3.245130	-0.000115	-2.367212
Mg8	0.520701	0.000039	-1.127996
Mg9	-2.046218	1.590511	-1.296198
Mg10	-2.046190	-1.590511	-1.296171
Mg11	-1.704635	0.000005	1.353634

@mg11-isomer15 bp86/6-31G(d) Etot=-2200.957278 Eb=-10.87

Mg1	-0.998891	0.000119	-1.548712
Mg2	-3.697826	-1.511876	-0.000143
Mg3	-3.697621	1.512027	-0.000057
Mg4	-0.998796	0.000035	1.549021
Mg5	1.763207	1.676013	-1.535266
Mg6	1.763094	-1.676176	1.535129
Mg7	3.858502	-0.000136	-0.000082
Mg8	1.763268	1.676012	1.535106
Mg9	1.762967	-1.676109	-1.535195
Mg10	-0.758808	2.630613	0.000149
Mg11	-0.759096	-2.630522	0.000049

@mg11-isomer16 bp86/6-31G(d) Etot=-2200.956095 Eb=-10.80

Mg1	-0.716506	1.093847	-1.519517
Mg2	-0.716121	0.768858	1.707393
Mg3	1.979451	1.881758	0.189641
Mg4	-0.716091	-1.863623	-0.187417
Mg5	1.844473	1.428679	3.172660
Mg6	1.844053	2.033494	-2.823678
Mg7	1.979575	-0.776183	-1.724289
Mg8	1.845197	-3.461606	-0.349277
Mg9	-6.245628	0.000142	-0.000001
Mg10	-3.078397	-0.000652	0.000185
Mg11	1.979993	-1.104714	1.534299

@mg11-isomer17 bp86/6-31G(d) Etot=-2200.954692 Eb=-10.72

Mg1	-0.979842	-0.341520	-1.257050
Mg2	2.062182	0.669750	-1.602104
Mg3	-3.932236	-1.073552	-0.135092
Mg4	-0.000012	2.440004	-0.000040
Mg5	-2.062038	0.669713	1.602087
Mg6	-1.255831	-2.458305	0.994017
Mg7	3.164314	1.983718	0.881427
Mg8	1.255856	-2.458302	-0.994101
Mg9	0.979886	-0.341689	1.257053
Mg10	-3.164473	1.983677	-0.881335
Mg11	3.932194	-1.073493	0.135139

@mg11-isomer18 bp86/6-31G(d) Etot=-2200.953208 Eb=-10.64

Mg1	0.560279	0.039680	-0.000077
Mg2	3.176222	0.373815	-1.537858
Mg3	0.759182	-1.504050	2.660508
Mg4	-1.602209	2.281094	-0.000327
Mg5	-1.960156	-0.313983	1.714187
Mg6	1.680498	2.752079	-0.000537
Mg7	-1.960139	-0.314385	-1.714187
Mg8	-0.190620	-2.833053	0.000596
Mg9	-4.398359	0.649452	-0.000102
Mg10	3.176177	0.374555	1.537728
Mg11	0.759124	-1.505205	-2.659931

@mg11-isomer19 bp86/6-31G(d) Etot=-2200.952052 Eb=-10.57

Mg1	-0.367957	-0.538395	1.452204
Mg2	-2.681514	1.743837	0.405453
Mg3	0.294740	-2.465955	-0.850918
Mg4	-0.368151	0.538437	-1.452399
Mg5	-2.680959	-1.743863	-0.405556
Mg6	2.344913	-2.201900	1.420705
Mg7	-5.046654	-0.000444	0.000135
Mg8	2.344836	2.201953	-1.420598
Mg9	2.932946	0.865955	1.276485
Mg10	0.294217	2.466120	0.850533
Mg11	2.933584	-0.865744	-1.276045

@mg11-isomer20 bp86/6-31G(d) Etot=-2200.951423 Eb=-10.53

Mg1	-0.523084	-0.000014	1.158405
Mg2	1.984103	-2.137854	0.488846
Mg3	-3.475596	1.493406	-0.149711
Mg4	-1.042679	2.938955	1.139953
Mg5	-1.042538	-2.938984	1.140005
Mg6	-3.475491	-1.493487	-0.149697
Mg7	1.984003	2.137900	0.488921
Mg8	-0.460057	-1.657875	-1.507062
Mg9	-0.460069	1.657844	-1.507061
Mg10	2.348180	0.000038	-1.766444
Mg11	4.163228	0.000070	0.663846

@mg11-isomer21 bp86/6-31G(d) Etot=-2200.951349 Eb=-10.53

Mg1	-1.651422	-2.679504	-0.416900
Mg2	0.956799	-2.651442	1.393538
Mg3	-0.058260	1.720478	-1.330414
Mg4	-3.111380	1.801134	-0.369573
Mg5	-4.176325	-0.980337	-0.270602
Mg6	-0.725957	2.775300	1.451236
Mg7	0.920524	-1.380353	-1.381102
Mg8	-0.882894	-0.196415	1.100242
Mg9	3.014939	0.916450	-1.755531
Mg10	2.187720	1.724454	1.014967
Mg11	3.526254	-1.049764	0.564139

@mg11-isomer22 bp86/6-31G(d) Etot=-2200.950094 Eb=-10.46

Mg1	1.297092	1.601728	-0.485864
Mg2	0.297514	-1.494975	-1.285658
Mg3	4.150331	1.416905	0.718017
Mg4	-0.971779	-0.001117	1.246023
Mg5	-0.632586	-2.973196	1.230575
Mg6	2.131208	-1.093379	1.256000
Mg7	-1.601388	1.068057	-1.679578
Mg8	-2.877407	-1.808966	-0.675401
Mg9	-1.349556	2.940716	0.708988
Mg10	3.506685	-0.701569	-1.396296
Mg11	-3.950115	1.045798	0.363194

@mg11-isomer23 bp86/6-31G(d) Etot=-2200.949547 Eb=-10.43

Mg1	-1.769972	1.525710	0.814825
Mg2	1.270430	1.926481	1.655517
Mg3	-1.941714	-0.638848	-1.489505
Mg4	0.655434	1.310297	-1.230292
Mg5	3.116718	-0.337589	0.125078
Mg6	-0.048589	-1.126962	0.987702
Mg7	-4.516772	1.127926	-0.511695
Mg8	3.369870	2.643071	-0.531500
Mg9	1.056481	-1.977319	-1.738738
Mg10	-3.470160	-1.317323	1.068632

Mg11	2.278274	-3.135443	0.849978
@mg11-isomer24 bp86/6-31G(d) Etot=-2200.949192 Eb=-10.41			
Mg1	-0.190674	1.888091	1.346198
Mg2	-1.303908	0.457103	-1.285998
Mg3	-3.453136	1.653390	0.487928
Mg4	4.220462	-1.358650	0.114995
Mg5	2.977559	1.482798	0.591351
Mg6	-0.510242	-2.589434	-0.668078
Mg7	-1.752084	-0.881246	1.543543
Mg8	1.749541	-0.540029	-1.538713
Mg9	-3.950756	-1.395459	-0.613406
Mg10	0.885186	2.604887	-1.402983
Mg11	1.328053	-1.321451	1.425163
@mg11-isomer25 bp86/6-31G(d) Etot=-2200.948905 Eb=-10.39			
Mg1	1.852098	0.477198	-1.345505
Mg2	-1.376244	-0.500360	-1.356207
Mg3	-4.528434	-1.165099	-0.339236
Mg4	-0.494507	2.550854	-1.135528
Mg5	3.711069	-2.081516	-0.992556
Mg6	3.141415	-0.171013	1.347274
Mg7	-3.191824	1.537908	0.324750
Mg8	-0.081291	0.673164	1.247510
Mg9	0.858617	-2.237595	0.173640
Mg10	2.123220	2.756682	0.761065
Mg11	-2.014120	-1.840222	1.314792
@mg11-isomer26 bp86/6-31G(d) Etot=-2200.948903 Eb=-10.39			
Mg1	-0.887889	2.469068	-0.337475
Mg2	-0.097686	0.221249	1.591002
Mg3	3.429198	-0.152150	1.033809
Mg4	1.680209	1.043651	-1.231067
Mg5	-3.820124	1.534435	-0.987019
Mg6	1.339682	-2.219547	0.041832
Mg7	-4.152976	-1.239310	0.231191
Mg8	3.500520	-1.241183	-1.882694
Mg9	-1.236866	-0.609434	-1.171909
Mg10	-1.493918	-2.450789	1.257198
Mg11	1.739852	2.644010	1.455131
@mg11-isomer27 bp86/6-31G(d) Etot=-2200.947679 Eb=-10.32			
Mg1	-3.442055	-1.779548	0.488111
Mg2	-1.397364	0.972845	1.008800
Mg3	2.794297	-1.335452	-1.323546
Mg4	0.618974	1.226383	-1.374464
Mg5	-2.401486	0.050442	-1.749101
Mg6	-0.242397	-1.812443	-0.409381
Mg7	1.124460	2.914224	1.133122
Mg8	-4.543085	1.125100	0.234121
Mg9	2.125428	-3.085114	1.116464
Mg10	1.806442	-0.085588	1.348050
Mg11	3.556785	1.809152	-0.472176
@mg11-isomer28 bp86/6-31G(d) Etot=-2200.946740 Eb=-10.27			
Mg1	-1.209714	-2.611405	0.873708
Mg2	-0.138286	0.000642	2.020178
Mg3	3.007800	0.000592	2.179972
Mg4	1.505112	-1.744917	-0.227770
Mg5	-3.857733	-1.537497	-0.397630
Mg6	1.505203	1.744708	-0.228586
Mg7	-3.857856	1.537177	-0.397978
Mg8	3.864004	-0.000313	-0.861644
Mg9	-1.091705	-0.000245	-0.957218

Mg10	-1.209665	2.611981	0.872219	
Mg11	1.482840	-0.000723	-2.875251	
@mg11-isomer29 bp86/6-31G(d) Etot=-2200.945397 Eb=-10.19				
Mg1	-3.327321	2.118718	-0.324275	
Mg2	-0.366160	-2.555755	0.582558	
Mg3	-3.327249	-2.118865	-0.324242	
Mg4	2.874354	-2.970310	0.750897	
Mg5	-1.109082	-0.000034	-1.239262	
Mg6	1.632061	1.617497	-1.712748	
Mg7	1.415178	0.000028	0.980226	
Mg8	2.874208	2.970392	0.750928	
Mg9	-1.931850	-0.000027	1.666094	
Mg10	-0.366285	2.555746	0.582573	
Mg11	1.632146	-1.617388	-1.712749	
@mg11-isomer30 bp86/6-31G(d) Etot=-2200.945197 Eb=-10.18				
Mg1	2.283249	3.259014	-0.550159	
Mg2	-0.140612	2.480767	1.493284	
Mg3	-3.136139	1.413067	0.176885	
Mg4	2.133840	0.505329	0.656996	
Mg5	-0.236423	1.464068	-1.329849	
Mg6	-0.976449	-0.717600	1.007406	
Mg7	-4.228251	-1.537461	0.561532	
Mg8	1.658016	-2.438707	1.490264	
Mg9	-2.299470	-0.959578	-1.743026	
Mg10	4.055744	-1.792952	-0.395432	
Mg11	0.886495	-1.675946	-1.367901	
@mg11-isomer31 bp86/6-31G(d) Etot=-2200.945192 Eb=-10.18				
Mg1	-1.781471	-1.083281	-1.093930	
Mg2	-2.406817	-0.057474	1.706078	
Mg3	2.237291	2.889716	1.309189	
Mg4	0.321370	-1.868552	1.166904	
Mg5	-3.363433	1.832931	-0.564924	
Mg6	2.448039	2.024604	-1.634795	
Mg7	-4.778523	-0.859663	-0.120763	
Mg8	3.029928	-3.038050	0.172281	
Mg9	3.026236	0.036919	0.686369	
Mg10	-0.075463	1.342246	0.025977	
Mg11	1.342843	-1.219395	-1.652386	
@mg11-isomer32 bp86/6-31G(d) Etot=-2200.944921 Eb=-10.16				
Mg1	-0.303885	-0.236971	-0.505917	
Mg2	-0.966483	2.081438	1.692212	
Mg3	2.091323	1.430123	1.030924	
Mg4	2.653329	0.343059	-1.749206	
Mg5	2.116688	-2.223853	0.233457	
Mg6	-3.107591	1.583598	-0.512317	
Mg7	-0.952955	-3.016718	0.218739	
Mg8	-3.261201	-1.447737	-1.307902	
Mg9	0.042347	2.669836	-1.149186	
Mg10	4.479838	-0.459878	0.494094	
Mg11	-2.791409	-0.722897	1.555101	
@mg11-isomer33 bp86/6-31G(d) Etot=-2200.944805 Eb=-10.16				
Mg1	0.000025	-1.140136	-1.225870	
Mg2	-2.689059	-2.603043	-0.342008	
Mg3	2.689071	-2.603009	-0.342080	
Mg4	1.652192	-0.059730	1.339470	
Mg5	0.000062	-2.757107	1.389225	
Mg6	-2.572439	0.644130	-1.506782	
Mg7	-3.023827	2.919121	0.583334	
Mg8	-1.652091	-0.059749	1.339487	

Mg9	-0.000034	2.096055	-0.311332
Mg10	3.023698	2.919182	0.583408
Mg11	2.572402	0.644286	-1.506852
@mg11-isomer34 bp86/6-31G(d) Etot=-2200.944316 Eb=-10.13			
Mg1	-0.253965	2.113001	-0.895719
Mg2	-1.867448	-0.612741	-1.571782
Mg3	-3.510614	1.970506	-0.536870
Mg4	1.300465	1.752931	1.775421
Mg5	-1.530535	-2.803263	0.572084
Mg6	3.680544	-0.480263	1.422892
Mg7	-1.441814	0.368178	1.323053
Mg8	0.991380	-1.113742	-0.125248
Mg9	2.969585	1.419217	-0.871683
Mg10	3.824430	-1.496377	-1.457840
Mg11	-4.162028	-1.117449	0.365694
@mg11-isomer35 bp86/6-31G(d) Etot=-2200.943623 Eb=-10.09			
Mg1	-3.323291	0.386242	1.721824
Mg2	-2.594704	1.024892	-1.164300
Mg3	1.121675	-2.341680	-0.116941
Mg4	-0.127819	0.567250	0.866676
Mg5	-1.911700	-1.930226	0.047736
Mg6	4.104097	-2.079618	-0.776160
Mg7	-4.792696	-1.145982	-0.470008
Mg8	2.153747	2.674912	0.982225
Mg9	2.253697	0.481315	-1.262155
Mg10	0.067992	2.702341	-1.400365
Mg11	3.049002	-0.339444	1.571468
@mg11-isomer36 bp86/6-31G(d) Etot=-2200.943252 Eb=-10.07			
Mg1	-1.596652	1.457028	-1.581331
Mg2	-1.596893	1.457132	1.581048
Mg3	-5.457336	-2.421795	-0.000022
Mg4	-0.000333	3.567644	-0.000100
Mg5	-2.631595	-0.979282	-0.000160
Mg6	1.596463	1.457464	1.581322
Mg7	0.000336	-1.297571	-1.573402
Mg8	1.596719	1.457387	-1.581096
Mg9	0.000048	-1.297499	1.573615
Mg10	2.631886	-0.978698	0.000286
Mg11	5.457358	-2.421811	-0.000159
@mg11-isomer37 bp86/6-31G(d) Etot=-2200.942870 Eb=-10.05			
Mg1	0.550910	1.595596	0.057868
Mg2	3.144918	2.456078	-1.358166
Mg3	-3.969278	-1.347355	-0.549927
Mg4	-4.571690	1.532699	0.633235
Mg5	-0.364963	-1.503366	-0.977458
Mg6	-2.259882	1.162808	-1.353002
Mg7	2.928206	-0.554225	-0.785907
Mg8	1.170686	-1.286623	1.698811
Mg9	3.238966	1.494498	1.576803
Mg10	-1.839103	-0.110623	1.402115
Mg11	1.971229	-3.439487	-0.344372
@mg11-isomer38 bp86/6-31G(d) Etot=-2200.942491 Eb=-10.02			
Mg1	-3.847324	2.034173	-1.197840
Mg2	-1.529841	-0.056230	-1.269368
Mg3	-3.624006	-0.231528	0.987247
Mg4	-2.089431	-2.966486	-0.054266
Mg5	-1.633800	2.201471	0.924574
Mg6	0.899256	-1.905911	-0.993772
Mg7	1.236235	1.317645	-0.115986

Mg8	-0.437293	-0.976470	1.556806
Mg9	4.345709	1.775877	0.533901
Mg10	3.015477	-0.940296	1.257796
Mg11	3.665018	-0.252245	-1.629093
@mg11-isomer39 bp86/6-31G(d) Etot=-2200.941653 Eb=-9.98			
Mg1	-1.992321	-3.513968	-0.258363
Mg2	-0.390155	-1.643126	1.676536
Mg3	2.890517	-0.947280	1.172925
Mg4	-2.009658	-0.544812	-0.821429
Mg5	0.811207	-1.925879	-1.093798
Mg6	0.963509	1.169799	-0.032573
Mg7	4.141355	1.891434	0.583809
Mg8	-1.637952	2.539916	-1.193566
Mg9	3.332194	-0.005979	-1.665767
Mg10	-4.368253	1.533667	-0.013545
Mg11	-1.740444	1.446228	1.645773
@mg11-isomer40 bp86/6-31G(d) Etot=-2200.941612 Eb=-9.97			
Mg1	1.237406	-2.474131	1.730754
Mg2	3.173948	-2.782684	-0.715509
Mg3	1.659473	-0.000066	0.000138
Mg4	-0.216012	-2.308803	-1.013299
Mg5	-1.413662	-0.699869	1.399081
Mg6	3.174208	2.782561	0.715471
Mg7	-3.611806	-1.438299	-0.647085
Mg8	-1.413617	0.700018	-1.399059
Mg9	-3.611802	1.438527	0.647042
Mg10	1.237692	2.473854	-1.730802
Mg11	-0.215827	2.308893	1.013268
@mg11-isomer41 bp86/6-31G(d) Etot=-2200.940797 Eb=-9.93			
Mg1	-3.744955	-2.251882	0.000069
Mg2	-2.167711	0.000036	1.446614
Mg3	-0.647720	2.738388	0.000005
Mg4	3.595606	-0.000035	1.465763
Mg5	2.558092	-2.572003	0.000044
Mg6	-2.167803	-0.000079	-1.446575
Mg7	-3.744920	2.251869	-0.000044
Mg8	3.595611	-0.000030	-1.465791
Mg9	0.813368	0.000036	-0.000042
Mg10	2.558145	2.571981	0.000015
Mg11	-0.647713	-2.738281	-0.000057
@mg11-isomer42 bp86/6-31G(d) Etot=-2200.940623 Eb=-9.92			
Mg1	-0.498977	-1.589706	1.573989
Mg2	-2.939454	-2.621995	0.000051
Mg3	-3.276758	-0.000016	-1.583418
Mg4	1.629906	-0.000017	-0.000005
Mg5	4.730423	-0.000055	0.000044
Mg6	-0.498964	-1.589795	-1.573972
Mg7	-0.498954	1.589700	-1.574022
Mg8	-0.498944	1.589777	1.573966
Mg9	-2.939403	2.622022	-0.000046
Mg10	-3.276764	0.000053	1.583431
Mg11	8.067889	0.000034	-0.000018
@mg11-isomer43 bp86/6-31G(d) Etot=-2200.940326 Eb=-9.90			
Mg1	2.691197	2.693899	-0.048940
Mg2	1.351183	0.000010	-1.327570
Mg3	-0.443591	1.853687	0.455890
Mg4	1.962059	-0.000009	1.546622
Mg5	-2.285473	0.000010	-1.482531
Mg6	-3.326767	2.785731	-0.239480

Mg7	4.371929	0.000024	-0.334254
Mg8	-3.241466	-0.000016	1.262821
Mg9	-0.443563	-1.853697	0.455881
Mg10	-3.326730	-2.785751	-0.239513
Mg11	2.691224	-2.693888	-0.048927
@mg11-isomer44 bp86/6-31G(d) Etot=-2200.939320 Eb=-9.84			
Mg1	0.917871	-1.669928	0.551936
Mg2	0.671683	1.001727	-1.064429
Mg3	1.313766	1.167468	1.951577
Mg4	3.543151	0.108135	0.204842
Mg5	-0.969748	3.156288	0.640156
Mg6	6.422807	-0.722093	-0.974584
Mg7	-1.467928	-1.450859	-1.541025
Mg8	-1.672063	0.284845	1.136732
Mg9	-2.379176	1.553263	-1.691285
Mg10	-2.034403	-2.689933	1.224280
Mg11	-4.345960	-0.738912	-0.438199
@mg11-isomer45 bp86/6-31G(d) Etot=-2200.938732 Eb=-9.81			
Mg1	4.114646	-1.175732	-0.367579
Mg2	1.348401	-0.897651	-2.259602
Mg3	2.840664	1.599045	-0.551833
Mg4	1.243435	-0.687391	0.865703
Mg5	3.856837	0.517763	2.175561
Mg6	-1.182049	-1.868648	-0.840563
Mg7	-0.533426	1.284209	-1.296025
Mg8	-1.882401	0.304216	1.583177
Mg9	-3.455508	-2.383644	1.187512
Mg10	-2.582975	3.071276	0.158955
Mg11	-3.767626	0.236557	-0.655304
@mg11-isomer46 bp86/6-31G(d) Etot=-2200.938458 Eb=-9.79			
Mg1	-6.104709	0.228475	0.466693
Mg2	-2.934977	0.105397	0.288621
Mg3	-1.009472	0.137868	-2.104068
Mg4	1.519098	2.097546	-1.676310
Mg5	1.982577	-1.035125	-1.107081
Mg6	1.507115	-4.060357	-0.284418
Mg7	-0.786016	-2.104842	0.125641
Mg8	-0.106182	1.024812	0.828132
Mg9	1.193839	4.094257	0.674979
Mg10	1.832711	-1.689425	1.843304
Mg11	2.906016	1.201395	0.944509
@mg11-isomer47 bp86/6-31G(d) Etot=-2200.938107 Eb=-9.77			
Mg1	5.957117	-1.513828	0.636831
Mg2	3.003993	-0.416666	0.121739
Mg3	0.497159	-2.005843	-1.316938
Mg4	2.014153	2.568398	0.709835
Mg5	0.125907	0.153500	1.063144
Mg6	1.108841	1.026589	-1.799417
Mg7	-1.925253	-2.193775	0.839905
Mg8	-1.070482	2.816145	-0.368638
Mg9	-1.952272	-0.021287	-1.391298
Mg10	-2.905825	0.862684	1.405250
Mg11	-4.853340	-1.275915	0.099587
@mg11-isomer48 bp86/6-31G(d) Etot=-2200.937683 Eb=-9.75			
Mg1	1.858237	0.550741	-1.207038
Mg2	-0.129792	1.896986	1.056362
Mg3	0.404481	-1.266975	1.065223
Mg4	-1.348453	0.060493	-1.209718
Mg5	3.579784	-1.854750	-0.048270

Mg6	3.106549	0.781530	1.492675
Mg7	-3.134575	2.488065	-0.313601
Mg8	-4.412663	-0.438460	-1.085466
Mg9	-2.290083	-2.783581	-0.020859
Mg10	-2.639183	-0.089631	1.480974
Mg11	5.005698	0.655584	-1.210285

@mg11-isomer49 bp86/6-31G(d) Etot=-2200.937580 Eb=-9.74

Mg1	2.593043	2.031446	-1.464839
Mg2	-1.289486	-1.324875	-1.789263
Mg3	1.903155	-1.014345	-1.087441
Mg4	-0.274103	1.497052	-0.643174
Mg5	1.457545	4.139622	0.532883
Mg6	0.522618	-3.792137	-0.489013
Mg7	-2.901332	0.315699	0.329831
Mg8	2.109364	0.924143	1.375972
Mg9	-0.447333	-1.267773	1.201735
Mg10	-6.045007	0.797162	0.400006
Mg11	2.371535	-2.305995	1.633303

@mg11-isomer50 bp86/6-31G(d) Etot=-2200.937102 Eb=-9.72

Mg1	1.224942	2.343583	0.508206
Mg2	-0.000032	0.000002	2.294988
Mg3	3.382462	1.220260	-1.632528
Mg4	3.610128	0.421731	1.294400
Mg5	-1.366416	0.970011	-0.352674
Mg6	1.366439	-0.970050	-0.352629
Mg7	4.344805	-1.656053	-0.964903
Mg8	-1.224954	-2.343594	0.508183
Mg9	-3.610136	-0.421732	1.294376
Mg10	-3.382471	-1.220239	-1.632530
Mg11	-4.344766	1.656082	-0.964889

@mg11-isomer51 bp86/6-31G(d) Etot=-2200.936849 Eb=-9.70

Mg1	-4.057344	0.767244	1.101304
Mg2	-4.098312	0.623861	-1.993703
Mg3	-1.266954	-0.645931	2.305643
Mg4	-2.943768	-1.698515	-0.284201
Mg5	-1.341549	1.033089	-0.441377
Mg6	1.263959	1.008154	1.445187
Mg7	0.482913	-1.639325	-0.074752
Mg8	1.584139	1.487375	-1.577987
Mg9	3.725414	-0.323004	-0.317005
Mg10	3.054256	-3.327339	-0.491460
Mg11	3.597247	2.714392	0.328350

@mg11-isomer52 bp86/6-31G(d) Etot=-2200.936791 Eb=-9.70

Mg1	-0.000009	0.667491	0.000080
Mg2	2.439336	-1.073153	0.973413
Mg3	-2.841112	2.031658	-0.909714
Mg4	-5.392615	0.408803	-0.117941
Mg5	-2.439311	-1.073138	-0.973467
Mg6	-0.593570	-2.101352	1.416621
Mg7	-2.808875	0.400213	1.692576
Mg8	0.593610	-2.101261	-1.416667
Mg9	2.808804	0.400344	-1.692580
Mg10	2.841152	2.031640	0.909820
Mg11	5.392590	0.408754	0.117857

@mg11-isomer53 bp86/6-31G(d) Etot=-2200.936572 Eb=-9.69

Mg1	4.570964	0.000029	0.000049
Mg2	2.574960	2.604145	0.030758
Mg3	1.768175	0.018462	-1.564573
Mg4	2.574923	-2.604180	-0.030750

Mg5	1.768163	-0.018484	1.564584
Mg6	-0.487681	-1.577304	-0.018668
Mg7	-1.280038	0.030900	-2.607806
Mg8	-1.280051	-0.030911	2.607766
Mg9	-0.487644	1.577319	0.018622
Mg10	-3.224239	-0.000001	-0.000053
Mg11	-6.497532	0.000026	0.000071

@mg11-isomer54 bp86/6-31G(d) Etot=-2200.936305 Eb=-9.67

Mg1	-0.463939	-0.943776	-0.764717
Mg2	2.396171	0.766373	-1.167025
Mg3	-3.685690	-2.096187	-0.043605
Mg4	-3.422140	0.507990	-1.588937
Mg5	-0.521257	2.108100	-0.763742
Mg6	-2.332769	0.421216	1.320850
Mg7	5.330326	-0.484267	-1.074890
Mg8	0.949010	0.590832	1.520043
Mg9	2.922763	-1.834954	0.371525
Mg10	4.299600	0.663372	1.505794
Mg11	-5.472077	0.301301	0.684703

@mg11-isomer55 bp86/6-31G(d) Etot=-2200.936014 Eb=-9.65

Mg1	-4.046294	-2.367869	0.417802
Mg2	-1.019386	-1.962452	0.212331
Mg3	4.196012	-0.914748	-1.158688
Mg4	1.890748	-1.077299	0.889527
Mg5	4.651222	0.203216	1.771749
Mg6	0.716424	-0.550894	-2.003304
Mg7	-2.713532	0.147229	-1.413254
Mg8	-2.833581	3.041188	-0.173893
Mg9	2.893962	1.693252	-0.309764
Mg10	-3.390582	0.500131	1.490688
Mg11	-0.344994	1.288247	0.276807

@mg11-isomer56 bp86/6-31G(d) Etot=-2200.934422 Eb=-9.56

Mg1	-1.373157	0.399440	1.050915
Mg2	-3.976050	2.040736	0.727041
Mg3	1.076152	-1.533309	0.688535
Mg4	-2.143709	1.615058	-1.744944
Mg5	-1.782727	-2.866170	0.887856
Mg6	6.694344	0.141737	-0.957122
Mg7	3.781439	0.112899	0.437637
Mg8	1.503164	1.216420	2.130510
Mg9	1.003961	1.144717	-0.913523
Mg10	-3.833682	-0.747038	-0.593318
Mg11	-0.949736	-1.524489	-1.713586

@mg11-isomer57 bp86/6-31G(d) Etot=-2200.931479 Eb=-9.40

Mg1	-1.762978	-2.010530	1.464892
Mg2	1.127549	-0.987274	0.933585
Mg3	3.921403	0.315002	-0.018137
Mg4	-3.817779	0.591903	1.753335
Mg5	-1.258301	0.905679	-0.047810
Mg6	1.584528	2.133310	0.712194
Mg7	7.094139	-0.157759	0.248834
Mg8	-3.648517	-0.996871	-0.861856
Mg9	1.428727	0.397377	-1.795909
Mg10	-4.023907	2.029046	-0.953426
Mg11	-0.644864	-2.219883	-1.435701

@mg11-isomer58 bp86/6-31G(d) Etot=-2200.930545 Eb=-9.34

Mg1	-0.024964	-2.227929	1.626456
Mg2	0.632695	0.729104	1.527514
Mg3	-1.674415	-0.305781	-0.291772

Mg4	3.109374	-1.604673	1.246936
Mg5	1.062222	-1.283489	-1.151382
Mg6	-4.775042	-0.137816	-0.220080
Mg7	1.999366	3.379482	0.981330
Mg8	3.342403	1.065836	-0.467590
Mg9	-8.103753	-0.002336	-0.230155
Mg10	0.398380	1.990402	-1.321251
Mg11	4.033734	-1.602800	-1.700007

@mg11-isomer59 bp86/6-31G(d) Etot=-2200.930488 Eb=-9.34

Mg1	6.228857	-0.090449	0.000792
Mg2	1.542075	1.837650	-0.000872
Mg3	-1.376784	3.160582	-0.000082
Mg4	3.420178	-0.063619	-1.470542
Mg5	-3.831824	-1.011042	1.464484
Mg6	-4.145840	1.676293	0.000099
Mg7	-1.597102	-2.766864	-0.000270
Mg8	-1.208893	0.154347	-0.000782
Mg9	3.419191	-0.063245	1.470735
Mg10	-3.833447	-1.011804	-1.463041
Mg11	1.383589	-1.821848	-0.000520

@mg11-isomer60 bp86/6-31G(d) Etot=-2200.929657 Eb=-9.29

Mg1	0.457435	0.636718	-1.264104
Mg2	3.074239	-0.648744	-0.059363
Mg3	2.760058	2.646870	-0.370337
Mg4	-2.346745	-1.314140	-1.635634
Mg5	-4.959889	-0.076138	-0.380928
Mg6	-0.042263	-1.765227	0.613782
Mg7	5.635630	-2.629277	-0.186527
Mg8	1.056932	1.028454	1.599311
Mg9	-2.090349	0.933405	0.575346
Mg10	-3.270782	-2.292347	1.018325
Mg11	-0.274267	3.480426	0.090129

@mg11-isomer61 bp86/6-31G(d) Etot=-2200.929601 Eb=-9.29

Mg1	0.930942	-1.023645	1.060705
Mg2	1.103266	1.338038	-1.056695
Mg3	-2.189497	-1.699670	1.580038
Mg4	2.349951	1.649531	1.790315
Mg5	-1.520363	-0.551748	-1.212742
Mg6	-4.068448	0.446720	0.177567
Mg7	-3.966111	-2.509413	-0.884311
Mg8	3.679349	-0.272415	-0.231748
Mg9	-1.065887	1.520040	1.192344
Mg10	-1.840228	2.579146	-1.523202
Mg11	6.587026	-1.476583	-0.892272

@mg11-isomer62 bp86/6-31G(d) Etot=-2200.929151 Eb=-9.26

Mg1	-4.635464	0.858418	1.036753
Mg2	-1.594668	0.903815	0.252443
Mg3	0.450001	-1.577253	1.458407
Mg4	2.789165	-1.815316	-0.743162
Mg5	0.000022	3.633696	0.000013
Mg6	-2.789273	-1.815244	0.743388
Mg7	3.723183	-0.186198	1.779716
Mg8	-3.722990	-0.186501	-1.779828
Mg9	4.635348	0.858165	-1.037173
Mg10	-0.449975	-1.577444	-1.458131
Mg11	1.594652	0.903862	-0.252426

@mg11-isomer63 bp86/6-31G(d) Etot=-2200.929096 Eb=-9.26

Mg1	0.060556	-1.369920	0.000400
Mg2	-1.508365	1.040403	1.524264

Mg3	-1.508347	1.039809	-1.524523
Mg4	-2.968940	-1.264127	0.000159
Mg5	1.332101	1.784551	-0.000299
Mg6	1.340708	-0.033080	2.630713
Mg7	-1.000390	3.758594	-0.000622
Mg8	2.981141	-0.689743	0.000254
Mg9	5.911983	-1.876326	-0.000042
Mg10	1.340650	-0.034419	-2.630488
Mg11	-5.981097	-2.355742	0.000184

@mg11-isomer64 bp86/6-31G(d) Etot=-2200.924178 Eb=-8.98

Mg1	-0.986077	-1.218976	-0.977344
Mg2	0.812566	0.934372	0.729472
Mg3	-2.287916	0.323371	1.407086
Mg4	2.210674	-1.857125	-0.319667
Mg5	3.776911	0.786338	-0.110498
Mg6	0.149464	-4.111393	-0.560119
Mg7	6.590065	2.407159	-0.216219
Mg8	-0.100413	-2.115463	1.747116
Mg9	-4.156162	0.073735	-1.137504
Mg10	-4.309013	2.728178	0.464858
Mg11	-1.700098	2.049805	-1.027180

@mg11-isomer65 bp86/6-31G(d) Etot=-2200.920944 Eb=-8.79

Mg1	-0.966071	0.000077	1.149094
Mg2	1.406672	1.557115	-0.115369
Mg3	1.406756	-1.557120	-0.115047
Mg4	-1.060895	-0.000197	-1.873879
Mg5	-3.708982	-0.000189	-0.480222
Mg6	4.195014	0.000198	0.488876
Mg7	-6.813311	0.000158	0.413361
Mg8	6.959533	-0.000145	-1.147956
Mg9	1.991329	0.000291	2.512276
Mg10	-1.704957	-2.648724	-0.415343
Mg11	-1.705088	2.648536	-0.415791

@mg11-isomer66 bp86/6-31G(d) Etot=-2200.914179 Eb=-8.41

Mg1	2.239216	0.365805	0.000568
Mg2	5.328618	0.863759	0.000202
Mg3	-0.692816	1.157111	0.000282
Mg4	-2.676755	-1.470795	-0.000263
Mg5	-3.407258	1.116133	1.504472
Mg6	-3.406868	1.116474	-1.504600
Mg7	8.627169	1.368017	-0.000405
Mg8	0.329107	-1.646183	-1.450564
Mg9	0.328725	-1.646437	1.450796
Mg10	-1.068204	-4.086814	-0.000326
Mg11	-5.600934	2.862930	-0.000163

@mg11-isomer67 bp86/6-31G(d) Etot=-2200.913080 Eb=-8.35

Mg1	1.131380	-0.145097	-0.176536
Mg2	-1.536368	-1.591281	-0.544317
Mg3	-1.330623	0.927749	1.473795
Mg4	-4.151842	0.543780	-0.166638
Mg5	4.227526	-0.135729	-0.042163
Mg6	-1.086018	1.689419	-1.379679
Mg7	-3.733445	-1.939602	1.663427
Mg8	-3.075752	3.373784	0.385516
Mg9	6.915196	-0.521516	1.693368
Mg10	-4.424225	-2.255652	-1.352024
Mg11	7.064170	0.054143	-1.554749

@mg11-isomer68 bp86/6-31G(d) Etot=-2200.912731 Eb=-8.33

Mg1	0.136592	2.247274	-0.062785
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Mg2	-0.220787	-0.758684	0.866519
Mg3	2.509932	0.384263	-0.234672
Mg4	-2.453855	-2.074170	-1.052238
Mg5	5.535349	-0.297456	0.116225
Mg6	-2.647470	3.733854	0.459645
Mg7	8.830657	-0.736071	0.397734
Mg8	0.063829	-0.074142	-2.041341
Mg9	-2.955647	0.712942	-0.098571
Mg10	-5.526376	-1.485011	-0.223851
Mg11	-3.272225	-1.652799	1.873333

@mg12-isomer01 bp86/6-31G(d) Etot=-2401.066331 Eb=-12.02

Mg1	-0.672502	-2.280994	0.000198
Mg2	0.614792	0.124786	1.540187
Mg3	0.614649	0.124624	-1.540175
Mg4	-2.132062	1.662410	-1.560147
Mg5	-2.131966	1.662585	1.559882
Mg6	-1.885657	-1.201621	2.636851
Mg7	0.261287	2.718138	-0.000189
Mg8	-1.885696	-1.202053	-2.636602
Mg9	2.328892	-2.055131	-0.000070
Mg10	-3.337754	-0.699793	0.000072
Mg11	4.977826	-0.645521	0.000018
Mg12	3.248190	1.792570	-0.000024

@mg12-isomer02 bp86/6-31G(d) Etot=-2401.063762 Eb=-11.88

Mg1	-0.901618	-1.519350	-2.586062
Mg2	0.461526	-2.324041	0.000327
Mg3	-4.219171	1.091550	-0.000156
Mg4	-0.901746	-1.518547	2.586391
Mg5	-2.589756	-1.443762	0.000128
Mg6	0.791966	2.731509	-0.000393
Mg7	-1.486273	1.323055	-1.507118
Mg8	1.390516	0.172136	1.593344
Mg9	-1.486390	1.323710	1.506823
Mg10	1.390703	0.171648	-1.593492
Mg11	3.940605	1.574242	-0.000130
Mg12	3.609638	-1.582152	0.000337

@mg12-isomer03 bp86/6-31G(d) Etot=-2401.063484 Eb=-11.87

Mg1	-0.105445	1.577792	1.538028
Mg2	2.649494	-2.282832	0.297423
Mg3	-0.320845	2.606421	-1.302484
Mg4	-2.877842	1.514376	-0.082111
Mg5	-2.505378	0.000224	2.576841
Mg6	2.649877	2.282682	0.297480
Mg7	-2.878181	-1.514219	-0.082079
Mg8	-1.781667	-0.000017	-2.560095
Mg9	4.608109	-0.000244	0.067142
Mg10	0.988701	-0.000060	-0.986112
Mg11	-0.105651	-1.577667	1.538198
Mg12	-0.321174	-2.606454	-1.302232

@mg12-isomer04 bp86/6-31G(d) Etot=-2401.061643 Eb=-11.77

Mg1	-1.669174	1.637854	-1.901631
Mg2	3.834458	-1.524488	-0.049492
Mg3	-1.669033	-1.637160	-1.902254
Mg4	-0.919019	-0.000692	3.508689
Mg5	-3.817290	0.000012	-0.500374
Mg6	0.996387	0.000393	-1.801677
Mg7	1.082687	-0.000186	1.259655
Mg8	0.857011	-2.624789	-0.352051
Mg9	-1.693558	-1.647239	1.069312
Mg10	3.834327	1.524585	-0.049016

Mg11	0.856853	2.624971	-0.351072
Mg12	-1.693649	1.646740	1.069910
@mg12-isomer05 bp86/6-31G(d) Etot=-2401.061334 Eb=-11.76			
Mg1	1.179528	-0.359440	-1.561683
Mg2	-0.331357	2.205886	1.492975
Mg3	-0.638518	-2.289798	0.000002
Mg4	2.505872	2.255215	0.000037
Mg5	4.195160	-0.202720	-0.000018
Mg6	1.179525	-0.359470	1.561743
Mg7	2.381188	-2.651051	-0.000040
Mg8	-3.598428	-1.472003	-0.000048
Mg9	-1.781975	-0.397226	-2.313101
Mg10	-2.977652	1.461951	0.000016
Mg11	-0.331328	2.205945	-1.492969
Mg12	-1.782015	-0.397289	2.313085
@mg12-isomer06 bp86/6-31G(d) Etot=-2401.061262 Eb=-11.75			
Mg1	1.822087	-1.592606	-0.000538
Mg2	4.984166	-1.450040	0.000091
Mg3	-0.831172	-1.521362	1.542807
Mg4	-1.155591	2.655239	0.000551
Mg5	-3.004821	0.271055	0.000294
Mg6	-1.789029	1.255091	2.637933
Mg7	-3.182398	-2.727260	-0.000352
Mg8	3.790997	1.410152	-0.000238
Mg9	-1.789632	1.256145	-2.637215
Mg10	-0.831441	-1.520717	-1.543380
Mg11	0.993227	0.982453	-1.547069
Mg12	0.993606	0.981849	1.547117
@mg12-isomer07 bp86/6-31G(d) Etot=-2401.061060 Eb=-11.74			
Mg1	-2.922355	1.437370	0.195346
Mg2	-0.869575	2.353040	-1.931305
Mg3	1.317805	-0.526427	1.649999
Mg4	-3.614275	-1.476760	0.369175
Mg5	4.289610	-0.513586	-0.266973
Mg6	3.043078	2.096841	0.553983
Mg7	0.937302	0.091260	-1.321820
Mg8	-0.019009	2.108557	1.042536
Mg9	-1.964596	-0.558193	-2.179348
Mg10	-1.634807	-0.174570	2.456107
Mg11	2.148749	-2.602967	-0.664494
Mg12	-0.711928	-2.234564	0.096795
@mg12-isomer08 bp86/6-31G(d) Etot=-2401.060746 Eb=-11.73			
Mg1	2.218607	0.525003	1.548751
Mg2	-0.025213	-1.292084	-2.623444
Mg3	-1.636840	-1.136586	-0.000844
Mg4	1.280178	-2.094495	-0.000876
Mg5	-0.026001	-1.294482	2.621957
Mg6	2.219102	0.526369	-1.547821
Mg7	-0.700398	1.477304	-1.547532
Mg8	-4.866764	-1.430654	0.000079
Mg9	-3.497844	1.532229	-0.000039
Mg10	-0.700863	1.475937	1.548367
Mg11	4.271852	-1.288641	-0.000011
Mg12	1.464184	3.000100	0.001414
@mg12-isomer09 bp86/6-31G(d) Etot=-2401.059249 Eb=-11.65			
Mg1	-3.471388	-1.674324	-0.281634
Mg2	-0.699778	-2.192838	-1.506968
Mg3	-0.880920	-1.637971	1.438769
Mg4	-2.313392	0.486495	-2.142547

Mg5	-2.533045	1.106080	0.798932
Mg6	1.878496	-1.658093	0.086097
Mg7	-1.133283	0.607617	3.442475
Mg8	0.823079	0.504091	-1.878185
Mg9	4.927146	-1.141604	0.213699
Mg10	0.662283	1.125193	1.080058
Mg11	-0.820741	2.860046	-0.975302
Mg12	3.561542	1.615307	-0.275394

@mg12-isomer10 bp86/6-31G(d) Etot=-2401.058340 Eb=-11.60

Mg1	0.381418	1.535325	1.556773
Mg2	5.729103	-0.000231	0.000001
Mg3	2.531029	-0.000046	0.000054
Mg4	-2.340390	-1.541319	-0.000050
Mg5	-0.514463	4.178844	-0.000038
Mg6	-2.037932	0.000022	2.616858
Mg7	-2.340244	1.541471	0.000020
Mg8	0.381441	1.535296	-1.556691
Mg9	-2.037843	0.000090	-2.616895
Mg10	0.381385	-1.535321	-1.556730
Mg11	0.381348	-1.535314	1.556700
Mg12	-0.514852	-4.178816	0.000000

@mg12-isomer11 bp86/6-31G(d) Etot=-2401.057710 Eb=-11.57

Mg1	-1.541090	-1.607489	-1.306286
Mg2	1.556038	1.397009	-0.403142
Mg3	-4.183485	-0.299383	0.025915
Mg4	-1.556199	1.396904	-0.403259
Mg5	-0.000172	1.651017	2.199966
Mg6	0.000070	0.506357	-2.897336
Mg7	1.541391	-1.607393	-1.306247
Mg8	-1.523647	-0.980569	1.703817
Mg9	0.000155	-3.550334	0.599849
Mg10	1.523649	-0.980428	1.703902
Mg11	-0.000228	4.373216	0.056797
Mg12	4.183515	-0.298907	0.026024

@mg12-isomer12 bp86/6-31G(d) Etot=-2401.057585 Eb=-11.56

Mg1	-2.147998	-1.452830	1.066802
Mg2	-0.612205	0.331285	3.006055
Mg3	0.938895	-0.197722	-1.793668
Mg4	0.938867	1.652180	0.725574
Mg5	0.938947	-1.454543	1.068045
Mg6	-2.147962	1.650324	0.724785
Mg7	-4.843168	0.000090	0.000019
Mg8	-2.147946	-0.197473	-1.791554
Mg9	-0.612246	2.437642	-1.789958
Mg10	3.526949	-0.000025	0.000037
Mg11	-0.612267	-2.769015	-1.216128
Mg12	6.780136	0.000088	-0.000009

@mg12-isomer13 bp86/6-31G(d) Etot=-2401.056938 Eb=-11.53

Mg1	4.816210	1.111537	-0.184726
Mg2	1.008949	-0.960524	2.178879
Mg3	1.658367	1.144869	-0.021972
Mg4	3.571822	-1.741335	0.235857
Mg5	-2.329455	-0.167350	-1.500644
Mg6	-2.324524	-3.057298	-0.706056
Mg7	-0.646222	1.613251	2.067117
Mg8	0.344032	-1.657570	-0.687774
Mg9	-3.465749	1.634040	0.757912
Mg10	0.364472	0.609668	-2.765281
Mg11	-1.024169	2.524089	-0.850582
Mg12	-1.973732	-1.053378	1.477270

@mg12-isomer14 bp86/6-31G(d) Etot=-2401.056853 Eb=-11.52

Mg1	-0.066113	0.302206	-2.532931
Mg2	-3.922380	0.616910	1.743246
Mg3	-0.948057	1.341895	1.637727
Mg4	0.910075	-1.046398	2.205974
Mg5	0.715997	-2.029100	-0.610193
Mg6	-0.460019	2.886014	-0.969746
Mg7	1.685432	1.009196	0.030883
Mg8	-1.962140	-2.056895	-1.992239
Mg9	3.767620	-1.620719	0.315329
Mg10	4.852197	1.419052	0.090682
Mg11	-2.689188	0.769347	-0.955591
Mg12	-1.883425	-1.591508	1.036859

@mg12-isomer15 bp86/6-31G(d) Etot=-2401.056377 Eb=-11.50

Mg1	0.084783	1.497994	1.776559
Mg2	-2.901254	1.550093	0.528127
Mg3	1.377362	-1.310464	2.123184
Mg4	0.562520	-2.186435	-0.630334
Mg5	2.295083	0.408977	-0.319453
Mg6	-0.203059	2.101313	-1.154093
Mg7	2.329116	3.280618	0.396941
Mg8	-1.590402	-1.145268	1.461251
Mg9	-4.554024	-1.187588	0.190981
Mg10	-1.963191	-0.506642	-1.562310
Mg11	0.704482	-0.216967	-2.967120
Mg12	3.858586	-2.285632	0.156267

@mg12-isomer16 bp86/6-31G(d) Etot=-2401.055959 Eb=-11.48

Mg1	-4.295589	0.709424	0.705397
Mg2	-2.898655	-1.632788	-0.893819
Mg3	-0.000251	-2.948729	0.071966
Mg4	1.563622	-0.760829	1.676367
Mg5	4.295844	0.707744	0.704948
Mg6	-1.557105	1.660865	-0.307275
Mg7	0.000239	1.988366	-2.918675
Mg8	-0.001546	-0.772655	-1.877742
Mg9	2.896505	-1.632057	-0.895777
Mg10	0.001347	1.780961	2.366499
Mg11	-1.562522	-0.759639	1.676327
Mg12	1.558112	1.659337	-0.308218

@mg12-isomer17 bp86/6-31G(d) Etot=-2401.055867 Eb=-11.47

Mg1	-1.398996	0.810123	1.288712
Mg2	0.793718	-1.245687	2.395900
Mg3	1.421589	1.750597	1.842280
Mg4	-1.867235	0.352230	-1.790780
Mg5	1.931745	-3.177638	-0.083370
Mg6	-3.801564	-1.224009	0.385425
Mg7	2.733631	-0.383662	0.029755
Mg8	-0.778437	-1.899472	-0.078564
Mg9	3.640338	2.440054	-0.439145
Mg10	0.680111	1.788090	-1.111677
Mg11	-4.289429	1.816603	-0.010684
Mg12	0.934529	-1.027228	-2.427851

@mg12-isomer18 bp86/6-31G(d) Etot=-2401.055562 Eb=-11.46

Mg1	-0.777534	1.370853	2.228128
Mg2	0.288553	-2.453746	-0.720759
Mg3	-4.359014	-1.004634	-0.735760
Mg4	-3.219150	1.677717	0.102061
Mg5	4.358907	1.004711	-0.735816
Mg6	3.219252	-1.677708	0.102131

Mg7	-0.288534	2.453684	-0.720936
Mg8	0.777550	-1.370749	2.228134
Mg9	1.501978	0.201559	-1.865870
Mg10	-1.924896	-1.294867	0.992304
Mg11	-1.501971	-0.201765	-1.865871
Mg12	1.924860	1.294944	0.992253

@mg12-isomer19 bp86/6-31G(d) Etot=-2401.054945 Eb=-11.42

Mg1	0.338043	1.760666	-1.150001
Mg2	-1.867549	1.287060	1.181697
Mg3	-3.461850	-1.615321	0.836713
Mg4	-2.162475	-0.138938	-1.617384
Mg5	2.895643	-0.056498	-0.439593
Mg6	-4.712458	1.039694	-0.000883
Mg7	0.711543	-0.946914	-2.578407
Mg8	3.053039	2.963656	-0.254056
Mg9	1.193240	1.439938	1.776544
Mg10	-0.253725	-1.262178	0.522642
Mg11	2.210118	-1.555450	2.236859
Mg12	2.056432	-2.915715	-0.514131

@mg12-isomer20 bp86/6-31G(d) Etot=-2401.054857 Eb=-11.42

Mg1	2.335146	-2.056776	0.411241
Mg2	2.335221	2.056759	0.411136
Mg3	-0.599394	-2.616567	2.027787
Mg4	-0.439872	-2.364299	-1.028515
Mg5	-0.439855	2.364319	-1.028475
Mg6	-1.966696	0.000029	-2.231217
Mg7	-0.065726	-0.000013	0.899725
Mg8	1.263170	0.000000	-2.074960
Mg9	-3.131237	1.510165	0.310570
Mg10	-3.131270	-1.510127	0.310474
Mg11	4.439777	-0.000078	-0.035561
Mg12	-0.599264	2.616588	2.027795

@mg12-isomer21 bp86/6-31G(d) Etot=-2401.054615 Eb=-11.41

Mg1	-0.403470	1.289981	-0.856425
Mg2	0.331979	-1.895925	-0.817664
Mg3	0.580072	1.557803	2.100006
Mg4	-1.537080	-0.577041	1.373543
Mg5	-4.752090	-1.064713	0.266567
Mg6	1.988168	2.934246	-0.500160
Mg7	3.217599	-2.302155	-0.398136
Mg8	1.238597	-1.542283	2.124076
Mg9	-3.548843	1.775190	-0.097814
Mg10	3.099450	0.492232	0.699623
Mg11	-2.403936	-0.874926	-1.684999
Mg12	2.189556	0.207589	-2.208616

@mg12-isomer22 bp86/6-31G(d) Etot=-2401.054506 Eb=-11.40

Mg1	1.121967	-0.140845	-1.611560
Mg2	0.794674	2.847688	-1.479150
Mg3	-1.750135	0.958122	-1.812736
Mg4	1.445262	-0.875376	1.581335
Mg5	-0.200116	1.695289	1.038833
Mg6	3.964706	-1.080798	-0.376374
Mg7	-3.364880	0.828791	0.914303
Mg8	2.970308	1.755201	0.679523
Mg9	-4.036647	-1.264591	-1.231416
Mg10	-1.197084	-1.546264	0.037893
Mg11	1.432373	-2.935381	-0.755748
Mg12	-1.180429	-0.241837	3.015097

@mg12-isomer23 bp86/6-31G(d) Etot=-2401.054459 Eb=-11.40

Mg1	-1.215716	-1.569046	-2.140989
Mg2	1.000188	0.493310	-1.751254
Mg3	1.206161	-2.296867	-0.394009
Mg4	3.051478	2.287674	-0.179339
Mg5	3.832953	-0.602275	-0.978551
Mg6	1.980081	0.172034	1.626288
Mg7	0.491446	-2.307955	2.680151
Mg8	-3.980297	-0.958043	-0.569293
Mg9	-1.939344	1.368712	-1.357698
Mg10	-0.035595	2.412019	0.832435
Mg11	-1.033066	-0.525758	0.865226
Mg12	-3.358289	1.526196	1.367033

@mg12-isomer24 bp86/6-31G(d) Etot=-2401.054390 Eb=-11.39

Mg1	-0.049826	2.539782	-1.917920
Mg2	2.182485	1.431020	-0.297035
Mg3	-0.448063	2.046422	1.258859
Mg4	4.398995	0.194020	1.278423
Mg5	0.835042	-0.540652	-2.619114
Mg6	-3.878051	1.363174	0.837436
Mg7	-1.651761	0.166507	-1.102028
Mg8	2.850361	-1.717325	-0.571785
Mg9	1.322183	-0.488385	1.911326
Mg10	-3.719479	-1.890318	-0.332681
Mg11	-1.664195	-0.698205	1.850732
Mg12	-0.177693	-2.406040	-0.296213

@mg12-isomer25 bp86/6-31G(d) Etot=-2401.054240 Eb=-11.39

Mg1	2.778241	-3.004114	0.539608
Mg2	1.553823	0.192122	-2.313893
Mg3	0.114886	-2.093879	-0.719522
Mg4	0.192303	-1.553764	2.314175
Mg5	2.093857	0.114972	0.719770
Mg6	3.004206	2.777864	-0.540054
Mg7	-3.004376	-2.777927	-0.540013
Mg8	-0.114939	2.093968	-0.719772
Mg9	-2.093831	-0.115075	0.719864
Mg10	-0.192180	1.554063	2.313902
Mg11	-1.553918	-0.192199	-2.313808
Mg12	-2.778071	3.003968	0.539743

@mg12-isomer26 bp86/6-31G(d) Etot=-2401.053700 Eb=-11.36

Mg1	3.147368	-3.017908	0.204689
Mg2	2.940516	-0.000101	0.288053
Mg3	0.537088	1.624957	1.554140
Mg4	0.855707	1.642314	-1.481665
Mg5	-2.063717	-1.646547	-0.294091
Mg6	-1.284819	0.000075	-2.873922
Mg7	-4.592116	0.000301	0.346500
Mg8	-2.016642	0.000061	2.273289
Mg9	-2.063301	1.646461	-0.294105
Mg10	0.855440	-1.642210	-1.481683
Mg11	0.536827	-1.625090	1.554036
Mg12	3.147648	3.017688	0.204758

@mg12-isomer27 bp86/6-31G(d) Etot=-2401.053071 Eb=-11.33

Mg1	-1.312027	-1.225493	2.077838
Mg2	-3.025063	-2.937234	-0.171522
Mg3	-3.594900	2.356317	0.446853
Mg4	0.391348	-0.279547	-2.655763
Mg5	-2.063807	-0.175433	-0.744396
Mg6	1.640450	-0.479463	1.875299
Mg7	1.790909	1.477252	-0.456761
Mg8	3.006570	-1.356063	-0.889038

Mg9	-0.893429	2.448533	-1.458436
Mg10	0.118543	-2.300107	-0.345200
Mg11	4.537956	0.755154	0.750600
Mg12	-0.596550	1.716085	1.570526

@mg12-isomer28 bp86/6-31G(d) Etot=-2401.052825 Eb=-11.31

Mg1	-3.694283	1.657316	0.648938
Mg2	-1.081965	0.000184	1.525592
Mg3	-0.557974	2.358339	-0.384603
Mg4	1.488124	1.590929	1.757495
Mg5	-2.381093	-0.000106	-1.433945
Mg6	4.068972	-0.000021	0.814262
Mg7	2.301099	1.627888	-1.099517
Mg8	1.488042	-1.590592	1.757637
Mg9	2.301010	-1.628158	-1.099377
Mg10	-3.694258	-1.657231	0.649129
Mg11	-0.558070	-2.358413	-0.384184
Mg12	0.320398	-0.000134	-2.751426

@mg12-isomer29 bp86/6-31G(d) Etot=-2401.052191 Eb=-11.28

Mg1	-0.668962	-1.143662	1.563433
Mg2	0.292546	1.708982	-0.337109
Mg3	-2.078388	2.557019	-2.034153
Mg4	-0.947709	-3.131212	-0.621964
Mg5	-2.708839	1.317435	0.659886
Mg6	2.208852	0.217809	1.585983
Mg7	3.484287	1.537106	-0.919817
Mg8	4.469627	-1.281066	-0.159541
Mg9	1.451733	-1.179090	-1.133501
Mg10	-3.560335	-1.758619	0.402776
Mg11	-0.401555	1.553754	2.756156
Mg12	-1.541256	-0.398456	-1.762148

@mg12-isomer30 bp86/6-31G(d) Etot=-2401.052099 Eb=-11.27

Mg1	0.939004	0.694414	-1.076962
Mg2	0.693220	2.167077	1.740895
Mg3	-1.448931	0.076307	1.281729
Mg4	-3.589771	-2.001190	0.206830
Mg5	1.186622	-0.958289	2.294769
Mg6	-0.339314	-2.440821	-0.079319
Mg7	-1.368376	2.553663	-0.691181
Mg8	2.742682	-1.934629	-0.251906
Mg9	3.766535	0.233106	-2.148413
Mg10	-1.884342	-0.363491	-1.836781
Mg11	3.449687	0.856220	0.836403
Mg12	-4.147016	1.117632	-0.276064

@mg12-isomer31 bp86/6-31G(d) Etot=-2401.052001 Eb=-11.27

Mg1	1.716042	0.276739	1.385507
Mg2	-1.255812	-0.820060	1.043618
Mg3	1.177873	-2.627404	1.709267
Mg4	-0.220939	1.373611	-1.170151
Mg5	-4.495845	-1.327202	0.133841
Mg6	-2.194590	-0.828209	-1.921040
Mg7	-0.569364	2.141101	1.851245
Mg8	-3.279709	1.550176	0.002599
Mg9	2.061668	2.952960	0.122940
Mg10	3.648274	-1.745929	-0.068268
Mg11	2.683109	0.708138	-1.863864
Mg12	0.729293	-1.653920	-1.225693

@mg12-isomer32 bp86/6-31G(d) Etot=-2401.051954 Eb=-11.27

Mg1	0.328960	2.070283	1.911474
Mg2	-0.578576	1.843420	-1.091674

Mg3	2.443563	0.081139	1.147214
Mg4	-2.434163	0.702512	1.216451
Mg5	-0.155042	-1.028122	2.402753
Mg6	-1.229237	-1.277279	-0.868599
Mg7	2.315784	2.580979	-0.537807
Mg8	-4.327487	-1.660703	0.004285
Mg9	4.237523	-1.480555	-0.759505
Mg10	-3.487176	0.884991	-1.594390
Mg11	1.323509	-2.547813	0.066823
Mg12	1.562343	-0.168851	-1.897024

@mg12-isomer33 bp86/6-31G(d) Etot=-2401.051950 Eb=-11.27

Mg1	-2.605901	2.151121	0.163763
Mg2	-1.447168	-0.047698	1.968287
Mg3	0.414252	2.064976	0.844729
Mg4	-4.232395	-0.743131	0.864821
Mg5	-2.302137	-0.455511	-1.378416
Mg6	1.281903	-1.152153	1.034414
Mg7	-0.387071	1.719690	-2.166105
Mg8	2.439672	0.818178	-1.220155
Mg9	3.404206	1.236142	1.549559
Mg10	-1.224406	-2.661181	0.349835
Mg11	0.432384	-1.463597	-2.075903
Mg12	4.226661	-1.466837	0.065170

@mg12-isomer34 bp86/6-31G(d) Etot=-2401.051860 Eb=-11.26

Mg1	0.375569	0.632518	-1.581020
Mg2	2.915981	0.864617	0.000040
Mg3	-2.343236	-0.737678	1.551098
Mg4	1.605578	-1.841690	0.000268
Mg5	0.079457	-2.235945	-2.626622
Mg6	0.375362	0.632814	1.580841
Mg7	-3.416226	4.714650	0.000007
Mg8	0.079010	-2.235403	2.627011
Mg9	-1.143316	-3.170185	0.000175
Mg10	-1.961278	1.864405	-0.000380
Mg11	5.776096	2.249904	0.000011
Mg12	-2.342999	-0.738007	-1.551429

@mg12-isomer35 bp86/6-31G(d) Etot=-2401.051624 Eb=-11.25

Mg1	6.162241	0.323069	0.000655
Mg2	3.006542	-0.025035	-0.026384
Mg3	0.456100	1.493738	-0.463464
Mg4	-1.173912	4.301231	0.065418
Mg5	0.740660	-1.528125	-1.361878
Mg6	-1.086384	0.393844	-2.903488
Mg7	0.702197	-0.909400	1.696840
Mg8	-1.063583	1.568842	2.205877
Mg9	-0.567857	-3.622275	0.623787
Mg10	-2.585414	1.098652	-0.345851
Mg11	-2.295179	-1.872610	-1.253632
Mg12	-2.295410	-1.221931	1.762119

@mg12-isomer36 bp86/6-31G(d) Etot=-2401.051098 Eb=-11.22

Mg1	0.000208	0.415143	3.545145
Mg2	1.691810	-0.321549	1.164527
Mg3	-1.691654	-0.321650	1.164755
Mg4	-2.748062	2.272951	-0.426048
Mg5	3.277023	-2.892369	-0.140167
Mg6	-3.277071	-2.892275	-0.140086
Mg7	0.000004	-2.480187	-0.317295
Mg8	-0.000024	2.334789	1.154255
Mg9	1.600741	-0.349615	-1.844673
Mg10	-1.600869	-0.349636	-1.844488

Mg11	2.747981	2.273074	-0.426188
Mg12	-0.000086	2.311325	-1.889737
@mg12-isomer37 bp86/6-31G(d) Etot=-2401.050853 Eb=-11.21			
Mg1	0.000034	1.105390	1.399636
Mg2	-1.568142	-1.082846	-2.046004
Mg3	-2.653223	1.061460	-0.159876
Mg4	0.000032	1.569398	-1.588923
Mg5	-5.461061	2.564205	0.099158
Mg6	-0.000012	-3.439642	-0.919522
Mg7	1.603022	-1.610538	0.943698
Mg8	-1.603064	-1.610480	0.943564
Mg9	2.653288	1.061396	-0.159846
Mg10	1.568113	-1.082885	-2.045860
Mg11	-0.000140	-1.099596	3.434830
Mg12	5.461155	2.564138	0.099146
@mg12-isomer38 bp86/6-31G(d) Etot=-2401.050506 Eb=-11.19			
Mg1	-4.865934	0.268859	-0.867740
Mg2	-1.809792	0.504847	-2.341302
Mg3	-1.899939	1.900090	0.330612
Mg4	0.752183	1.909940	-1.377148
Mg5	-2.060515	-1.146156	0.236826
Mg6	0.915239	1.766714	1.699106
Mg7	0.685624	-1.098720	-1.516913
Mg8	-1.495423	0.302763	2.890967
Mg9	0.809906	-1.271258	1.603783
Mg10	-0.281759	-3.554129	-0.068865
Mg11	3.060583	0.297354	0.054316
Mg12	6.189827	0.119695	-0.643642
@mg12-isomer39 bp86/6-31G(d) Etot=-2401.050498 Eb=-11.19			
Mg1	-3.135108	1.689623	-0.087609
Mg2	2.225436	2.547357	1.980868
Mg3	2.997943	-0.165784	0.902124
Mg4	-0.546155	1.435263	-2.418957
Mg5	-1.686329	-1.095900	-0.981153
Mg6	0.482456	-2.150937	1.025659
Mg7	1.287834	-0.920749	-1.788302
Mg8	-0.061911	1.079163	0.714747
Mg9	-4.715659	-0.947446	0.095962
Mg10	2.204665	2.138327	-1.054869
Mg11	-2.244873	-0.678327	2.000535
Mg12	3.191701	-2.930588	-0.389006
@mg12-isomer40 bp86/6-31G(d) Etot=-2401.050470 Eb=-11.19			
Mg1	-0.235297	1.366498	1.216916
Mg2	8.556894	-0.000143	-0.000179
Mg3	-3.299101	1.343194	1.197698
Mg4	5.247224	-0.000045	0.000410
Mg5	-3.298652	-1.710137	0.564991
Mg6	-0.234933	-1.736461	0.573848
Mg7	-3.298207	0.364638	-1.762466
Mg8	-0.234229	0.372012	-1.791671
Mg9	-1.784813	-2.262926	-2.017144
Mg10	2.153378	0.000317	0.000924
Mg11	-1.785429	-0.615184	2.968123
Mg12	-1.786835	2.878237	-0.951450
@mg12-isomer41 bp86/6-31G(d) Etot=-2401.050179 Eb=-11.17			
Mg1	-0.807670	2.919763	0.000070
Mg2	1.636714	1.675436	-1.544466
Mg3	-2.294434	0.257836	-0.000092
Mg4	0.203340	-0.996193	-1.568963

Mg5	1.636632	1.675316	1.544688
Mg6	-1.726106	-2.673962	-0.000207
Mg7	-4.946071	-2.118350	0.000088
Mg8	-1.227792	1.479012	2.634666
Mg9	2.849874	-0.634939	0.000020
Mg10	0.203230	-0.996314	1.568812
Mg11	-1.227645	1.479244	-2.634657
Mg12	5.699928	-2.066849	0.000041

@mg12-isomer42 bp86/6-31G(d) Etot=-2401.050046 Eb=-11.17

Mg1	-3.338341	-2.791339	0.307986
Mg2	-1.131196	-1.631923	-1.593349
Mg3	-3.163433	0.246143	0.051132
Mg4	-2.471349	3.129135	-0.453320
Mg5	-0.757282	-1.458302	1.496393
Mg6	0.918437	0.178850	-3.127390
Mg7	0.001274	1.363710	-0.595837
Mg8	-1.161781	1.696074	2.088526
Mg9	1.708508	-1.474869	-0.471761
Mg10	1.722968	0.409022	1.997079
Mg11	3.250735	1.376891	-0.628805
Mg12	4.421460	-1.043393	0.929346

@mg12-isomer43 bp86/6-31G(d) Etot=-2401.049983 Eb=-11.16

Mg1	-0.124542	0.385854	-0.000099
Mg2	2.148394	-0.960540	1.560930
Mg3	-1.010742	-1.232011	2.561835
Mg4	2.148366	-0.961125	-1.560693
Mg5	-1.010754	-1.232752	-2.561528
Mg6	-0.643283	3.222898	-0.000184
Mg7	2.513947	2.188247	-0.000167
Mg8	-2.747563	1.278477	-1.513709
Mg9	-2.747655	1.278751	1.513311
Mg10	-0.140636	-2.662282	0.000370
Mg11	4.604080	0.132508	-0.000142
Mg12	-2.989612	-1.438025	0.000078

@mg12-isomer44 bp86/6-31G(d) Etot=-2401.049971 Eb=-11.16

Mg1	1.249699	0.345855	2.173239
Mg2	-1.261481	-1.463179	2.175451
Mg3	-2.759353	-0.559805	-0.343310
Mg4	-1.390903	1.579689	1.411651
Mg5	-4.433268	1.917058	0.334740
Mg6	1.043142	1.274788	-0.755526
Mg7	-1.722324	1.948220	-1.663414
Mg8	-1.473063	-3.205861	-0.558055
Mg9	3.655181	-0.332289	-0.020380
Mg10	1.041534	-1.750595	-0.002449
Mg11	6.534722	1.044874	-0.231514
Mg12	-0.483886	-0.798754	-2.520432

@mg12-isomer45 bp86/6-31G(d) Etot=-2401.049949 Eb=-11.16

Mg1	2.382151	1.188195	-1.743040
Mg2	1.711749	-0.006814	0.925865
Mg3	4.881682	1.586991	0.265610
Mg4	-0.551632	-1.421599	2.362403
Mg5	-0.668548	1.632594	2.093516
Mg6	1.404844	-3.219281	0.672313
Mg7	0.694420	-1.333765	-1.734769
Mg8	-0.494593	1.469358	-0.946783
Mg9	-2.807018	3.510098	0.157155
Mg10	-1.561837	-2.749471	-0.250935
Mg11	-2.730090	0.018142	0.551076
Mg12	-2.261128	-0.674447	-2.352410

@mg12-isomer46 bp86/6-31G(d) Etot=-2401.049784 Eb=-11.15

Mg1	2.931553	2.541232	-0.000011
Mg2	-2.528519	0.180446	-1.806360
Mg3	-1.565246	0.111734	1.203631
Mg4	-0.111770	-1.565473	-1.203876
Mg5	0.111690	1.565335	-1.203752
Mg6	-2.541194	2.931327	-0.000010
Mg7	0.180421	2.528332	1.806498
Mg8	-2.931420	-2.540964	0.000126
Mg9	1.565440	-0.111716	1.203595
Mg10	2.541104	-2.931546	0.000025
Mg11	-0.180487	-2.528277	1.806501
Mg12	2.528428	-0.180431	-1.806367

@mg12-isomer47 bp86/6-31G(d) Etot=-2401.049397 Eb=-11.13

Mg1	3.765292	-1.713550	-0.040059
Mg2	-2.094892	0.646023	0.944892
Mg3	2.799947	1.128159	-0.759211
Mg4	-1.451940	-1.620650	-1.336338
Mg5	3.062826	0.431474	2.143822
Mg6	0.518971	2.272070	1.132768
Mg7	0.744993	-0.894437	0.687337
Mg8	-4.299141	-1.447417	0.095247
Mg9	-0.274957	1.343585	-1.727730
Mg10	-1.789794	-2.340411	1.660335
Mg11	-2.380484	3.348001	-0.390228
Mg12	1.399178	-1.152847	-2.410835

@mg12-isomer48 bp86/6-31G(d) Etot=-2401.048791 Eb=-11.10

Mg1	-1.287562	0.734265	-1.334423
Mg2	-1.525402	-0.016337	1.666883
Mg3	0.174429	2.489540	1.040671
Mg4	-3.916940	1.873741	0.208860
Mg5	-0.702515	-2.153193	-0.382712
Mg6	1.662167	-0.057889	0.652333
Mg7	1.586195	1.896299	-1.674304
Mg8	2.437239	-2.819930	-0.272922
Mg9	0.989576	-1.012699	-2.590206
Mg10	0.695398	-2.215425	2.393615
Mg11	3.563536	2.421144	0.746133
Mg12	-3.676121	-1.139516	-0.453930

@mg12-isomer49 bp86/6-31G(d) Etot=-2401.048744 Eb=-11.10

Mg1	0.736105	0.495809	-3.033856
Mg2	1.987151	0.936580	0.049177
Mg3	-0.884410	1.763110	-0.933351
Mg4	0.837284	-1.706468	-1.083467
Mg5	4.881021	2.350552	0.264163
Mg6	-2.066387	-0.880783	-2.003295
Mg7	-0.317515	1.823049	2.009112
Mg8	-3.175459	3.054431	0.586816
Mg9	-1.563140	-2.844386	0.361119
Mg10	-2.540737	-0.070924	0.975738
Mg11	1.663696	-3.850331	0.893298
Mg12	0.442392	-1.070639	1.914547

@mg12-isomer50 bp86/6-31G(d) Etot=-2401.048601 Eb=-11.09

Mg1	-0.330704	1.857717	1.550650
Mg2	-0.435425	-1.172085	-1.586635
Mg3	-3.055554	1.980946	0.000085
Mg4	-3.225167	-1.060965	-0.000174
Mg5	-2.815132	0.458000	2.625642
Mg6	1.784044	0.272275	0.000067

Mg7	4.896490	0.110114	0.000036
Mg8	-2.814966	0.458377	-2.625710
Mg9	-1.465183	-3.500668	-0.000130
Mg10	8.227717	-0.089382	-0.000045
Mg11	-0.330665	1.857897	-1.550335
Mg12	-0.435455	-1.172225	1.586547
@mg12-isomer51 bp86/6-31G(d) Etot=-2401.048595 Eb=-11.09			
Mg1	0.658015	2.015990	-0.940956
Mg2	-1.988475	0.503799	-0.658427
Mg3	-1.635211	-1.312539	2.008295
Mg4	-1.363516	-2.477812	-0.859114
Mg5	1.005094	-1.136419	0.518612
Mg6	2.778277	1.147306	1.376121
Mg7	-2.147221	3.419332	-0.159743
Mg8	3.043464	0.024775	-1.460118
Mg9	0.157674	-0.422260	-2.736850
Mg10	4.159904	-1.696631	0.810561
Mg11	-0.382220	1.592202	1.856135
Mg12	-4.285785	-1.657744	0.245484
@mg12-isomer52 bp86/6-31G(d) Etot=-2401.048396 Eb=-11.08			
Mg1	-1.121024	-1.336162	-0.992918
Mg2	-4.187852	-0.525356	-0.745522
Mg3	2.037681	0.921628	0.965843
Mg4	1.214868	0.827557	-1.975418
Mg5	-1.739498	1.494482	-2.013377
Mg6	-0.126416	-1.266618	1.957015
Mg7	1.815664	-1.819270	-0.416001
Mg8	-0.042645	1.784244	2.911846
Mg9	-0.071701	-4.379725	0.429397
Mg10	0.060840	3.189795	-0.085102
Mg11	4.284797	0.169525	-0.970249
Mg12	-2.124714	0.939900	0.934486
@mg12-isomer53 bp86/6-31G(d) Etot=-2401.048347 Eb=-11.08			
Mg1	1.844079	-1.857351	0.320608
Mg2	-1.166551	-2.213946	0.200563
Mg3	0.111342	-0.759266	-2.264003
Mg4	2.605080	0.991388	-1.046508
Mg5	-1.892483	2.820829	0.893876
Mg6	-2.507035	0.495533	-1.004777
Mg7	0.175072	0.683686	1.023534
Mg8	-2.713167	0.016509	1.979053
Mg9	-4.216761	-2.016355	-0.186534
Mg10	4.786849	-1.097082	-0.054402
Mg11	-0.200475	2.287732	-1.783349
Mg12	3.174051	0.648323	1.921938
@mg12-isomer54 bp86/6-31G(d) Etot=-2401.047778 Eb=-11.05			
Mg1	1.800950	-0.695675	1.402771
Mg2	3.589882	1.754815	1.806554
Mg3	-0.630025	-2.352832	0.594931
Mg4	-0.982606	0.817187	1.012058
Mg5	2.245897	-2.796845	-0.868182
Mg6	0.409726	-0.494991	-1.783162
Mg7	-2.833891	-0.918022	-1.155147
Mg8	-3.414917	-1.074497	1.793764
Mg9	-1.319104	1.998335	-1.814202
Mg10	3.696419	0.054662	-0.867307
Mg11	-3.983779	1.544671	0.207868
Mg12	1.421447	2.163189	-0.329946
@mg12-isomer55 bp86/6-31G(d) Etot=-2401.047698 Eb=-11.04			

Mg1	-3.474420	-2.075563	-0.320030
Mg2	1.409524	1.605124	-1.320281
Mg3	2.856279	2.220464	1.303620
Mg4	-1.679316	2.737061	-1.530213
Mg5	3.959219	-0.063594	-0.500343
Mg6	-1.123580	-0.236877	-1.327771
Mg7	1.310889	-0.552232	0.998690
Mg8	-0.543830	2.084601	1.152474
Mg9	-3.497772	1.119840	0.379771
Mg10	-1.693774	-0.993507	1.833768
Mg11	-0.325610	-2.953494	-0.183369
Mg12	2.802391	-2.891822	-0.486315

@mg12-isomer56 bp86/6-31G(d) Etot=-2401.047654 Eb=-11.04

Mg1	1.069901	0.159833	1.063379
Mg2	-1.217506	-1.837978	-0.133236
Mg3	-4.159536	-1.339548	0.852508
Mg4	1.568365	-1.551583	-1.477641
Mg5	2.808161	1.326683	-1.577473
Mg6	1.430456	-2.727831	1.384744
Mg7	-0.313337	0.713882	-2.158978
Mg8	-3.436196	0.057930	-1.843021
Mg9	0.553308	2.899563	-0.106164
Mg10	-2.071127	1.156151	0.586534
Mg11	-0.229990	2.064229	2.921884
Mg12	3.997502	-0.921330	0.487464

@mg12-isomer57 bp86/6-31G(d) Etot=-2401.047594 Eb=-11.04

Mg1	-1.794177	-0.000061	-1.972337
Mg2	-3.295586	-2.363381	-0.104684
Mg3	1.445510	-0.000029	-1.453864
Mg4	-0.012542	-0.000131	3.618326
Mg5	-0.277905	2.522179	-0.950287
Mg6	1.489716	1.569299	1.435350
Mg7	-1.349815	-0.000130	0.952540
Mg8	2.938896	-2.775161	-0.953003
Mg9	-0.277914	-2.522162	-0.949839
Mg10	1.490362	-1.568827	1.435247
Mg11	-3.295435	2.363363	-0.104603
Mg12	2.938889	2.775042	-0.952846

@mg12-isomer58 bp86/6-31G(d) Etot=-2401.047389 Eb=-11.03

Mg1	-0.418344	-2.155852	0.441405
Mg2	1.233799	0.062792	-1.214806
Mg3	-0.427400	1.112923	1.274878
Mg4	-3.268165	-0.527072	1.295751
Mg5	-0.269074	2.811104	-1.207594
Mg6	2.660987	-2.731805	-0.525477
Mg7	-3.061918	2.512234	0.212444
Mg8	4.282469	0.016931	-0.332387
Mg9	-2.043937	0.035084	-1.378514
Mg10	-3.228736	-2.836463	-0.675746
Mg11	2.122306	-0.750015	1.660913
Mg12	2.418012	2.450139	0.449132

@mg12-isomer59 bp86/6-31G(d) Etot=-2401.047004 Eb=-11.01

Mg1	-0.368327	-2.540200	-0.000015
Mg2	1.268511	-0.313135	-1.500015
Mg3	-0.377448	2.459742	1.530137
Mg4	-2.075737	-0.370237	1.536007
Mg5	-0.377488	2.459745	-1.530118
Mg6	2.770176	-2.756728	-0.000035
Mg7	-3.070306	2.122372	0.000001
Mg8	4.242700	-0.121260	-0.000033

Mg9	-2.075827	-0.370277	-1.536054
Mg10	-3.613876	-2.567660	0.000058
Mg11	1.268570	-0.313199	1.500066
Mg12	2.409052	2.310837	0.000001

@mg12-isomer60 bp86/6-31G(d) Etot=-2401.046994 Eb=-11.01

Mg1	-4.143602	-1.506840	0.691919
Mg2	-2.182824	-0.782304	-1.542819
Mg3	-3.125752	1.441549	0.536868
Mg4	-0.281985	2.334997	1.835359
Mg5	1.388699	-2.572761	1.666106
Mg6	0.106126	0.051472	-3.544684
Mg7	1.978477	0.377916	1.134298
Mg8	-1.084220	-0.735047	1.421464
Mg9	0.872539	-1.588753	-1.117641
Mg10	2.566280	3.088879	-0.060702
Mg11	-0.128357	1.649015	-1.033254
Mg12	4.034621	-1.758123	0.013085

@mg12-isomer61 bp86/6-31G(d) Etot=-2401.046915 Eb=-11.00

Mg1	3.314265	-1.504511	-0.757853
Mg2	0.302757	-0.000078	-2.122848
Mg3	0.882050	0.000131	1.133553
Mg4	-2.353725	1.620210	-1.304157
Mg5	3.918566	0.000110	1.904754
Mg6	0.347893	-2.616262	-0.388998
Mg7	-1.791773	-1.637393	1.668937
Mg8	-2.353656	-1.620449	-1.304062
Mg9	-4.136414	-0.000044	0.649030
Mg10	0.347747	2.616310	-0.389220
Mg11	3.314177	1.504443	-0.758002
Mg12	-1.791886	1.637532	1.668866

@mg12-isomer62 bp86/6-31G(d) Etot=-2401.046844 Eb=-11.00

Mg1	-2.702998	-0.870880	-1.562138
Mg2	-1.080782	-2.860869	-0.000371
Mg3	-3.787634	1.621439	-0.000105
Mg4	-1.183240	2.045494	1.547954
Mg5	0.539614	-0.663122	-1.535970
Mg6	1.488475	1.949896	0.000527
Mg7	-1.182913	2.046035	-1.547452
Mg8	3.525233	-0.691459	0.000356
Mg9	0.539283	-0.663593	1.536288
Mg10	4.524246	2.215647	-0.000496
Mg11	2.024063	-3.257221	-0.000124
Mg12	-2.703348	-0.871368	1.561531

@mg12-isomer63 bp86/6-31G(d) Etot=-2401.046822 Eb=-11.00

Mg1	-0.805825	-2.905898	-0.070809
Mg2	-0.907786	-0.994545	-2.572045
Mg3	1.013358	-0.627047	1.569482
Mg4	0.880002	1.237744	-0.892090
Mg5	-1.219061	1.561097	1.416918
Mg6	-1.669120	-1.360344	2.564996
Mg7	-2.753243	-0.645179	-0.185757
Mg8	1.767467	-1.683759	-1.255272
Mg9	-1.936211	1.892059	-1.586229
Mg10	3.567912	0.246672	0.211917
Mg11	-4.484470	1.953656	0.411478
Mg12	6.546977	1.325544	0.387411

@mg12-isomer64 bp86/6-31G(d) Etot=-2401.046707 Eb=-10.99

Mg1	-4.634102	1.464149	0.003868
Mg2	1.130193	-0.899750	1.867673

Mg3	-2.289135	0.511954	-1.809932
Mg4	-0.487641	-1.842755	-0.703244
Mg5	2.574566	-1.111208	-1.121595
Mg6	-1.734652	0.412324	1.235306
Mg7	1.837243	-3.482380	0.562952
Mg8	0.503409	1.439646	-0.688787
Mg9	3.237425	1.414107	0.753670
Mg10	0.650415	2.042221	2.411511
Mg11	3.082241	1.671166	-2.296201
Mg12	-3.869962	-1.619475	-0.215221

@mg12-isomer65 bp86/6-31G(d) Etot=-2401.046676 Eb=-10.99

Mg1	-2.378392	0.169383	-1.875622
Mg2	3.273827	0.149000	0.945932
Mg3	0.950580	2.032373	1.806650
Mg4	3.319460	-0.329062	-2.055786
Mg5	-4.528574	1.757949	-0.199919
Mg6	-0.889457	-2.209872	-0.280118
Mg7	0.720806	-1.125143	2.235737
Mg8	2.585139	2.544345	-0.878788
Mg9	-4.089492	-1.401856	0.085571
Mg10	-1.721523	0.601054	1.164465
Mg11	2.186637	-2.565133	-0.030533
Mg12	0.570990	0.376962	-0.917588

@mg12-isomer66 bp86/6-31G(d) Etot=-2401.046122 Eb=-10.96

Mg1	-2.892592	0.756757	1.577123
Mg2	1.873886	-1.485538	-1.527418
Mg3	-0.732477	2.641350	-0.000077
Mg4	-0.484483	-0.306923	0.000044
Mg5	-2.892748	0.756756	-1.576923
Mg6	0.262006	1.244460	2.569286
Mg7	0.261774	1.244222	-2.569402
Mg8	2.210440	1.885313	-0.000164
Mg9	-0.431835	-3.194137	-0.000046
Mg10	1.873866	-1.485563	1.527471
Mg11	4.332736	-0.184057	0.000047
Mg12	-3.380573	-1.872640	0.000060

@mg12-isomer67 bp86/6-31G(d) Etot=-2401.046114 Eb=-10.96

Mg1	-0.010761	0.475206	-1.072461
Mg2	1.282433	-2.326026	-0.488821
Mg3	4.141648	-2.074488	0.419584
Mg4	-1.140298	-1.260455	1.369594
Mg5	1.817131	2.896463	-0.016744
Mg6	-1.743336	-2.227851	-1.433889
Mg7	-4.150871	-2.025815	0.357172
Mg8	3.317455	0.413203	-1.178750
Mg9	-3.196772	0.835469	-0.052400
Mg10	-0.742769	1.960034	1.632331
Mg11	1.936046	0.109359	1.482644
Mg12	-1.509907	3.224901	-1.018260

@mg12-isomer68 bp86/6-31G(d) Etot=-2401.045967 Eb=-10.95

Mg1	3.504907	0.322728	-1.558312
Mg2	0.666906	1.666857	2.558876
Mg3	3.505006	0.322701	1.558205
Mg4	-1.003529	2.417208	0.000083
Mg5	2.857829	-2.315697	-0.000040
Mg6	-1.594700	-0.332755	1.790886
Mg7	-3.932884	1.189324	-0.000057
Mg8	0.666849	1.666940	-2.558795
Mg9	-1.594740	-0.332663	-1.790824
Mg10	-0.445253	-2.722118	-0.000044

Mg11	-3.533326	-1.952602	0.000004	
Mg12	0.902934	0.070075	0.000020	
@mg12-isomer69 bp86/6-31G(d) Etot=-2401.045585 Eb=-10.93				
Mg1	-3.954294	-0.934532	-1.305979	
Mg2	-1.042204	-2.481775	-0.819428	
Mg3	-1.391705	0.768520	-1.320821	
Mg4	-2.452671	-0.883562	1.335248	
Mg5	-3.691604	1.780347	0.330206	
Mg6	1.391954	-0.768721	-1.321051	
Mg7	-0.520502	1.550726	1.780735	
Mg8	0.520362	-1.550526	1.780778	
Mg9	3.954418	0.934517	-1.305818	
Mg10	3.691525	-1.780384	0.330507	
Mg11	1.042302	2.481780	-0.819579	
Mg12	2.452419	0.883611	1.335202	
@mg12-isomer70 bp86/6-31G(d) Etot=-2401.044049 Eb=-10.85				
Mg1	-1.433611	0.000029	-0.818194	
Mg2	-2.669709	2.532204	0.402518	
Mg3	2.921049	-2.646232	-0.131394	
Mg4	0.217043	1.585916	1.421026	
Mg5	-0.025223	2.713140	-1.370253	
Mg6	1.925493	-0.000044	-1.421289	
Mg7	0.216798	-1.585865	1.421123	
Mg8	-2.670040	-2.532002	0.402404	
Mg9	-4.381962	0.000241	0.135272	
Mg10	2.921336	2.646016	-0.131356	
Mg11	-0.025508	-2.713262	-1.370087	
Mg12	3.004335	-0.000140	1.460230	
@mg12-isomer71 bp86/6-31G(d) Etot=-2401.043935 Eb=-10.85				
Mg1	1.307660	-1.362855	-2.151294	
Mg2	3.003082	-3.025737	-0.162610	
Mg3	-2.599888	-2.190708	1.472487	
Mg4	-4.320354	0.000115	0.000015	
Mg5	-1.663172	0.840792	1.322962	
Mg6	3.305982	0.000018	-0.000204	
Mg7	0.459485	1.521939	-0.860864	
Mg8	-1.663279	-0.840812	-1.322907	
Mg9	3.003051	3.025823	0.162745	
Mg10	1.307725	1.362643	2.151348	
Mg11	-2.599703	2.190769	-1.472631	
Mg12	0.459410	-1.521987	0.860953	
@mg12-isomer72 bp86/6-31G(d) Etot=-2401.043918 Eb=-10.85				
Mg1	0.784297	-1.098141	1.901616	
Mg2	-2.443728	0.591516	-1.826364	
Mg3	-4.145184	-1.596482	-0.259905	
Mg4	3.017471	1.416993	-2.199261	
Mg5	0.346628	1.948013	2.290009	
Mg6	-0.896539	-1.939368	-0.692594	
Mg7	3.015338	1.108457	0.843896	
Mg8	1.397659	-3.944883	0.488678	
Mg9	2.199200	-1.348207	-1.025471	
Mg10	-1.943606	0.277477	1.205311	
Mg11	0.356019	1.180132	-0.814861	
Mg12	-1.687554	3.404494	0.088945	
@mg12-isomer73 bp86/6-31G(d) Etot=-2401.043710 Eb=-10.84				
Mg1	0.745495	2.016339	0.000130	
Mg2	-2.319270	2.240046	0.000140	
Mg3	-0.553451	-0.890465	-0.000131	
Mg4	2.005184	-0.388516	-1.604218	

Mg5	4.273804	1.091937	0.000120
Mg6	2.005157	-0.388831	1.604174
Mg7	-2.507203	-3.104357	-0.000020
Mg8	-3.234559	-0.455255	1.518257
Mg9	-0.715696	1.214045	-2.536785
Mg10	-3.234561	-0.455135	-1.518401
Mg11	-0.715672	1.213736	2.536906
Mg12	4.250773	-2.093544	-0.000170

@mg12-isomer74 bp86/6-31G(d) Etot=-2401.042849 Eb=-10.79

Mg1	0.055977	0.000040	0.750751
Mg2	-2.548199	1.562064	1.233969
Mg3	2.481257	-1.559840	-0.368060
Mg4	0.642056	-0.000400	-2.492078
Mg5	-0.462388	2.540493	-1.102346
Mg6	-2.267204	-0.000199	-1.413476
Mg7	5.232717	0.000127	0.570376
Mg8	-5.318649	0.000185	0.725562
Mg9	-2.548285	-1.561706	1.234383
Mg10	2.481239	1.559690	-0.368542
Mg11	2.713910	0.000382	2.331068
Mg12	-0.462431	-2.540833	-1.101607

@mg12-isomer75 bp86/6-31G(d) Etot=-2401.042624 Eb=-10.78

Mg1	0.566566	-1.047778	1.742153
Mg2	-2.599392	-1.074700	1.737028
Mg3	1.453175	0.246327	-1.262255
Mg4	3.612126	-0.495735	0.958304
Mg5	-0.742831	-1.844162	-0.887142
Mg6	-1.171221	1.373779	0.109177
Mg7	-4.118946	1.607889	1.188516
Mg8	-1.042269	0.349972	-3.010069
Mg9	-3.569033	-0.292332	-1.097929
Mg10	2.075079	-2.964670	-0.103644
Mg11	1.616343	2.025977	1.314704
Mg12	3.920403	2.115433	-0.688844

@mg12-isomer76 bp86/6-31G(d) Etot=-2401.042357 Eb=-10.77

Mg1	-1.069668	1.695819	1.604316
Mg2	-3.467978	-2.551919	-0.209860
Mg3	-3.467830	2.552021	-0.209916
Mg4	0.864700	-0.000025	-0.083802
Mg5	-2.085773	0.000011	-1.257381
Mg6	-0.325229	2.548101	-1.295574
Mg7	1.111432	-0.000002	2.968926
Mg8	3.790788	-0.000073	1.042184
Mg9	-1.069719	-1.695783	1.604333
Mg10	3.022315	1.640225	-1.433775
Mg11	3.022292	-1.640241	-1.433879
Mg12	-0.325329	-2.548132	-1.295572

@mg12-isomer77 bp86/6-31G(d) Etot=-2401.042327 Eb=-10.76

Mg1	2.315449	2.581875	-0.058339
Mg2	2.380305	-0.000111	1.695514
Mg3	-2.539855	0.000080	-0.485601
Mg4	-0.419897	-1.651040	1.430015
Mg5	4.045337	-0.000179	-0.773754
Mg6	-0.419577	1.651552	1.429803
Mg7	-0.800380	-2.717775	-1.361789
Mg8	-3.429412	-2.769053	0.295830
Mg9	0.782112	-0.000127	-1.047286
Mg10	-3.429091	2.769234	0.295987
Mg11	-0.800159	2.717708	-1.362104
Mg12	2.315167	-2.582164	-0.058274

@mg12-isomer78 bp86/6-31G(d) Etot=-2401.042296 Eb=-10.76

Mg1	0.148357	0.527141	-1.010617
Mg2	0.483810	-2.744779	-0.776858
Mg3	-1.347434	-1.000281	1.278631
Mg4	-2.303479	-1.376137	-1.545615
Mg5	3.453754	0.534273	-0.111787
Mg6	3.540796	-2.523798	-0.536730
Mg7	1.811852	-1.406470	1.667017
Mg8	-1.131053	3.401663	-0.085640
Mg9	-3.205511	1.289704	-0.198386
Mg10	1.961007	3.053483	-0.924629
Mg11	1.016169	1.735880	1.648412
Mg12	-4.428267	-1.490679	0.596202

@mg12-isomer79 bp86/6-31G(d) Etot=-2401.042046 Eb=-10.75

Mg1	-4.076296	1.935838	-0.237188
Mg2	-1.187256	1.800399	0.927043
Mg3	3.285990	-0.915506	-0.261166
Mg4	-1.633455	1.427710	-2.067438
Mg5	-3.114373	-0.951254	-0.039035
Mg6	1.355248	2.065114	-0.979534
Mg7	-1.180504	-3.261556	0.337320
Mg8	1.501965	-3.038241	-1.704663
Mg9	0.074709	-0.673847	-0.516127
Mg10	1.663896	0.670290	1.880641
Mg11	-0.869617	-1.054108	2.461688
Mg12	4.179694	1.995160	0.198460

@mg12-isomer80 bp86/6-31G(d) Etot=-2401.041856 Eb=-10.74

Mg1	-0.000060	0.101368	-0.443624
Mg2	-2.672908	0.595039	1.281644
Mg3	1.738489	2.730865	-0.784202
Mg4	-0.000027	2.379661	1.742457
Mg5	-4.415113	-1.898977	0.456496
Mg6	2.672886	0.595020	1.281627
Mg7	-1.561879	-2.574122	-0.018355
Mg8	3.049587	-0.093345	-1.585001
Mg9	-3.049614	-0.093377	-1.585008
Mg10	4.415215	-1.898939	0.456428
Mg11	-1.738486	2.730855	-0.784243
Mg12	1.561910	-2.574049	-0.018219

@mg12-isomer81 bp86/6-31G(d) Etot=-2401.041717 Eb=-10.73

Mg1	-1.665512	0.262811	1.294561
Mg2	-0.980960	-2.843389	0.125922
Mg3	2.274114	-2.834532	0.253415
Mg4	-2.267836	-0.523329	-1.586800
Mg5	-3.881000	-1.836254	0.496852
Mg6	-0.785709	2.576851	-0.755002
Mg7	2.622213	2.277331	-0.660112
Mg8	-3.786188	1.839763	-0.283439
Mg9	0.752193	-0.264787	-0.666150
Mg10	3.729031	-0.657860	-1.436195
Mg11	3.145581	-0.103750	1.407319
Mg12	0.844074	2.107144	1.809629

@mg12-isomer82 bp86/6-31G(d) Etot=-2401.041479 Eb=-10.72

Mg1	1.625343	-1.366467	0.226991
Mg2	-1.044270	-1.127668	-1.491196
Mg3	-0.327333	1.105465	0.895570
Mg4	-1.998158	2.082119	-1.453349
Mg5	-3.365743	-2.890711	-0.535548
Mg6	-2.815361	2.759576	1.492807

Mg7	-3.418514	0.003877	0.528579
Mg8	2.943168	1.646645	0.581685
Mg9	4.109203	-0.310358	-1.382759
Mg10	-1.176010	-2.118480	1.449433
Mg11	1.042634	1.005048	-1.988627
Mg12	4.425042	-0.789047	1.676415

@mg12-isomer83 bp86/6-31G(d) Etot=-2401.041459 Eb=-10.72

Mg1	2.860399	-2.481258	0.227156
Mg2	-2.014760	0.000010	-0.996949
Mg3	-2.138474	1.583280	1.699184
Mg4	-0.066534	-2.549839	-0.470952
Mg5	0.765839	0.000028	1.251131
Mg6	1.731888	-0.000048	-1.545006
Mg7	4.548740	-0.000021	0.061843
Mg8	2.860435	2.481247	0.227139
Mg9	-2.138557	-1.583274	1.699177
Mg10	-3.171229	2.852825	-0.840805
Mg11	-0.066495	2.549822	-0.471044
Mg12	-3.171252	-2.852772	-0.840874

@mg12-isomer84 bp86/6-31G(d) Etot=-2401.041288 Eb=-10.71

Mg1	-1.798604	0.364906	-1.372294
Mg2	0.910743	-1.410245	-1.067928
Mg3	-4.052098	-1.020306	0.299813
Mg4	3.391757	0.651219	-0.282715
Mg5	-2.817862	1.805349	1.102698
Mg6	-1.215403	-1.644396	1.328403
Mg7	2.238442	3.445113	-0.210619
Mg8	3.950264	-2.388729	-0.348215
Mg9	-2.040454	-2.787076	-1.305464
Mg10	-0.908406	3.217479	-0.848236
Mg11	1.981959	-1.399019	1.750578
Mg12	0.359662	1.165706	0.953977

@mg12-isomer85 bp86/6-31G(d) Etot=-2401.041150 Eb=-10.70

Mg1	1.284580	-1.575144	-0.229216
Mg2	3.967704	-0.000662	0.469756
Mg3	-3.633693	1.561485	1.317701
Mg4	-1.564201	2.525808	-0.991193
Mg5	-3.351959	0.000553	-1.272894
Mg6	1.667877	-0.000756	2.425727
Mg7	-1.060971	-0.000368	1.068620
Mg8	1.284891	1.574778	-0.228566
Mg9	-1.564714	-2.525261	-0.992433
Mg10	-0.459128	0.000519	-2.444713
Mg11	7.063693	0.000605	-0.439738
Mg12	-3.634078	-1.561556	1.316948

@mg12-isomer86 bp86/6-31G(d) Etot=-2401.041061 Eb=-10.70

Mg1	-2.244725	-0.652022	0.615866
Mg2	0.895236	-0.223722	1.906706
Mg3	-0.817223	-2.829998	2.058964
Mg4	0.376453	1.227145	-0.870960
Mg5	2.999090	-0.047431	-0.351798
Mg6	-1.467510	-0.661739	-2.532290
Mg7	6.156573	0.091646	-0.321714
Mg8	-2.539314	1.890110	-0.980786
Mg9	-0.745101	4.516392	0.072613
Mg10	-1.969846	-3.332693	-0.774521
Mg11	-1.315371	1.935598	1.886047
Mg12	0.671738	-1.913286	-0.708126

@mg12-isomer87 bp86/6-31G(d) Etot=-2401.040738 Eb=-10.68

Mg1	0.963896	1.623667	-1.082437
Mg2	0.708357	-1.278486	-2.022789
Mg3	-1.617380	3.071442	-1.702914
Mg4	-1.895302	0.175507	-1.161510
Mg5	1.922137	1.710598	1.972226
Mg6	3.109886	-0.238453	-0.125556
Mg7	6.029403	-1.449318	-0.121779
Mg8	-1.103349	2.141044	1.218098
Mg9	-4.662633	-1.793234	-0.038165
Mg10	-2.459151	-0.550963	1.963108
Mg11	0.476194	-0.792072	1.267691
Mg12	-1.472057	-2.619731	-0.165973

@mg12-isomer88 bp86/6-31G(d) Etot=-2401.039941 Eb=-10.64

Mg1	-0.038159	-0.652975	1.496309
Mg2	0.033300	-0.054859	-1.557317
Mg3	0.373201	2.405606	0.423543
Mg4	-3.144837	-1.395147	1.729775
Mg5	2.813590	0.283430	0.055146
Mg6	-1.591551	-2.684046	-0.476285
Mg7	1.502573	-2.607703	-0.360230
Mg8	-1.904479	2.394548	-1.671688
Mg9	-3.408272	-0.307443	-1.131949
Mg10	3.402143	3.225250	0.468035
Mg11	-2.521584	1.598607	1.171886
Mg12	4.484075	-2.205268	-0.147225

@mg12-isomer89 bp86/6-31G(d) Etot=-2401.039874 Eb=-10.64

Mg1	3.674342	-0.679369	0.703604
Mg2	1.667748	0.410268	-1.364579
Mg3	-1.047995	-1.347757	-1.434122
Mg4	-3.842060	2.411932	0.885495
Mg5	4.325069	2.159654	-0.559483
Mg6	0.398170	-0.774246	1.267604
Mg7	-1.249844	-3.344727	0.814915
Mg8	-0.990269	1.835538	-0.171932
Mg9	-3.559099	0.771226	-1.667394
Mg10	1.863956	2.091114	1.175472
Mg11	-2.959635	-0.682778	0.934985
Mg12	1.719617	-2.850855	-0.584565

@mg12-isomer90 bp86/6-31G(d) Etot=-2401.039735 Eb=-10.63

Mg1	2.540289	-2.318284	-1.053639
Mg2	-1.666389	-1.110934	1.416487
Mg3	-1.867970	0.224898	-1.409564
Mg4	0.651377	-0.556954	-3.032085
Mg5	-3.829275	1.237525	0.712403
Mg6	-4.325616	-1.709076	-0.176729
Mg7	3.767190	-0.335858	1.048148
Mg8	0.901868	-0.044778	0.030973
Mg9	2.407503	2.530005	0.944657
Mg10	1.331376	-2.302118	1.846856
Mg11	0.818292	2.354269	-1.684471
Mg12	-0.728645	2.031307	1.356965

@mg12-isomer91 bp86/6-31G(d) Etot=-2401.039732 Eb=-10.63

Mg1	3.897624	-1.636391	-0.307990
Mg2	1.081920	-2.911843	-1.207822
Mg3	-3.038998	1.381178	1.064016
Mg4	-4.308884	-1.412756	1.261239
Mg5	0.271789	1.488126	1.308479
Mg6	-1.084525	1.751595	-1.472598
Mg7	2.036059	2.969088	-0.741116
Mg8	-1.281029	-1.187521	0.000992

Mg9	1.482304	-1.502678	1.526088
Mg10	1.432761	0.072789	-1.359490
Mg11	-3.873419	-0.047545	-1.468967
Mg12	3.384398	1.035959	1.397169
@mg12-isomer92 bp86/6-31G(d) Etot=-2401.039566 Eb=-10.62			
Mg1	0.545836	-0.935651	0.816616
Mg2	-1.136367	2.295555	0.520568
Mg3	-2.448623	-0.449774	1.515622
Mg4	-1.827384	-0.252061	-1.558235
Mg5	1.099065	0.962382	-1.722043
Mg6	-4.571027	-1.925476	-0.449391
Mg7	2.056058	1.755173	1.176118
Mg8	-0.333374	1.104008	3.127845
Mg9	3.314158	-0.555694	-0.322842
Mg10	6.260195	-1.702938	-0.495695
Mg11	-1.573478	-2.922287	-0.173190
Mg12	-1.385059	2.626762	-2.435372
@mg12-isomer93 bp86/6-31G(d) Etot=-2401.039399 Eb=-10.61			
Mg1	-0.934899	0.093419	0.000026
Mg2	-1.538657	-2.800023	0.000059
Mg3	-1.735492	-1.251257	-2.668842
Mg4	-3.181739	1.414477	-1.554994
Mg5	-1.735359	-1.251151	2.668933
Mg6	1.890528	1.392327	-0.000081
Mg7	1.204380	-1.239987	-1.669331
Mg8	3.861058	-1.208572	-0.000068
Mg9	-0.933639	3.042478	-0.000274
Mg10	-3.181436	1.414733	1.555210
Mg11	5.080774	1.633465	0.000023
Mg12	1.204480	-1.239908	1.669339
@mg12-isomer94 bp86/6-31G(d) Etot=-2401.039344 Eb=-10.61			
Mg1	-0.927360	-2.136727	-0.566098
Mg2	0.812397	0.427534	-1.516229
Mg3	-2.560843	-0.858274	1.764537
Mg4	0.600212	-0.162501	1.478642
Mg5	4.984961	-1.723541	-0.015613
Mg6	-3.993223	-2.595629	-0.421161
Mg7	-1.180225	2.923766	-1.522498
Mg8	-1.725528	2.174990	1.373061
Mg9	2.089248	-2.285787	-0.239034
Mg10	-2.919000	0.418872	-0.922475
Mg11	3.541861	0.937580	0.160479
Mg12	1.277500	2.879718	0.426389
@mg12-isomer95 bp86/6-31G(d) Etot=-2401.037824 Eb=-10.53			
Mg1	-5.057875	-1.056256	-0.680871
Mg2	-3.613502	1.613642	-0.961430
Mg3	2.227965	1.907574	-1.510006
Mg4	-2.001147	-1.299132	-0.867132
Mg5	-0.457216	1.323837	0.087343
Mg6	1.062452	-1.301337	-1.213531
Mg7	2.816495	-2.653328	0.870523
Mg8	1.620504	3.220229	1.246977
Mg9	4.065385	-0.770169	-1.501708
Mg10	-3.188826	0.029609	1.630246
Mg11	2.575008	0.402699	1.148584
Mg12	-0.049245	-1.417368	1.751008
@mg12-isomer96 bp86/6-31G(d) Etot=-2401.036761 Eb=-10.47			
Mg1	-3.767301	1.560948	-0.848106
Mg2	1.366665	0.185091	-1.272149

Mg3	3.865974	0.171978	0.708321
Mg4	-4.064600	0.537757	2.021072
Mg5	3.163821	2.646012	-1.163397
Mg6	1.540320	2.061705	1.388054
Mg7	1.315288	-1.234728	1.929614
Mg8	-3.476296	-1.427814	-0.300651
Mg9	2.862122	-2.711521	-0.258534
Mg10	-0.242589	-2.271047	-0.519529
Mg11	-1.417587	-0.086287	-2.440236
Mg12	-1.145816	0.567906	0.755541

@mg12-isomer97 bp86/6-31G(d) Etot=-2401.036408 Eb=-10.45

Mg1	-0.393108	1.370505	-0.430704
Mg2	1.488742	0.054221	-2.445062
Mg3	1.583512	-1.070114	0.603186
Mg4	-0.808846	-1.713549	-1.379782
Mg5	-1.334524	-1.266281	1.708289
Mg6	-2.327521	1.937676	1.903591
Mg7	-3.091297	-3.149860	0.075951
Mg8	2.921294	1.809504	-0.054828
Mg9	-3.023722	2.822838	-0.995003
Mg10	4.310856	-0.711065	-0.912967
Mg11	4.172410	-0.016840	2.108599
Mg12	-3.497796	-0.067034	-0.181270

@mg12-isomer98 bp86/6-31G(d) Etot=-2401.035842 Eb=-10.42

Mg1	-1.196702	1.072958	-1.372494
Mg2	0.508674	3.703997	-0.578357
Mg3	1.988418	0.894793	-0.832667
Mg4	2.865441	-2.413569	-0.826309
Mg5	-2.454453	3.168208	0.496833
Mg6	2.390205	-0.838171	1.727120
Mg7	-0.220233	-1.606485	0.052201
Mg8	-2.770105	-1.680709	-1.740003
Mg9	-0.050801	1.435659	1.451668
Mg10	-2.964376	-0.156094	0.890575
Mg11	4.833698	-0.202666	-0.023879
Mg12	-2.929766	-3.377920	0.755311

@mg12-isomer99 bp86/6-31G(d) Etot=-2401.035638 Eb=-10.41

Mg1	-2.248892	0.000016	1.343520
Mg2	0.956113	-0.000028	1.659694
Mg3	-0.368527	-0.000023	-1.104748
Mg4	2.517256	1.565120	-0.551789
Mg5	-0.489106	2.591380	0.561889
Mg6	-3.246138	-1.556360	-1.172670
Mg7	2.517297	-1.565123	-0.551857
Mg8	5.058574	0.000045	-1.470326
Mg9	-3.246120	1.556365	-1.172689
Mg10	-5.406591	0.000037	0.431729
Mg11	4.445251	0.000007	1.465358
Mg12	-0.489117	-2.591437	0.561889

@mg12-isomer100 bp86/6-31G(d) Etot=-2401.034243 Eb=-10.34

Mg1	-0.903887	-0.800066	1.087365
Mg2	-2.033830	2.402181	1.243041
Mg3	-3.725444	-0.225738	-0.030815
Mg4	1.309725	-0.913007	-1.162723
Mg5	-0.211675	4.180632	-0.659698
Mg6	2.324214	-0.967641	1.706241
Mg7	4.180407	-2.277550	-0.431334
Mg8	-3.048823	-3.339564	0.707730
Mg9	-1.219512	1.281376	-1.396660
Mg10	-1.716260	-1.959133	-1.650287

Mg11	1.028127	1.782507	0.709129
Mg12	4.016958	0.836003	-0.121988
@mg12-isomer101 bp86/6-31G(d) Etot=-2401.033840 Eb=-10.32			
Mg1	-0.018384	-1.332457	0.657154
Mg2	-1.959561	0.044898	-1.297794
Mg3	-0.543550	1.827406	0.730395
Mg4	2.527660	0.840687	1.150053
Mg5	3.311603	-1.721829	-0.327915
Mg6	5.520447	-0.156520	1.157308
Mg7	1.193375	0.493459	-1.565206
Mg8	-2.862163	-2.757969	-0.076563
Mg9	4.512517	0.829370	-1.481279
Mg10	-3.658975	2.442356	0.046445
Mg11	-5.013153	-0.337441	-0.594596
Mg12	-3.009816	-0.171960	1.601997
@mg12-isomer102 bp86/6-31G(d) Etot=-2401.033455 Eb=-10.30			
Mg1	-0.981148	1.792313	-1.040780
Mg2	-4.235146	1.403493	-1.011663
Mg3	-2.229459	-1.179434	-0.414489
Mg4	2.227307	1.701931	-0.693202
Mg5	0.421057	-0.183412	1.008213
Mg6	5.306866	0.741218	-0.340307
Mg7	-5.153364	-0.759089	0.894963
Mg8	0.497601	-0.796231	-1.970489
Mg9	3.421296	0.771588	2.063630
Mg10	0.404350	-3.153485	-0.006324
Mg11	-2.764628	1.095545	1.611934
Mg12	3.085267	-1.434436	-0.101486
@mg12-isomer103 bp86/6-31G(d) Etot=-2401.033191 Eb=-10.29			
Mg1	-4.023447	-1.622836	-1.112986
Mg2	0.010614	0.501055	1.516612
Mg3	3.078607	1.435868	0.494759
Mg4	-2.179669	1.015771	-0.631598
Mg5	-5.343983	0.911876	-0.118645
Mg6	-0.958962	-1.979087	-0.043605
Mg7	0.395467	3.098681	-0.120199
Mg8	-3.432848	-0.695567	1.686401
Mg9	2.252571	-1.762893	0.475932
Mg10	5.222452	-0.704410	0.999040
Mg11	4.107791	-0.480918	-1.786394
Mg12	0.871407	0.282459	-1.359317
@mg12-isomer104 bp86/6-31G(d) Etot=-2401.032586 Eb=-10.25			
Mg1	-0.805835	1.338907	-1.998848
Mg2	-5.632530	0.415425	0.344188
Mg3	2.064148	0.177269	-1.338947
Mg4	0.673609	2.021422	0.638333
Mg5	-3.487640	-1.524630	1.448920
Mg6	-0.455031	-1.058041	0.059895
Mg7	4.925366	-0.778342	-0.180354
Mg8	-3.410641	-0.663113	-1.468433
Mg9	3.941240	2.080809	0.611753
Mg10	2.197765	-2.810199	-0.442591
Mg11	2.481402	-0.515889	1.604620
Mg12	-2.491853	1.316382	0.721464
@mg12-isomer105 bp86/6-31G(d) Etot=-2401.032463 Eb=-10.25			
Mg1	-0.762872	1.049991	1.114652
Mg2	-1.252975	-2.027965	0.454702
Mg3	-3.832045	-0.365884	1.483176
Mg4	1.772307	-1.238827	1.066049

Mg5	-2.639354	0.255177	-1.292453
Mg6	2.216328	1.876529	0.040420
Mg7	-4.078232	-2.615532	-0.634775
Mg8	0.560116	-0.336563	-1.555070
Mg9	4.584533	-2.817828	0.707130
Mg10	0.381777	3.925515	1.256662
Mg11	-0.640557	2.761767	-1.389832
Mg12	3.690972	-0.466381	-1.250662

@mg12-isomer106 bp86/6-31G(d) Etot=-2401.032305 Eb=-10.24

Mg1	1.997723	1.668616	0.412700
Mg2	-0.347381	0.541193	-1.453639
Mg3	-0.971605	-2.466629	-0.853113
Mg4	4.399561	-0.000084	0.000037
Mg5	-0.971550	2.466559	0.853233
Mg6	1.997664	-1.668675	-0.412637
Mg7	-3.045587	-2.214238	1.402135
Mg8	-3.045404	2.214378	-1.402189
Mg9	-3.612405	0.858266	1.279967
Mg10	7.558707	0.000073	-0.000075
Mg11	-3.612307	-0.858182	-1.280139
Mg12	-0.347416	-0.541278	1.453719

@mg12-isomer107 bp86/6-31G(d) Etot=-2401.031893 Eb=-10.22

Mg1	2.739069	-0.957232	1.205138
Mg2	4.530605	-0.230978	-1.155371
Mg3	0.403916	1.356555	1.753068
Mg4	3.548973	2.123396	1.055722
Mg5	-0.355371	-1.296598	0.128580
Mg6	-1.301279	1.851650	-0.870845
Mg7	-3.406026	-1.011641	-1.133712
Mg8	2.180451	-2.369728	-1.487986
Mg9	-4.347464	1.953932	-1.262511
Mg10	1.608778	0.868583	-1.080012
Mg11	-2.818767	0.419485	1.435461
Mg12	-2.782885	-2.707424	1.412467

@mg12-isomer108 bp86/6-31G(d) Etot=-2401.031487 Eb=-10.20

Mg1	-3.228328	0.412250	-1.085321
Mg2	-1.980920	3.215855	-1.107076
Mg3	2.048222	-0.523862	-1.233037
Mg4	-2.958344	2.007962	1.598764
Mg5	3.049617	1.394140	1.010614
Mg6	-2.324564	-1.261739	1.491740
Mg7	-0.247163	1.201477	0.373294
Mg8	4.261797	-1.380356	0.774795
Mg9	-3.738691	-2.596530	-0.980821
Mg10	-0.760438	-1.914181	-1.029343
Mg11	4.955230	0.758744	-1.460335
Mg12	0.923581	-1.313759	1.646727

@mg12-isomer109 bp86/6-31G(d) Etot=-2401.030787 Eb=-10.16

Mg1	0.429183	-0.000006	-0.999726
Mg2	-2.251000	0.000023	0.929843
Mg3	-2.313136	1.589025	-1.681716
Mg4	-0.324042	2.618603	0.680752
Mg5	2.600693	-1.732018	0.590062
Mg6	-3.438379	-3.002742	0.874533
Mg7	-2.313220	-1.588988	-1.681696
Mg8	2.600716	1.731979	0.590058
Mg9	5.071529	-0.000028	0.947874
Mg10	-3.438300	3.002763	0.874515
Mg11	3.700037	-0.000015	-1.805205
Mg12	-0.324080	-2.618595	0.680705

@mg12-isomer110 bp86/6-31G(d) Etot=-2401.030029 Eb=-10.12

Mg1	4.446860	-2.265449	-0.000008
Mg2	1.492793	-2.854785	0.000041
Mg3	-2.856682	-0.000285	1.448894
Mg4	-1.492763	-2.854799	0.000042
Mg5	1.868769	2.594450	-0.000023
Mg6	-2.856606	-0.000329	-1.448937
Mg7	-0.000008	0.003970	0.000046
Mg8	-1.868801	2.594443	-0.000024
Mg9	2.856617	-0.000306	-1.448944
Mg10	-4.446836	-2.265495	-0.000017
Mg11	-0.000020	5.048863	0.000038
Mg12	2.856679	-0.000278	1.448893

@mg12-isomer111 bp86/6-31G(d) Etot=-2401.030020 Eb=-10.12

Mg1	-0.858317	1.759421	1.157496
Mg2	-3.876571	1.232962	0.097282
Mg3	-4.142883	-1.855413	-0.568972
Mg4	0.957796	-1.135060	0.902114
Mg5	-1.190602	-3.143701	-0.376847
Mg6	-2.116770	-1.142715	1.690783
Mg7	-1.328608	-0.263848	-1.250937
Mg8	1.429296	1.569143	-1.018547
Mg9	3.784775	-0.275004	0.101718
Mg10	-1.652950	2.679535	-1.635630
Mg11	6.668393	-1.135865	-0.947144
Mg12	2.326441	1.710545	1.848684

@mg12-isomer112 bp86/6-31G(d) Etot=-2401.029045 Eb=-10.07

Mg1	-0.927510	1.402852	1.106617
Mg2	-1.738551	-1.734620	1.927387
Mg3	1.367422	-0.932146	1.219118
Mg4	-3.773561	0.093235	0.203915
Mg5	-3.457971	-2.837642	-0.380541
Mg6	-0.892763	-1.229438	-0.961597
Mg7	2.390030	-1.950771	-1.466528
Mg8	1.256643	1.103776	-1.199852
Mg9	-3.470455	3.107390	0.594974
Mg10	-1.769578	1.924542	-1.729758
Mg11	4.007471	0.303928	-0.170634
Mg12	7.008825	0.748894	0.856898

@mg12-isomer113 bp86/6-31G(d) Etot=-2401.028839 Eb=-10.06

Mg1	-1.755165	-1.818950	0.478512
Mg2	-4.083415	0.523268	1.317929
Mg3	-3.193220	0.263763	-1.481244
Mg4	1.204891	-1.077506	1.198687
Mg5	4.396660	-0.213997	1.798443
Mg6	0.256635	-0.709143	-1.661952
Mg7	5.704207	0.800321	-0.713311
Mg8	-4.759268	-2.108653	-0.149226
Mg9	3.598517	-1.394037	-0.965230
Mg10	-3.090410	3.170164	-0.106885
Mg11	-0.798364	1.217915	0.496689
Mg12	2.518930	1.346853	-0.212412

@mg12-isomer114 bp86/6-31G(d) Etot=-2401.028098 Eb=-10.02

Mg1	0.297643	1.376067	-1.938851
Mg2	-2.663166	0.066725	-1.426506
Mg3	0.315489	-1.002909	0.070017
Mg4	1.965578	1.797510	0.612872
Mg5	-5.584286	-1.007198	-0.431768
Mg6	-2.947315	-1.201622	1.313654

Mg7	-1.156544	1.568350	0.805796
Mg8	3.190474	-0.354671	-1.380729
Mg9	3.599110	-0.950384	1.489972
Mg10	5.063882	1.534190	0.282831
Mg11	2.343321	-3.265080	-0.262904
Mg12	-4.424186	1.439023	0.865617

@mg12-isomer115 bp86/6-31G(d) Etot=-2401.026990 Eb=-9.96

Mg1	-1.230817	-0.000001	0.995609
Mg2	-4.174176	-1.514631	1.077650
Mg3	1.363325	1.623447	0.496121
Mg4	0.050128	-0.000059	-1.786868
Mg5	-4.174315	1.514382	1.078019
Mg6	1.363405	-1.623285	0.496278
Mg7	4.158404	-2.779747	-0.081419
Mg8	4.301968	-0.000032	1.371175
Mg9	4.158457	2.779732	-0.081388
Mg10	3.460196	-0.000030	-1.431100
Mg11	-3.115065	0.000201	-1.463577
Mg12	-6.161509	0.000022	-0.670500

@mg12-isomer116 bp86/6-31G(d) Etot=-2401.025703 Eb=-9.89

Mg1	-1.722762	2.007523	0.783918
Mg2	-4.598275	-2.442301	-0.525346
Mg3	0.350538	-0.306525	0.283392
Mg4	2.697622	-2.432917	-0.258122
Mg5	2.935532	0.585117	-1.237508
Mg6	-2.589897	-1.168314	1.454511
Mg7	1.492793	2.631909	0.815243
Mg8	-4.956089	0.522974	0.399793
Mg9	3.311293	-0.075030	1.657307
Mg10	-2.440831	-0.098463	-1.396979
Mg11	5.533254	-1.291540	-0.221344
Mg12	-0.013179	2.067567	-1.754865

@mg12-isomer117 bp86/6-31G(d) Etot=-2401.024916 Eb=-9.85

Mg1	-0.175969	-0.853205	-0.311542
Mg2	2.723183	0.371291	-0.816507
Mg3	1.075854	1.809896	1.495587
Mg4	4.936504	-1.660700	0.178703
Mg5	-2.112644	1.743625	0.520417
Mg6	2.270462	-1.281949	1.701832
Mg7	2.377031	-2.962445	-0.904450
Mg8	-2.279500	0.342716	-2.243779
Mg9	-0.466161	4.403107	0.707745
Mg10	-3.162983	-1.066333	0.309158
Mg11	-5.496868	-3.176658	0.782685
Mg12	0.311091	2.330655	-1.419848

@mg12-isomer118 bp86/6-31G(d) Etot=-2401.024734 Eb=-9.84

Mg1	1.427907	0.279019	-2.033466
Mg2	-4.082253	2.976134	-0.481068
Mg3	1.814055	-1.776732	0.328255
Mg4	-0.049572	-4.065025	0.869186
Mg5	-0.651052	-2.400768	-1.617763
Mg6	-1.623683	0.785858	-1.209177
Mg7	-1.427230	-1.326760	1.151844
Mg8	0.865880	1.346104	0.792401
Mg9	6.552476	1.945795	0.482105
Mg10	-2.189820	1.735684	1.601192
Mg11	-4.379243	-0.074307	0.216702
Mg12	3.742535	0.574998	-0.100211

@mg12-isomer119 bp86/6-31G(d) Etot=-2401.024697 Eb=-9.84

Mg1	1.696001	-0.614418	1.131750
Mg2	-0.727337	0.899988	-0.641207
Mg3	-3.524869	-0.425259	0.370733
Mg4	0.746464	2.396131	1.733900
Mg5	1.637198	-1.263108	-1.802591
Mg6	0.038142	4.122488	-0.705049
Mg7	-6.338493	-0.487808	-1.177650
Mg8	2.274590	1.747816	-0.972782
Mg9	4.459500	-0.425836	-0.519183
Mg10	1.846780	-3.692193	0.291794
Mg11	-0.859446	-2.182108	-0.028745
Mg12	-1.248529	-0.075693	2.319030

@mg12-isomer120 bp86/6-31G(d) Etot=-2401.024083 Eb=-9.81

Mg1	-0.668592	0.651566	0.898453
Mg2	-2.857309	0.265839	-1.405662
Mg3	2.423193	0.778541	2.046081
Mg4	-3.129590	2.546428	0.719766
Mg5	1.932481	1.308224	-0.904966
Mg6	1.431644	-1.677633	0.334362
Mg7	4.223519	-0.597093	0.037387
Mg8	7.298661	-0.616644	-0.708855
Mg9	-1.538805	-2.374605	0.022064
Mg10	-3.826059	-0.498704	1.377536
Mg11	-4.440659	-2.447994	-0.951832
Mg12	-0.848485	2.662076	-1.464334

@mg12-isomer121 bp86/6-31G(d) Etot=-2401.023807 Eb=-9.80

Mg1	-0.472942	0.763857	1.674266
Mg2	-2.221587	-1.285641	-0.345282
Mg3	-3.939148	0.603768	1.452052
Mg4	1.401259	2.642030	-0.044885
Mg5	-5.195029	-2.114710	0.377310
Mg6	0.812317	-0.386093	-0.885730
Mg7	3.876431	0.699997	-1.302544
Mg8	-4.720001	0.379964	-1.425728
Mg9	2.832814	0.047133	1.444304
Mg10	3.452744	-2.287063	-0.619380
Mg11	5.820976	-0.817319	0.578339
Mg12	-1.647834	1.754077	-0.902722

@mg12-isomer122 bp86/6-31G(d) Etot=-2401.023352 Eb=-9.77

Mg1	-1.072295	-1.594600	-1.573376
Mg2	-3.511251	-2.623863	0.001769
Mg3	-3.849412	0.001545	1.585663
Mg4	-3.849198	-0.000728	-1.585948
Mg5	1.056694	-0.000712	0.000228
Mg6	4.136835	-0.000484	0.000250
Mg7	-1.071812	1.594188	1.573530
Mg8	-3.510075	2.624533	-0.002011
Mg9	6.906877	1.656841	0.001861
Mg10	6.907750	-1.656335	-0.002125
Mg11	-1.071587	1.591937	-1.575702
Mg12	-1.072526	-1.592321	1.575861

@mg12-isomer123 bp86/6-31G(d) Etot=-2401.022732 Eb=-9.74

Mg1	0.955889	0.719575	0.384266
Mg2	-1.459319	2.482991	-0.677116
Mg3	-0.377051	-2.383542	0.795206
Mg4	2.091392	-1.807636	-1.206036
Mg5	2.650544	-1.718215	1.762468
Mg6	-1.168721	-0.802888	-1.647356
Mg7	-4.053068	0.739913	-1.095064
Mg8	-3.431237	-2.373113	-0.374216

Mg9	4.059834	0.236724	-0.033841
Mg10	-2.130415	0.080877	1.235362
Mg11	-3.751398	2.741139	1.326263
Mg12	6.613550	2.084177	-0.469936

@mg12-isomer124 bp86/6-31G(d) Etot=-2401.022547 Eb=-9.73

Mg1	-0.089810	-1.156342	0.845349
Mg2	2.999025	-2.992261	0.463135
Mg3	2.929515	0.012955	1.415585
Mg4	-2.277189	1.418199	0.721756
Mg5	2.013327	-0.677360	-1.417444
Mg6	-3.050919	-1.464188	0.055221
Mg7	-1.145069	0.013153	-1.804062
Mg8	0.916162	1.999654	0.003305
Mg9	-5.273707	-3.746897	0.211368
Mg10	-0.838597	4.024699	1.489299
Mg11	-1.345155	3.457937	-1.496769
Mg12	5.162417	-0.889550	-0.486741

@mg12-isomer125 bp86/6-31G(d) Etot=-2401.019165 Eb=-9.55

Mg1	-1.573333	-0.375661	1.105998
Mg2	0.619391	0.523158	-1.158874
Mg3	1.305065	-1.924076	0.669623
Mg4	-3.993135	-2.031377	-0.343935
Mg5	-1.037924	-2.299060	-1.432699
Mg6	-1.358526	2.504022	0.349751
Mg7	-2.464179	0.483769	-1.792589
Mg8	3.592858	0.254080	0.127381
Mg9	1.213773	1.036806	1.821835
Mg10	-1.452122	5.665613	0.124734
Mg11	-1.419723	-3.374054	1.399584
Mg12	6.567853	-0.463219	-0.870808

@mg12-isomer126 bp86/6-31G(d) Etot=-2401.018575 Eb=-9.52

Mg1	-0.513045	0.163770	-1.506015
Mg2	-2.742542	0.019113	0.667609
Mg3	2.166599	-1.864413	-0.093270
Mg4	2.630469	1.152272	-0.950259
Mg5	-3.103675	-2.103330	-1.743210
Mg6	-0.791954	-2.646377	0.245371
Mg7	5.055162	-0.961975	-0.826278
Mg8	3.776585	0.171360	1.716158
Mg9	0.449571	0.502708	1.321435
Mg10	-3.722410	-2.916530	1.179704
Mg11	-1.365561	2.653792	0.034416
Mg12	-1.839200	5.829611	-0.045660

@mg12-isomer127 bp86/6-31G(d) Etot=-2401.017475 Eb=-9.46

Mg1	-1.092393	-0.773889	1.181802
Mg2	-0.324590	1.006342	-1.454051
Mg3	-3.076256	-0.768807	-1.402561
Mg4	1.768951	-0.537739	0.332986
Mg5	-2.793061	1.932128	0.215997
Mg6	-4.105532	-0.667115	1.468664
Mg7	-0.679173	4.216653	-0.758186
Mg8	0.149378	2.151645	1.374392
Mg9	4.855982	-0.499546	0.204731
Mg10	-0.231832	-2.125996	-1.534435
Mg11	-2.645970	-3.452373	0.235833
Mg12	8.174495	-0.481302	0.134828

@mg12-isomer128 bp86/6-31G(d) Etot=-2401.017474 Eb=-9.46

Mg1	0.020771	-1.805518	-0.220709
Mg2	1.747998	0.680616	-0.701826

Mg3	-3.127345	-1.169807	0.354110
Mg4	-0.600232	0.521740	1.631471
Mg5	4.789354	0.206187	-0.028650
Mg6	2.636735	-1.066769	1.690346
Mg7	-1.464013	0.791870	-1.275980
Mg8	3.249457	-2.133351	-1.086711
Mg9	7.531577	1.824506	-0.063619
Mg10	-4.790101	0.544295	-1.830032
Mg11	-6.126033	-0.220729	0.753345
Mg12	-3.868167	1.826961	0.778255

@mg12-isomer129 bp86/6-31G(d) Etot=-2401.015641 Eb=-9.37

Mg1	-4.031275	-0.140028	-1.443420
Mg2	-4.032155	-0.140561	1.442947
Mg3	-1.493877	1.318509	0.000897
Mg4	-4.275548	2.667195	0.000159
Mg5	1.150795	3.076510	-0.000711
Mg6	1.112677	-0.429347	0.001335
Mg7	3.708807	1.454217	-0.000853
Mg8	-1.569757	-1.870130	0.000336
Mg9	-4.436906	-2.938300	-0.000915
Mg10	6.305551	-0.337210	-0.001020
Mg11	3.781539	-1.329638	1.487641
Mg12	3.780149	-1.331218	-1.486395

@mg12-isomer130 bp86/6-31G(d) Etot=-2401.013404 Eb=-9.25

Mg1	-3.371850	-2.603758	0.002943
Mg2	-0.307282	-1.575158	0.001764
Mg3	-5.393082	0.000083	0.000003
Mg4	-2.574673	0.001758	1.557915
Mg5	-0.307247	1.575103	-0.001778
Mg6	2.420760	-0.000070	-0.000016
Mg7	0.469958	-0.003007	-2.609565
Mg8	-3.371750	2.603814	-0.002931
Mg9	0.469982	0.002902	2.609543
Mg10	5.592648	0.000031	-0.000010
Mg11	8.947215	0.000044	0.000018
Mg12	-2.574680	-0.001742	-1.557887

@mg12-isomer131 bp86/6-31G(d) Etot=-2401.013267 Eb=-9.24

Mg1	-2.257823	-1.225778	1.596543
Mg2	0.309639	-0.226756	0.143550
Mg3	-3.798483	2.933428	-1.287784
Mg4	-2.569653	0.105699	-1.221455
Mg5	3.397585	0.011354	0.054855
Mg6	6.031261	-1.628573	0.064016
Mg7	5.931291	1.138034	1.433545
Mg8	-4.624555	-2.252526	-0.190136
Mg9	-1.500412	-2.765959	-0.886337
Mg10	-1.913950	2.097420	1.085261
Mg11	5.817688	0.934605	-1.644424
Mg12	-4.822588	0.879055	0.852366

@mg12-isomer132 bp86/6-31G(d) Etot=-2401.011576 Eb=-9.16

Mg1	0.273361	-1.153185	0.682583
Mg2	-2.773236	-1.725117	1.773967
Mg3	0.166213	1.601401	-0.778483
Mg4	-1.637249	1.436074	1.792975
Mg5	0.504011	-1.043215	-2.390569
Mg6	2.895842	0.002975	-0.831199
Mg7	-4.597794	0.651320	0.908900
Mg8	-2.279628	-0.362060	-1.015772
Mg9	5.864619	-0.064627	0.177228
Mg10	9.126967	-0.157810	0.864940

Mg11	-2.721554	2.879925	-0.653285
Mg12	-4.821550	-2.065680	-0.531285
@mg12-isomer133 bp86/6-31G(d) Etot=-2401.011443 Eb=-9.15			
Mg1	0.000003	-2.196060	-0.971930
Mg2	-2.444671	-4.082617	-0.881133
Mg3	2.309412	0.031677	-1.268137
Mg4	1.673168	-1.195283	1.579901
Mg5	2.644890	2.016283	1.011277
Mg6	-3.114622	-1.107158	-0.735795
Mg7	-1.410407	-2.393160	1.611603
Mg8	-3.243890	1.884090	-0.060784
Mg9	4.669792	2.183803	-1.487361
Mg10	-0.508832	0.669608	0.550851
Mg11	-5.365441	4.334642	0.064456
Mg12	4.790597	-0.145825	0.587051
@mg12-isomer134 bp86/6-31G(d) Etot=-2401.009569 Eb=-9.05			
Mg1	1.710591	-0.624239	-0.730029
Mg2	1.470299	1.168584	1.723815
Mg3	4.867872	-1.571816	-1.546438
Mg4	-1.099066	0.809958	-0.006399
Mg5	-4.106415	0.178893	0.007922
Mg6	4.239596	1.163808	-0.194293
Mg7	-6.450987	-0.849486	1.757081
Mg8	-7.008961	1.032202	-0.624989
Mg9	4.235024	-1.416479	1.423943
Mg10	1.266392	2.448506	-1.017379
Mg11	-6.134138	-1.882764	-1.130872
Mg12	7.009793	-0.457169	0.337638
@mg12-isomer135 bp86/6-31G(d) Etot=-2401.008980 Eb=-9.02			
Mg1	1.236142	1.248303	-0.004138
Mg2	0.065902	-1.611027	-0.004617
Mg3	-2.846335	-1.763434	1.483862
Mg4	-5.035214	-0.210060	0.001557
Mg5	2.881007	-1.097354	1.433022
Mg6	-7.553540	1.772228	0.004806
Mg7	2.841663	3.893385	-0.002062
Mg8	-1.952315	0.777660	-0.001952
Mg9	2.886170	-1.098778	-1.432406
Mg10	5.736680	-1.467365	0.006019
Mg11	-2.849618	-1.762781	-1.486400
Mg12	4.589458	1.319221	0.002310
@mg12-isomer136 bp86/6-31G(d) Etot=-2401.007006 Eb=-8.92			
Mg1	0.079201	-0.060457	-0.903660
Mg2	-1.056009	-2.207758	0.938763
Mg3	-0.322248	0.642263	2.069188
Mg4	1.412055	-2.911958	-1.403663
Mg5	-2.800201	0.272983	0.222168
Mg6	2.405092	1.759473	0.738666
Mg7	-5.874964	0.550699	-0.181943
Mg8	3.244233	-0.295890	-1.542848
Mg9	-9.160700	0.837708	-0.620382
Mg10	2.183991	-1.438109	1.123777
Mg11	4.692402	2.540533	-1.274701
Mg12	5.197149	0.310512	0.834635
@mg12-isomer137 bp86/6-31G(d) Etot=-2401.005935 Eb=-8.86			
Mg1	-1.685808	0.503543	-0.000053
Mg2	-2.610656	-2.046868	-1.477361
Mg3	-0.862722	3.461527	0.000017
Mg4	-4.729841	-0.329808	-0.000047

Mg5	1.430306	1.020983	-0.000146
Mg6	0.240637	-2.023471	0.000047
Mg7	-2.610703	-2.046810	1.477348
Mg8	4.329510	1.108616	1.483393
Mg9	3.278344	-1.466324	0.000088
Mg10	-7.463302	1.352601	0.000080
Mg11	6.354621	-0.642384	0.000143
Mg12	4.329615	1.108395	-1.483510

@mg12-isomer138 bp86/6-31G(d) Etot=-2401.005746 Eb=-8.85

Mg1	3.113975	-0.149916	-0.003869
Mg2	2.196686	-1.787112	2.622922
Mg3	2.028817	2.686928	0.000746
Mg4	0.369331	-2.299922	0.002045
Mg5	0.297619	0.569804	1.526486
Mg6	3.247083	-3.127340	-0.005014
Mg7	0.291305	0.570774	-1.521474
Mg8	2.181520	-1.788485	-2.627476
Mg9	2.229208	5.888023	-0.003445
Mg10	-2.160044	-0.618349	0.005932
Mg11	-5.242498	-0.143353	0.009826
Mg12	-8.553001	0.198950	-0.006679

@mg12-isomer139 bp86/6-31G(d) Etot=-2401.002760 Eb=-8.70

Mg1	-3.263706	0.000095	-1.143136
Mg2	-0.429088	0.000246	-2.753360
Mg3	-3.867288	2.650484	0.475123
Mg4	-3.065259	-0.000173	1.873242
Mg5	1.926298	0.000078	-0.885274
Mg6	4.860403	0.000017	0.094716
Mg7	-5.865085	-0.000064	0.746433
Mg8	-0.785973	1.571612	-0.099383
Mg9	-0.785953	-1.571564	-0.099649
Mg10	7.571391	-1.641756	0.658436
Mg11	7.571541	1.641596	0.658224
Mg12	-3.867281	-2.650571	0.474629

@mg12-isomer140 bp86/6-31G(d) Etot=-2401.002701 Eb=-8.69

Mg1	-1.915201	1.060399	-0.000060
Mg2	0.986643	1.197648	1.447091
Mg3	3.005819	-0.820320	-0.000006
Mg4	6.123963	-0.737460	0.000004
Mg5	-0.259443	3.689794	0.000034
Mg6	9.454349	-0.723498	0.000027
Mg7	-2.935036	-1.891507	-0.000004
Mg8	-6.013578	-2.050175	0.000058
Mg9	-4.760374	0.345996	1.491454
Mg10	0.986715	1.197727	-1.447085
Mg11	-4.760436	0.345947	-1.491450
Mg12	0.086579	-1.614551	-0.000063

@mg12-isomer141 bp86/6-31G(d) Etot=-2400.998150 Eb=-8.45

Mg1	-1.276368	0.178350	-0.000282
Mg2	-4.491497	0.191604	0.000141
Mg3	-3.103363	2.908358	0.000210
Mg4	4.660041	-0.193412	0.000004
Mg5	1.777754	0.954308	-0.000359
Mg6	-2.987460	-2.119722	-1.504867
Mg7	-0.248059	2.745468	1.477310
Mg8	-5.560999	-2.836231	0.000097
Mg9	7.232599	-1.227499	1.641108
Mg10	-2.987141	-2.119819	1.504639
Mg11	-0.248196	2.746044	-1.477024
Mg12	7.232687	-1.227449	-1.640978

@mg12-isomer142 bp86/6-31G(d) Etot=-2400.996120 Eb=-8.35

Mg1	-1.384015	1.396004	-0.000044
Mg2	-4.173128	0.296985	1.448488
Mg3	1.520310	1.930518	-1.473827
Mg4	3.798419	0.501552	0.000047
Mg5	0.894529	-0.731706	0.000025
Mg6	6.748260	-0.519129	0.000004
Mg7	-5.433506	-2.291196	0.000029
Mg8	1.520262	1.930547	1.473836
Mg9	-7.144846	0.213125	-0.000026
Mg10	9.970274	-1.371521	-0.000035
Mg11	-2.143457	-1.652091	0.000040
Mg12	-4.173103	0.296913	-1.448538

@mg12-isomer143 bp86/6-31G(d) Etot=-2400.995755 Eb=-8.33

Mg1	3.677264	1.001552	-0.009263
Mg2	1.028550	2.890724	-0.026353
Mg3	1.109362	0.233630	1.568347
Mg4	-1.498922	1.279245	-0.011314
Mg5	3.170579	-1.981499	0.018093
Mg6	1.109082	0.204832	-1.572064
Mg7	-4.452469	0.358581	-0.003039
Mg8	-7.634602	-0.180727	0.001694
Mg9	6.070081	-1.167955	0.010367
Mg10	-10.808304	-1.287939	0.011464
Mg11	4.114453	-0.699416	-2.635126
Mg12	4.114925	-0.651030	2.647194

@mg12-isomer144 bp86/6-31G(d) Etot=-2400.995546 Eb=-8.32

Mg1	5.819443	-0.000178	-1.448692
Mg2	6.218400	-2.811836	-0.000379
Mg3	0.805485	0.000381	0.000686
Mg4	3.351506	-1.685578	0.000117
Mg5	-7.954249	1.642832	0.685043
Mg6	5.819927	-0.000185	1.448096
Mg7	-5.425157	0.001004	0.002585
Mg8	-7.953125	-1.416666	1.078345
Mg9	-7.949580	-0.227576	-1.767294
Mg10	-2.303546	0.000653	0.001730
Mg11	6.219018	2.811390	-0.000366
Mg12	3.351880	1.685758	0.000128

@mg13-isomer01 bp86/6-31G(d) Etot=-2601.163726 Eb=-12.43

Mg1	0.822754	-0.730193	2.142340
Mg2	-2.187363	-0.498528	1.836159
Mg3	2.260014	2.030259	2.046696
Mg4	-4.114743	-1.598129	-0.331182
Mg5	0.278759	0.963460	-2.554312
Mg6	-0.383159	-1.352747	-0.668165
Mg7	2.472581	-1.055280	-2.022196
Mg8	-0.201978	1.592035	0.374272
Mg9	-2.711215	0.763131	-1.657134
Mg10	1.984515	-2.938817	0.294110
Mg11	2.658410	1.975702	-0.961099
Mg12	-4.455111	1.232377	0.758382
Mg13	3.576536	-0.383269	0.742131

@mg13-isomer02 bp86/6-31G(d) Etot=-2601.160974 Eb=-12.30

Mg1	0.118575	1.006003	-1.687737
Mg2	2.241738	-1.198902	-1.993499
Mg3	-0.725797	-1.923730	-1.369674
Mg4	3.700626	-0.304338	0.652562
Mg5	1.433242	1.871205	0.942796

Mg6	3.148345	1.652177	-1.619821
Mg7	-0.780827	-0.308062	1.302570
Mg8	1.368036	-2.357658	0.753665
Mg9	-3.227228	0.472495	-1.697112
Mg10	1.782448	-0.366018	2.988636
Mg11	-3.539727	-1.921273	0.128973
Mg12	-4.048262	0.874673	1.164522
Mg13	-1.471170	2.503427	0.434119

@mg13-isomer03 bp86/6-31G(d) Etot=-2601.158862 Eb=-12.20

Mg1	-0.429394	-0.305499	-1.740425
Mg2	0.589931	2.398866	-1.600278
Mg3	-0.298599	1.735742	1.226030
Mg4	-2.608651	1.912339	-1.002484
Mg5	-1.496238	-2.977384	-1.004205
Mg6	-3.462007	0.923090	1.784480
Mg7	2.785348	0.007788	-2.055076
Mg8	2.837028	1.753139	0.482247
Mg9	1.305201	-2.118085	-0.054290
Mg10	4.037772	-0.931842	0.592690
Mg11	-3.725137	-0.924714	-0.616125
Mg12	1.598442	-0.322820	2.518939
Mg13	-1.133697	-1.150620	1.468496

@mg13-isomer04 bp86/6-31G(d) Etot=-2601.158034 Eb=-12.16

Mg1	-0.815659	-1.533550	1.334098
Mg2	3.251205	0.000001	-1.990662
Mg3	-0.526460	-2.880779	-1.413723
Mg4	1.996094	-1.952595	0.065800
Mg5	4.123519	-0.000108	0.924828
Mg6	1.495572	-0.000139	2.607356
Mg7	1.996232	1.952535	0.065936
Mg8	-0.050611	0.000107	-1.613474
Mg9	-3.270495	-1.519074	-0.855407
Mg10	-3.587139	-0.000016	1.809926
Mg11	-0.526365	2.881005	-1.413500
Mg12	-0.815550	1.533490	1.334139
Mg13	-3.270342	1.519121	-0.855317

@mg13-isomer05 bp86/6-31G(d) Etot=-2601.157919 Eb=-12.15

Mg1	3.511050	1.525904	-1.305422
Mg2	4.202517	-0.489216	0.789489
Mg3	1.764123	-1.933283	1.755064
Mg4	1.792019	1.284933	1.329820
Mg5	-3.793133	0.638535	1.646024
Mg6	-1.067123	2.445986	1.249296
Mg7	1.848837	-0.991931	-1.287547
Mg8	-0.862309	-0.464620	1.620912
Mg9	0.312361	1.747196	-1.412767
Mg10	-2.813262	1.298869	-1.140489
Mg11	-0.466218	-2.724498	-0.251241
Mg12	-1.040074	-0.771761	-2.506121
Mg13	-3.388788	-1.566114	-0.487018

@mg13-isomer06 bp86/6-31G(d) Etot=-2601.157248 Eb=-12.12

Mg1	-0.798726	1.519402	-2.129252
Mg2	-2.122688	2.005420	0.505901
Mg3	-2.122529	-2.004458	0.509555
Mg4	1.752668	-0.001483	-1.642927
Mg5	3.973063	-1.507814	-0.177713
Mg6	2.525101	0.001860	1.966546
Mg7	-0.798656	-1.523349	-2.126509
Mg8	-3.462295	-0.001373	-1.447433
Mg9	-3.952496	0.001419	1.606701

Mg10	-0.580539	0.002033	2.221081
Mg11	3.973055	1.507542	-0.180532
Mg12	0.806951	2.145389	0.445328
Mg13	0.807092	-2.144587	0.449255

@mg13-isomer07 bp86/6-31G(d) Etot=-2601.157006 Eb=-12.11

Mg1	0.581622	0.971483	1.881009
Mg2	3.660855	0.361555	1.697855
Mg3	-0.581732	0.972727	-1.880473
Mg4	-1.233546	-1.376719	2.288530
Mg5	2.400069	1.405224	-0.854636
Mg6	1.233633	-1.375119	-2.289370
Mg7	-3.660898	0.362380	-1.697650
Mg8	1.349593	-1.771536	0.768983
Mg9	-2.400202	1.404780	0.855406
Mg10	-0.000007	3.206612	0.001020
Mg11	4.023454	-1.194932	-0.863250
Mg12	-1.349429	-1.770959	-0.770013
Mg13	-4.023413	-1.195497	0.862590

@mg13-isomer08 bp86/6-31G(d) Etot=-2601.156178 Eb=-12.07

Mg1	2.920235	-1.069546	-1.585318
Mg2	3.866137	1.323278	-0.000185
Mg3	1.216348	1.589619	-1.590489
Mg4	2.920108	-1.069013	1.585801
Mg5	-0.081493	-1.071052	-2.614857
Mg6	0.601392	-2.517494	0.000503
Mg7	1.216240	1.590077	1.589962
Mg8	-3.358699	-1.120526	-1.652531
Mg9	-1.027672	2.983754	-0.000406
Mg10	-0.945897	0.057744	-0.000234
Mg11	-3.358587	-1.120294	1.652702
Mg12	-3.886444	1.493474	-0.000064
Mg13	-0.081669	-1.070020	2.615117

@mg13-isomer09 bp86/6-31G(d) Etot=-2601.156169 Eb=-12.07

Mg1	0.589714	0.000043	-0.912233
Mg2	-0.937635	-2.689382	-0.395509
Mg3	-0.937665	2.689408	-0.395482
Mg4	-3.865972	-1.934960	-0.001574
Mg5	3.428127	-0.000043	-2.005653
Mg6	2.324843	2.538507	-0.451818
Mg7	0.850129	1.554044	2.072844
Mg8	2.324800	-2.538500	-0.451800
Mg9	0.850111	-1.554035	2.072886
Mg10	3.353361	-0.000006	0.964202
Mg11	-3.865970	1.934952	-0.001559
Mg12	-2.381918	0.000000	-1.764278
Mg13	-1.731924	-0.000029	1.269972

@mg13-isomer10 bp86/6-31G(d) Etot=-2601.156023 Eb=-12.06

Mg1	0.910829	-1.888490	1.222755
Mg2	-2.243643	-2.620515	1.423161
Mg3	2.243655	-2.620461	-1.423198
Mg4	-3.719474	-0.585592	-0.310997
Mg5	3.719602	-0.585633	0.310981
Mg6	-0.910880	-1.888468	-1.222832
Mg7	-1.664305	1.009602	-2.031382
Mg8	1.664297	1.009601	2.031233
Mg9	-1.214466	0.264294	1.418407
Mg10	3.188340	2.460512	-0.230799
Mg11	1.214393	0.264272	-1.418089
Mg12	-3.188307	2.460464	0.230731
Mg13	-0.000042	2.720414	0.000029

@mg13-isomer11 bp86/6-31G(d) Etot=-2601.155712 Eb=-12.04

Mg1	3.764444	-2.539256	-0.000016
Mg2	1.303403	-1.494026	-1.536726
Mg3	3.143323	0.574775	0.000008
Mg4	1.739695	1.387671	-2.602249
Mg5	-4.281994	-2.632198	0.000030
Mg6	-1.251817	-2.241992	-0.000119
Mg7	1.303317	-1.494127	1.536563
Mg8	0.847673	2.625376	0.000122
Mg9	-1.011235	0.533438	-1.538523
Mg10	1.739680	1.387374	2.602365
Mg11	-1.011300	0.533367	1.538605
Mg12	-3.968820	0.377064	-0.000081
Mg13	-2.316368	2.982534	0.000021

@mg13-isomer12 bp86/6-31G(d) Etot=-2601.155373 Eb=-12.03

Mg1	0.460569	0.138808	-2.618990
Mg2	-2.421512	0.668260	1.621254
Mg3	-2.405119	3.183764	-0.000376
Mg4	1.297997	-1.309581	0.000359
Mg5	0.199155	1.668989	0.000007
Mg6	3.357634	1.033099	-1.530993
Mg7	3.357340	1.032903	1.531240
Mg8	0.459940	0.139108	2.619192
Mg9	4.485333	-1.389458	-0.000035
Mg10	-1.281299	-2.134434	1.571114
Mg11	-2.420999	0.667965	-1.621542
Mg12	-3.808176	-1.564708	-0.000250
Mg13	-1.280864	-2.134715	-1.570981

@mg13-isomer13 bp86/6-31G(d) Etot=-2601.155196 Eb=-12.02

Mg1	0.302309	1.411150	1.615255
Mg2	-0.808516	-1.739838	-1.229737
Mg3	-1.634663	2.535833	-0.542702
Mg4	1.559272	-1.332080	0.708986
Mg5	3.441270	1.581351	0.552376
Mg6	-3.350908	0.042428	-0.369277
Mg7	4.687482	-1.117771	1.110044
Mg8	-2.666978	1.602548	2.184846
Mg9	0.834244	0.839120	-1.438225
Mg10	-1.793015	0.652355	-2.913335
Mg11	-3.171621	-2.904801	0.252845
Mg12	3.888413	-0.417698	-1.762665
Mg13	-1.287291	-1.152597	1.831590

@mg13-isomer14 bp86/6-31G(d) Etot=-2601.155178 Eb=-12.02

Mg1	3.760576	1.451706	-0.959638
Mg2	-1.078736	-2.144953	-1.632612
Mg3	1.312724	-0.228020	-2.138323
Mg4	4.053937	-1.476637	-0.405001
Mg5	-3.805050	-1.077349	-0.819730
Mg6	-1.568894	0.794015	-1.935896
Mg7	3.094651	0.418581	1.843116
Mg8	0.864461	-1.548058	0.614506
Mg9	-2.044141	3.294228	-0.340808
Mg10	0.396130	1.593260	0.268356
Mg11	-2.720631	0.890859	1.223692
Mg12	-2.070045	-2.050300	1.457874
Mg13	-0.194981	0.082668	2.824464

@mg13-isomer15 bp86/6-31G(d) Etot=-2601.155158 Eb=-12.02

Mg1	-2.867198	-2.506615	-0.625171
Mg2	-1.247730	-1.910822	1.886896

Mg3	0.174760	-2.419092	-0.819193
Mg4	-3.039265	0.304418	0.671025
Mg5	1.347761	-0.277356	1.265109
Mg6	-1.559735	-0.038381	-2.005790
Mg7	-3.184829	2.573433	-1.282586
Mg8	-0.893078	0.988550	2.846807
Mg9	-0.427752	2.102547	-0.008777
Mg10	1.521898	0.301753	-1.664926
Mg11	3.194276	-2.383315	-0.298559
Mg12	4.388162	0.422019	-0.133074
Mg13	2.592730	2.842860	0.168237

@mg13-isomer16 bp86/6-31G(d) Etot=-2601.154950 Eb=-12.01

Mg1	-1.517430	2.603141	-1.350763
Mg2	1.009985	2.154454	0.122237
Mg3	1.638278	-2.338297	-1.893648
Mg4	-1.311278	0.581517	1.344673
Mg5	-2.772582	-2.047840	-0.166653
Mg6	3.208398	-1.414281	0.552155
Mg7	-4.341407	-0.106686	1.684090
Mg8	0.174998	-2.077297	0.872789
Mg9	-0.315587	-0.135441	-1.592761
Mg10	2.769125	0.508558	-1.892496
Mg11	3.798817	1.488348	0.995496
Mg12	-3.795312	0.593809	-1.266307
Mg13	1.453995	0.190015	2.591187

@mg13-isomer17 bp86/6-31G(d) Etot=-2601.154819 Eb=-12.00

Mg1	-2.329342	3.141685	-0.000019
Mg2	-3.591781	-2.697100	0.000267
Mg3	-3.108965	0.265631	-0.000042
Mg4	-1.008146	-1.629683	-1.487801
Mg5	0.752190	2.528948	-0.000020
Mg6	-1.007835	-1.629490	1.487516
Mg7	-1.076899	1.327732	-2.233759
Mg8	3.644096	1.728853	-0.000166
Mg9	1.547352	-2.930577	0.000073
Mg10	1.580624	-0.046789	-1.560963
Mg11	4.094807	-1.340517	-0.000021
Mg12	-1.076976	1.327793	2.233731
Mg13	1.580876	-0.046485	1.561202

@mg13-isomer18 bp86/6-31G(d) Etot=-2601.154755 Eb=-12.00

Mg1	2.514487	-1.797147	1.327262
Mg2	4.003906	-0.543975	-1.036101
Mg3	3.119514	1.131789	1.213683
Mg4	0.000019	-0.000155	2.020660
Mg5	-3.119646	-1.132069	1.213483
Mg6	-0.383270	-2.611021	0.718167
Mg7	0.953800	-1.186112	-1.481965
Mg8	-2.026984	-1.626068	-1.751840
Mg9	2.027081	1.626414	-1.751585
Mg10	-0.953771	1.186469	-1.481866
Mg11	0.383227	2.610954	0.718610
Mg12	-4.003896	0.544137	-1.036078
Mg13	-2.514468	1.796785	1.327570

@mg13-isomer19 bp86/6-31G(d) Etot=-2601.154742 Eb=-12.00

Mg1	-4.328033	1.334376	-0.798446
Mg2	-2.990938	-1.333435	-0.263556
Mg3	-1.877986	-1.377046	2.589341
Mg4	-2.100352	1.360792	1.336141
Mg5	-1.425470	1.176863	-1.722055
Mg6	-0.048803	-2.308054	0.322188

Mg7	3.193030	-1.563772	0.816836
Mg8	-0.914623	-1.702785	-2.503055
Mg9	0.656569	0.185534	1.926150
Mg10	0.439598	2.639666	0.170484
Mg11	1.343387	-0.047186	-1.326209
Mg12	3.519620	1.550047	0.971608
Mg13	4.534003	0.084999	-1.519427

@mg13-isomer20 bp86/6-31G(d) Etot=-2601.154411 Eb=-11.98

Mg1	1.608873	0.357613	-1.529855
Mg2	-0.056966	1.602232	0.860513
Mg3	-2.138838	-2.303352	0.892232
Mg4	3.978519	-1.680269	0.108574
Mg5	-1.187418	-0.314437	2.976863
Mg6	-3.472316	-1.239430	-1.668589
Mg7	-2.356080	3.267421	-0.172074
Mg8	-1.362745	1.019052	-1.906079
Mg9	-0.507167	-1.884859	-1.781538
Mg10	4.623737	1.014887	-1.154127
Mg11	3.184967	0.928749	1.554012
Mg12	-3.136704	0.578732	0.830610
Mg13	0.822138	-1.346340	0.989459

@mg13-isomer21 bp86/6-31G(d) Etot=-2601.154261 Eb=-11.97

Mg1	1.200547	1.957029	-0.000016
Mg2	-1.954192	-1.384042	2.615313
Mg3	-1.299563	1.403992	-1.588309
Mg4	0.855120	-0.709232	1.605691
Mg5	-3.315897	-0.613534	0.000047
Mg6	-1.954310	-1.383987	-2.615300
Mg7	3.565432	-1.668255	-0.000095
Mg8	3.995326	0.920788	-1.524572
Mg9	-3.656928	2.425291	0.000047
Mg10	0.855062	-0.709188	-1.605784
Mg11	3.995316	0.920647	1.524659
Mg12	-1.299511	1.403964	1.588350
Mg13	-0.986401	-2.563475	-0.000030

@mg13-isomer22 bp86/6-31G(d) Etot=-2601.153932 Eb=-11.96

Mg1	-3.219004	2.623697	0.000002
Mg2	0.000007	2.788526	0.000010
Mg3	-1.544228	0.452796	1.530460
Mg4	-1.544354	0.452757	-1.530532
Mg5	3.219002	2.623711	-0.000165
Mg6	1.544414	0.452813	1.530522
Mg7	-4.084975	-0.498513	0.000115
Mg8	1.544183	0.452649	-1.530420
Mg9	-0.000010	-1.991903	2.510556
Mg10	4.085000	-0.498484	0.000008
Mg11	-0.000116	-1.991958	-2.510563
Mg12	-1.734684	-2.433021	0.000034
Mg13	1.734766	-2.433070	-0.000027

@mg13-isomer23 bp86/6-31G(d) Etot=-2601.153872 Eb=-11.96

Mg1	-2.981009	2.721371	-0.000111
Mg2	1.525418	0.335363	-1.620383
Mg3	2.981144	2.721297	-0.000023
Mg4	-0.000083	-2.276214	-1.710400
Mg5	-4.178807	0.012729	0.000151
Mg6	1.525625	0.335559	1.620647
Mg7	-1.525466	0.335587	1.620469
Mg8	2.522588	-2.418985	0.000013
Mg9	-1.525628	0.335451	-1.620608
Mg10	0.000043	2.580208	-0.000074

Mg11	4.178857	0.012635	-0.000196	
Mg12	-0.000016	-2.276051	1.710446	
Mg13	-2.522665	-2.418950	0.000069	
@mg13-isomer24 bp86/6-31G(d) Etot=-2601.153390 Eb=-11.93				
Mg1	-1.826632	3.071149	1.690330	
Mg2	2.470058	0.279907	-1.918064	
Mg3	1.982360	-0.765890	1.519336	
Mg4	-0.521735	-2.717154	1.752774	
Mg5	-1.055278	0.197934	2.134715	
Mg6	-0.161168	-1.307273	-0.816181	
Mg7	-2.984062	-1.146668	-2.248932	
Mg8	-3.261830	-1.627999	0.735108	
Mg9	3.860272	1.464616	0.533449	
Mg10	0.484177	1.848722	0.032717	
Mg11	-2.802012	1.242604	-0.419822	
Mg12	4.422586	-1.413596	-0.304794	
Mg13	-0.606737	0.873646	-2.690637	
@mg13-isomer25 bp86/6-31G(d) Etot=-2601.153356 Eb=-11.93				
Mg1	-0.775865	-1.533871	1.554741	
Mg2	2.031214	0.000033	1.431995	
Mg3	-0.775846	1.533875	1.554776	
Mg4	-3.019232	0.000039	3.049366	
Mg5	-1.625951	-2.452126	-1.219774	
Mg6	1.441778	-2.677642	-0.484640	
Mg7	4.217713	1.555615	-0.064414	
Mg8	-3.215361	-0.000029	0.071104	
Mg9	0.236396	-0.000051	-1.291571	
Mg10	-1.625999	2.452104	-1.219729	
Mg11	1.441691	2.677565	-0.484753	
Mg12	4.217710	-1.555522	-0.064334	
Mg13	-2.548248	0.000011	-2.832767	
@mg13-isomer26 bp86/6-31G(d) Etot=-2601.153068 Eb=-11.92				
Mg1	1.102751	0.018270	-1.487660	
Mg2	-2.079835	0.721007	1.559356	
Mg3	3.068514	-2.101331	0.009262	
Mg4	2.885545	2.930743	0.005216	
Mg5	-1.204986	-1.912318	2.631852	
Mg6	-2.060992	0.731763	-1.565180	
Mg7	-0.114855	2.502590	0.013130	
Mg8	1.084619	0.005998	1.506014	
Mg9	0.176765	-2.646243	-0.003308	
Mg10	4.556611	0.497278	-0.002748	
Mg11	-1.176391	-1.893888	-2.648062	
Mg12	-3.427398	2.997637	-0.002511	
Mg13	-2.810348	-1.851506	-0.015362	
@mg13-isomer27 bp86/6-31G(d) Etot=-2601.152575 Eb=-11.89				
Mg1	3.629642	1.633741	-0.010840	
Mg2	1.181217	-0.296122	-1.317377	
Mg3	-0.827460	-1.686421	0.738060	
Mg4	-1.919126	-0.246520	-1.760455	
Mg5	-3.495012	-0.091971	0.891910	
Mg6	-0.256946	2.194717	-2.361504	
Mg7	4.145183	-1.370528	-0.276039	
Mg8	-1.107018	1.036077	2.481282	
Mg9	1.777549	-3.151854	0.005661	
Mg10	0.794836	2.468468	0.507043	
Mg11	-2.252530	2.542143	0.049826	
Mg12	-3.339637	-2.804894	-0.633162	
Mg13	1.669303	-0.226835	1.685596	

@mg13-isomer28 bp86/6-31G(d) Etot=-2601.152534 Eb=-11.89

Mg1	3.187962	-0.227394	-0.000049
Mg2	4.470631	2.544283	0.000027
Mg3	3.670356	-3.243172	0.000014
Mg4	1.438913	2.626692	0.000062
Mg5	-2.402396	0.959104	2.637378
Mg6	-1.586023	2.332679	0.000015
Mg7	0.291487	0.179139	-1.528864
Mg8	0.291469	0.179077	1.528822
Mg9	-2.402402	0.959148	-2.637374
Mg10	-3.635672	0.118348	0.000004
Mg11	0.599539	-2.538686	-0.000028
Mg12	-1.961921	-1.944574	-1.541359
Mg13	-1.961943	-1.944643	1.541350

@mg13-isomer29 bp86/6-31G(d) Etot=-2601.152417 Eb=-11.89

Mg1	-3.582087	0.334056	-1.759010
Mg2	0.612558	0.559089	-2.943008
Mg3	-0.835927	1.754270	-0.612449
Mg4	2.278321	1.748744	-0.610388
Mg5	-0.835958	-1.407450	-1.213089
Mg6	-3.582114	1.356304	1.168757
Mg7	-3.582207	-1.690340	0.590174
Mg8	2.278107	-1.403042	-1.209120
Mg9	0.612325	2.269310	1.955654
Mg10	4.582740	-0.000199	0.000137
Mg11	-0.836037	-0.346760	1.825338
Mg12	2.277981	-0.345648	1.819614
Mg13	0.612298	-2.828334	0.987388

@mg13-isomer30 bp86/6-31G(d) Etot=-2601.152206 Eb=-11.87

Mg1	0.446330	2.106500	-0.061712
Mg2	0.746245	0.903387	2.913403
Mg3	-2.632226	-2.387022	0.156078
Mg4	3.330563	2.635575	-1.078943
Mg5	0.333039	-1.698105	1.493452
Mg6	-4.307642	0.159184	-0.387501
Mg7	3.027284	0.313248	0.863724
Mg8	-1.309649	0.042698	-1.566505
Mg9	1.795769	-0.090885	-1.842038
Mg10	0.105300	-2.696763	-1.273188
Mg11	2.951597	-2.581747	-0.106698
Mg12	-2.630293	2.757925	-0.560354
Mg13	-1.856316	0.536005	1.450281

@mg13-isomer31 bp86/6-31G(d) Etot=-2601.152194 Eb=-11.87

Mg1	-2.975061	-2.662721	-0.073586
Mg2	-4.367271	-0.000075	-0.045572
Mg3	-1.680409	0.000179	1.676429
Mg4	-1.226167	-0.000054	-1.423233
Mg5	-2.975207	2.662646	-0.073457
Mg6	-0.034669	-2.287191	0.515515
Mg7	1.313295	-1.520814	-2.107178
Mg8	-0.034651	2.287334	0.515191
Mg9	1.313355	1.520553	-2.107444
Mg10	2.882663	-2.654521	0.758432
Mg11	1.498936	0.000147	2.013278
Mg12	3.402486	-0.000033	-0.406604
Mg13	2.882701	2.654550	0.758229

@mg13-isomer32 bp86/6-31G(d) Etot=-2601.152084 Eb=-11.87

Mg1	-1.247981	0.000053	1.299132
Mg2	3.072502	2.632232	0.117625
Mg3	1.860663	0.000042	1.284474

Mg4	0.242557	2.634726	1.604708
Mg5	-2.104209	-0.000075	-1.991096
Mg6	0.418794	-1.550804	-1.290812
Mg7	3.142379	-0.000040	-1.505126
Mg8	0.242572	-2.634550	1.605010
Mg9	-2.440268	-2.507936	-0.122194
Mg10	-4.237932	-0.000008	0.293771
Mg11	3.072427	-2.632270	0.117581
Mg12	0.418819	1.550689	-1.290908
Mg13	-2.440323	2.507941	-0.122166

@mg13-isomer33 bp86/6-31G(d) Etot=-2601.152007 Eb=-11.87

Mg1	0.933120	1.751733	-0.622193
Mg2	-1.560424	0.307750	-1.666299
Mg3	-1.193706	0.654211	1.380702
Mg4	-4.129941	1.305955	0.159244
Mg5	-0.785005	-2.575471	-0.952941
Mg6	1.782125	0.052231	1.867357
Mg7	2.125649	-2.636298	0.085169
Mg8	-3.285328	-1.609581	0.409477
Mg9	-1.820920	3.165790	-0.306739
Mg10	1.195265	-0.848530	-2.452738
Mg11	3.541339	2.663861	0.741780
Mg12	3.547703	-0.055028	-0.616884
Mg13	-0.349878	-2.176624	1.974066

@mg13-isomer34 bp86/6-31G(d) Etot=-2601.151878 Eb=-11.86

Mg1	-0.136471	2.103073	2.508347
Mg2	-3.153722	-2.610225	0.978957
Mg3	-1.208505	1.194746	-2.268885
Mg4	-1.441181	-1.794940	-1.419265
Mg5	-3.690394	0.183589	-0.452312
Mg6	3.732310	-1.922909	0.011479
Mg7	1.314819	-0.424371	-1.545306
Mg8	0.982041	2.426380	-0.434847
Mg9	-0.989485	-0.386894	1.160011
Mg10	0.867973	-2.854302	0.474585
Mg11	3.826479	1.233820	-0.688942
Mg12	2.047428	0.107339	1.516447
Mg13	-2.151292	2.744694	0.159730

@mg13-isomer35 bp86/6-31G(d) Etot=-2601.151836 Eb=-11.86

Mg1	1.076182	-0.359215	1.499965
Mg2	0.897142	0.099785	-1.493411
Mg3	-1.152556	-2.643521	1.217075
Mg4	1.934522	2.584144	0.258157
Mg5	3.862117	-1.027157	-0.193757
Mg6	-3.081228	-0.570439	0.156962
Mg7	4.783206	1.838248	-0.013262
Mg8	-1.656257	-0.110074	2.844540
Mg9	1.473027	-2.800346	-0.447100
Mg10	-1.292222	-2.143218	-1.801222
Mg11	-3.911562	2.503899	-0.236986
Mg12	-1.981303	0.840174	-2.267711
Mg13	-0.951069	1.787721	0.476752

@mg13-isomer36 bp86/6-31G(d) Etot=-2601.151832 Eb=-11.86

Mg1	-0.258462	0.673552	-2.066220
Mg2	-1.243981	0.477092	0.899220
Mg3	-4.394907	1.238420	0.250435
Mg4	0.902847	2.471280	0.087160
Mg5	1.535043	-1.802296	-2.682757
Mg6	2.774399	0.227567	-0.873726
Mg7	-3.479529	-1.671164	0.576777

Mg8	2.071543	-2.543642	0.329076
Mg9	-0.927731	-2.196581	-0.890110
Mg10	-2.188755	2.957694	-0.818930
Mg11	-0.437674	-2.190719	2.075046
Mg12	1.746671	0.071866	2.034693
Mg13	3.900536	2.286931	1.079336

@mg13-isomer37 bp86/6-31G(d) Etot=-2601.151669 Eb=-11.85

Mg1	3.951948	0.700342	-1.474733
Mg2	1.203824	-0.077177	-2.623392
Mg3	-4.197605	1.199777	-0.000278
Mg4	0.959328	1.481452	-0.000339
Mg5	-1.665562	0.474168	-1.713739
Mg6	3.951980	0.700879	1.474495
Mg7	-1.643461	3.016544	-0.000546
Mg8	-0.575294	-2.305645	-1.512590
Mg9	1.203776	-0.076027	2.623408
Mg10	2.288129	-1.535074	0.000295
Mg11	-3.236233	-1.749029	0.000368
Mg12	-1.665664	0.474780	1.713582
Mg13	-0.575166	-2.304990	1.513468

@mg13-isomer38 bp86/6-31G(d) Etot=-2601.151412 Eb=-11.84

Mg1	0.863171	-0.597556	2.743161
Mg2	2.609347	1.918242	2.043291
Mg3	3.188069	-0.487919	0.403176
Mg4	2.357488	2.185838	-0.975405
Mg5	-0.180493	1.198459	0.692181
Mg6	-2.199709	-0.835346	1.942395
Mg7	2.890619	-2.785528	-1.469337
Mg8	0.264611	-2.166228	0.218119
Mg9	1.045547	-0.402620	-2.120714
Mg10	-3.492630	1.671252	-0.097143
Mg11	-0.676234	2.118862	-2.035256
Mg12	-2.111320	-0.685357	-1.522225
Mg13	-4.558465	-1.132099	0.177756

@mg13-isomer39 bp86/6-31G(d) Etot=-2601.151236 Eb=-11.83

Mg1	0.812079	-2.659856	0.660920
Mg2	-2.477382	-2.660121	1.248339
Mg3	3.746200	-1.841298	-0.039280
Mg4	-0.814666	0.000020	1.453544
Mg5	2.290211	-0.000010	1.833292
Mg6	3.746249	1.841249	-0.039287
Mg7	-3.755467	0.000056	0.270664
Mg8	-2.477310	2.660235	1.248149
Mg9	1.327528	0.000061	-1.033810
Mg10	-1.487085	-1.638235	-1.320357
Mg11	0.812106	2.659907	0.660869
Mg12	-1.487020	1.638173	-1.320493
Mg13	-0.235443	-0.000181	-3.622549

@mg13-isomer40 bp86/6-31G(d) Etot=-2601.151200 Eb=-11.83

Mg1	3.139007	1.740782	-1.540514
Mg2	-2.722281	2.654363	-0.097922
Mg3	2.194914	1.220325	1.183937
Mg4	1.044635	-0.493607	-1.179747
Mg5	-0.639330	1.907615	2.194016
Mg6	0.203675	2.490402	-0.868470
Mg7	4.101009	-0.924884	-0.230772
Mg8	-2.633340	-0.180452	1.096737
Mg9	0.249583	-1.046920	2.133471
Mg10	2.089724	-3.077898	0.309793
Mg11	-1.950983	0.215709	-1.845991

Mg12	-4.040045	-2.021908	-0.878590	
Mg13	-1.036569	-2.483528	-0.275949	
@mg13-isomer41 bp86/6-31G(d) Etot=-2601.151127 Eb=-11.82				
Mg1	-1.079528	1.591782	1.579709	
Mg2	-3.345905	2.999834	-0.000423	
Mg3	-1.079033	-1.591171	1.579970	
Mg4	-1.079549	1.591199	-1.580196	
Mg5	1.285952	0.000559	2.648287	
Mg6	-1.079177	-1.591881	-1.579608	
Mg7	-3.323821	-0.000190	-0.000015	
Mg8	1.743658	-1.608089	0.000185	
Mg9	1.742815	1.607960	-0.000217	
Mg10	4.137070	0.000007	-1.481035	
Mg11	-3.345419	-3.000213	0.000598	
Mg12	4.137053	0.000504	1.481051	
Mg13	1.285885	-0.000303	-2.648306	
@mg13-isomer42 bp86/6-31G(d) Etot=-2601.150767 Eb=-11.81				
Mg1	-0.727604	-2.201762	0.591831	
Mg2	-1.128477	0.577444	-1.472390	
Mg3	2.928194	2.962210	-0.307859	
Mg4	-3.382366	2.289837	-0.082688	
Mg5	0.500332	-1.191767	3.105797	
Mg6	-0.289806	3.084838	-0.082941	
Mg7	-1.586662	0.696245	1.766261	
Mg8	3.902139	0.081101	-0.875531	
Mg9	2.653789	-2.319397	0.691085	
Mg10	-3.596504	-0.913814	0.022760	
Mg11	1.285978	0.540391	0.647085	
Mg12	-1.806282	-2.315278	-2.109295	
Mg13	1.247269	-1.290048	-1.894115	
@mg13-isomer43 bp86/6-31G(d) Etot=-2601.150658 Eb=-11.80				
Mg1	0.943212	1.253933	-1.758000	
Mg2	3.843266	0.911516	-0.455450	
Mg3	1.719385	2.717160	0.832514	
Mg4	-1.263617	2.917700	-0.013867	
Mg5	-0.870795	1.331911	2.574965	
Mg6	1.315657	-0.298065	0.919572	
Mg7	4.030332	-2.075528	-0.098647	
Mg8	-2.098503	1.299976	-2.413850	
Mg9	-0.895407	-1.230279	-1.284432	
Mg10	-1.260902	-1.675544	1.651828	
Mg11	1.202583	-3.162761	-0.176645	
Mg12	-3.024365	0.515781	0.450345	
Mg13	-3.640846	-2.505799	-0.228333	
@mg13-isomer44 bp86/6-31G(d) Etot=-2601.150463 Eb=-11.79				
Mg1	1.533702	-2.379163	0.368462	
Mg2	3.037409	0.378457	1.786708	
Mg3	0.000008	0.283348	0.972584	
Mg4	-1.533698	-2.379309	0.368427	
Mg5	2.605977	0.442654	-1.141878	
Mg6	-3.037349	0.378543	1.786749	
Mg7	1.653266	2.871379	0.510004	
Mg8	-0.000071	-1.118913	-2.189731	
Mg9	-1.653211	2.871362	0.509967	
Mg10	-4.428754	-1.866072	0.090895	
Mg11	-0.000025	1.941110	-2.011109	
Mg12	-2.606103	0.442662	-1.141868	
Mg13	4.428851	-1.866058	0.090790	
@mg13-isomer45 bp86/6-31G(d) Etot=-2601.150389 Eb=-11.79				

Mg1	-0.431124	1.425096	1.917359
Mg2	-3.571096	-2.128726	-0.239651
Mg3	0.380350	0.722649	-1.091956
Mg4	-2.440317	0.115868	-2.171153
Mg5	3.570859	1.077243	-0.477260
Mg6	4.408212	-1.760870	0.574202
Mg7	-1.575989	-1.432589	2.148436
Mg8	-0.648280	-2.238610	-0.766926
Mg9	1.630438	3.271655	0.255893
Mg10	2.284184	-1.557294	-1.607525
Mg11	-3.287617	0.737091	0.734407
Mg12	-1.654522	2.839193	-0.619514
Mg13	1.334902	-1.070706	1.343688

@mg13-isomer46 bp86/6-31G(d) Etot=-2601.150322 Eb=-11.78

Mg1	4.556266	-0.095782	1.516882
Mg2	1.643741	1.033872	1.783265
Mg3	2.550554	-1.569025	-0.299289
Mg4	3.228548	1.265184	-0.989337
Mg5	-0.079945	-1.486169	1.598267
Mg6	-1.340109	1.304675	1.707302
Mg7	0.259642	2.263692	-0.756097
Mg8	1.082988	-0.103142	-2.690333
Mg9	-2.969234	-2.514202	0.282578
Mg10	-4.126817	0.159109	0.974718
Mg11	-1.635121	-0.103124	-1.200786
Mg12	-0.163936	-2.686176	-1.145238
Mg13	-3.006575	2.531088	-0.781932

@mg13-isomer47 bp86/6-31G(d) Etot=-2601.150081 Eb=-11.77

Mg1	-2.709729	0.000111	-2.055910
Mg2	-0.854436	2.281508	-1.087293
Mg3	0.654931	0.000018	-2.356204
Mg4	-3.366429	1.500589	0.659974
Mg5	-0.854509	-2.281459	-1.087426
Mg6	-3.366446	-1.500592	0.659942
Mg7	3.876933	-0.000037	-1.489933
Mg8	2.074253	1.896217	0.165256
Mg9	-0.614579	2.674533	1.963419
Mg10	2.074117	-1.896152	0.165263
Mg11	-0.351531	-0.000027	0.923541
Mg12	4.052085	-0.000096	1.576049
Mg13	-0.614659	-2.674613	1.963323

@mg13-isomer48 bp86/6-31G(d) Etot=-2601.149999 Eb=-11.77

Mg1	-2.321361	1.209520	1.014994
Mg2	-1.583625	2.408600	-1.805804
Mg3	0.516102	2.291175	0.544801
Mg4	-1.958574	-2.053203	0.293904
Mg5	-4.485647	-0.807634	1.348873
Mg6	0.340610	-0.542542	1.929861
Mg7	-3.614730	-0.001158	-1.507254
Mg8	2.857471	1.315161	2.291957
Mg9	-0.008426	-0.107089	-1.376589
Mg10	3.078321	1.401254	-0.880177
Mg11	0.958806	-2.684147	-0.200801
Mg12	3.511580	-1.170603	0.695494
Mg13	2.709472	-1.259334	-2.349259

@mg13-isomer49 bp86/6-31G(d) Etot=-2601.149921 Eb=-11.76

Mg1	4.794833	-1.632796	0.000000
Mg2	2.798883	0.581014	-0.000091
Mg3	2.006862	-2.743446	0.000050
Mg4	2.988517	3.647610	0.000021

Mg5	0.197574	-0.636827	1.525238
Mg6	0.197537	-0.636821	-1.525172
Mg7	0.069799	2.138601	0.000072
Mg8	-1.172509	-2.995734	-0.000034
Mg9	-1.555162	1.500972	2.659839
Mg10	-1.555038	1.501041	-2.659795
Mg11	-2.914279	-1.117205	1.557328
Mg12	-2.914278	-1.117173	-1.557431
Mg13	-2.942738	1.510765	-0.000025

@mg13-isomer50 bp86/6-31G(d) Etot=-2601.149777 Eb=-11.76

Mg1	-1.110603	-2.020974	-1.887371
Mg2	-3.763121	-1.490897	-0.575984
Mg3	-1.261000	-1.995264	1.101870
Mg4	1.520093	-1.970303	-0.232480
Mg5	4.567132	-2.374596	0.013677
Mg6	3.658241	0.595409	-0.015182
Mg7	-2.452019	0.920170	-1.969782
Mg8	0.676055	0.590201	-1.728155
Mg9	-1.284082	-0.127320	3.508071
Mg10	-2.620841	0.983873	0.994446
Mg11	0.585357	0.662700	1.269906
Mg12	2.316929	3.288976	-0.069966
Mg13	-0.832142	2.938026	-0.409049

@mg13-isomer51 bp86/6-31G(d) Etot=-2601.149726 Eb=-11.76

Mg1	-1.484905	2.704268	0.640431
Mg2	1.495023	2.553329	2.011303
Mg3	3.062152	-0.000010	1.307508
Mg4	1.166639	1.721750	-0.795392
Mg5	3.692393	0.000061	-1.702157
Mg6	-4.113184	1.543716	-0.156321
Mg7	-0.221632	-0.000038	1.570583
Mg8	1.495081	-2.553406	2.011187
Mg9	0.936049	0.000074	-3.244711
Mg10	-1.596229	0.000006	-1.330999
Mg11	1.166651	-1.721715	-0.795471
Mg12	-1.484872	-2.704309	0.640356
Mg13	-4.113165	-1.543725	-0.156317

@mg13-isomer52 bp86/6-31G(d) Etot=-2601.149715 Eb=-11.75

Mg1	0.558134	-1.820549	-1.514751
Mg2	0.558121	-1.820434	1.514802
Mg3	-2.094774	-0.838346	0.000032
Mg4	-3.673433	1.427398	1.517549
Mg5	-1.504253	-3.741768	0.000096
Mg6	2.054822	0.894507	1.748224
Mg7	-0.874475	0.642032	2.652440
Mg8	-0.411626	1.876222	-0.000028
Mg9	2.054782	0.894441	-1.748257
Mg10	-3.673480	1.427320	-1.517621
Mg11	-0.874518	0.641887	-2.652434
Mg12	4.523559	1.673802	-0.000068
Mg13	3.357142	-1.256512	0.000015

@mg13-isomer53 bp86/6-31G(d) Etot=-2601.149694 Eb=-11.75

Mg1	-2.334795	0.000152	2.416615
Mg2	-2.238992	1.984397	-0.000160
Mg3	-4.391258	-0.000087	0.000003
Mg4	0.344041	1.491136	1.575956
Mg5	3.299077	-0.000121	-1.498385
Mg6	0.344152	-1.490784	1.576203
Mg7	2.781867	2.612719	-0.000307
Mg8	-2.238793	-1.984411	0.000128

Mg9	0.344106	1.490698	-1.576179
Mg10	2.782226	-2.612556	0.000338
Mg11	3.298947	0.000313	1.498409
Mg12	0.344233	-1.491201	-1.575942
Mg13	-2.334810	-0.000254	-2.416680

@mg13-isomer54 bp86/6-31G(d) Etot=-2601.149558 Eb=-11.75

Mg1	-3.361168	0.794153	-1.694531
Mg2	-4.709585	0.345302	1.083596
Mg3	-1.806198	1.300925	0.936687
Mg4	-0.161349	2.538470	-1.368657
Mg5	-0.323264	-0.369557	-1.678217
Mg6	-2.770192	-1.758676	0.216954
Mg7	1.198392	1.642144	1.346330
Mg8	4.295327	1.258952	1.292572
Mg9	2.594396	1.039072	-1.352124
Mg10	2.319572	-1.871636	-2.089032
Mg11	-0.154274	-0.929431	2.361306
Mg12	0.212888	-2.782638	0.012038
Mg13	2.665454	-1.207082	0.933077

@mg13-isomer55 bp86/6-31G(d) Etot=-2601.149458 Eb=-11.74

Mg1	2.448870	-2.303274	-0.423657
Mg2	4.312090	0.102703	-0.166821
Mg3	1.315165	0.312922	1.297203
Mg4	-0.368960	-2.397852	1.007059
Mg5	1.248215	0.369524	-1.684185
Mg6	-0.354035	-2.288108	-1.950441
Mg7	2.868062	2.768194	-0.038669
Mg8	-0.478361	-0.654584	3.535634
Mg9	-3.099487	-2.065220	-0.540197
Mg10	-0.293114	2.592881	-0.166254
Mg11	-2.110591	0.361964	1.169180
Mg12	-1.980294	0.476357	-1.814041
Mg13	-3.507559	2.724494	-0.224810

@mg13-isomer56 bp86/6-31G(d) Etot=-2601.149278 Eb=-11.73

Mg1	-1.455558	1.078732	-1.670118
Mg2	-1.943460	-1.808499	-2.446798
Mg3	-0.252691	3.624906	-0.559196
Mg4	-3.499851	-0.653663	0.051675
Mg5	-2.485992	2.056774	0.979507
Mg6	0.919171	-1.114020	-1.369973
Mg7	2.799250	3.262504	-0.098199
Mg8	-1.295249	-2.735785	0.344872
Mg9	0.420552	1.043738	0.883902
Mg10	-1.631159	-0.605083	2.567761
Mg11	3.426801	0.333518	-0.066156
Mg12	1.302420	-1.731645	1.586735
Mg13	3.695767	-2.751478	-0.204011

@mg13-isomer57 bp86/6-31G(d) Etot=-2601.149213 Eb=-11.73

Mg1	-1.209036	-0.433626	-1.228455
Mg2	-4.482658	0.081938	-1.137940
Mg3	-2.521514	2.400610	-0.851710
Mg4	1.598976	-0.309825	-2.525714
Mg5	0.581954	2.227595	-1.102793
Mg6	-0.922072	1.177465	1.428311
Mg7	-3.920194	-2.281109	0.676319
Mg8	4.248631	-2.000878	-1.221568
Mg9	1.283249	-1.984073	-0.061063
Mg10	1.806581	2.665716	1.724553
Mg11	-1.079329	-1.861831	1.742738
Mg12	3.081595	0.628302	0.016885

Mg13	1.533814	-0.310284	2.540437
@mg13-isomer58 bp86/6-31G(d) Etot=-2601.149169 Eb=-11.73			
Mg1	2.141060	-0.075204	1.785036
Mg2	3.421467	-2.095226	-0.012118
Mg3	-2.238898	-1.434611	2.382523
Mg4	4.093309	1.287453	-0.118694
Mg5	0.331931	-2.354834	0.654707
Mg6	-0.665831	0.821794	1.090337
Mg7	1.414438	0.138020	-1.212712
Mg8	1.511348	2.948700	0.186885
Mg9	-1.902069	3.228364	-0.241516
Mg10	-3.663961	0.770193	0.406302
Mg11	-1.572751	0.742872	-1.984826
Mg12	-0.263963	-2.010956	-2.460343
Mg13	-2.606080	-1.966564	-0.475583
@mg13-isomer59 bp86/6-31G(d) Etot=-2601.149144 Eb=-11.73			
Mg1	-4.508751	-1.462558	-0.026307
Mg2	1.947003	2.209311	-1.007742
Mg3	-1.565719	-1.488505	-1.108806
Mg4	-0.785120	1.308865	-2.252374
Mg5	3.604743	-2.884636	-0.252717
Mg6	0.780437	-2.614634	0.755250
Mg7	-2.130101	-1.568320	1.860076
Mg8	0.012271	0.393502	0.899086
Mg9	3.240052	-0.009037	0.651672
Mg10	-3.065732	1.199708	0.144111
Mg11	-0.879884	3.290996	0.202651
Mg12	1.441920	-0.846004	-1.846925
Mg13	1.908881	2.471312	1.982026
@mg13-isomer60 bp86/6-31G(d) Etot=-2601.148979 Eb=-11.72			
Mg1	-1.476731	-1.959929	1.973751
Mg2	4.288876	-0.875202	0.398075
Mg3	-2.720142	-1.878528	-0.826339
Mg4	1.697108	-1.639754	1.783626
Mg5	0.298861	-2.876347	-0.507497
Mg6	-0.229634	0.766843	1.500639
Mg7	-3.313776	0.361124	1.098884
Mg8	3.684148	2.095657	-0.176209
Mg9	-1.524360	1.037363	-1.336978
Mg10	-0.515684	-1.289152	-3.018587
Mg11	0.758252	2.974335	-0.354974
Mg12	-2.485556	3.316692	0.443252
Mg13	1.538638	-0.033101	-0.977643
@mg13-isomer61 bp86/6-31G(d) Etot=-2601.148896 Eb=-11.72			
Mg1	0.804780	-1.404472	2.515607
Mg2	2.440731	-2.229701	0.000074
Mg3	-3.776204	-1.769802	0.000130
Mg4	2.248196	3.026854	-0.000044
Mg5	0.648076	0.490327	-0.000297
Mg6	-1.238868	2.955682	-0.000111
Mg7	-3.991241	1.701640	-0.000031
Mg8	3.280839	0.449216	-1.508869
Mg9	3.280413	0.449401	1.509171
Mg10	-0.732935	-2.487924	0.000032
Mg11	-1.884260	0.111806	1.600173
Mg12	-1.884468	0.111603	-1.600224
Mg13	0.804942	-1.404630	-2.515609
@mg13-isomer62 bp86/6-31G(d) Etot=-2601.148658 Eb=-11.70			
Mg1	-0.877961	1.737228	2.788787

Mg2	-3.227653	1.778181	0.573741
Mg3	-0.000227	2.128101	0.000111
Mg4	-3.904071	-1.142192	-0.278904
Mg5	-1.021269	-0.823024	1.258746
Mg6	-1.850432	0.329290	-1.867365
Mg7	1.850202	0.329512	1.867459
Mg8	0.877262	1.737682	-2.788779
Mg9	3.227318	1.778739	-0.573734
Mg10	-1.510564	-2.944673	-0.688722
Mg11	1.021548	-0.822374	-1.258419
Mg12	1.511484	-2.945017	0.687963
Mg13	3.904362	-1.141453	0.279117

@mg13-isomer63 bp86/6-31G(d) Etot=-2601.148405 Eb=-11.69

Mg1	-3.203123	-1.655263	0.672480
Mg2	-0.466974	-3.149926	1.280023
Mg3	-0.303413	-0.258722	1.868177
Mg4	-0.467040	2.683446	2.087992
Mg5	-3.203117	1.410095	1.097042
Mg6	2.440778	-1.840865	0.747842
Mg7	-0.303444	-1.488415	-1.158058
Mg8	-3.202821	0.245105	-1.769995
Mg9	2.440659	1.568275	1.219996
Mg10	4.597452	-0.000003	0.000393
Mg11	-0.303492	1.747209	-0.709925
Mg12	2.441073	0.272562	-1.968028
Mg13	-0.466538	0.466503	-3.367939

@mg13-isomer64 bp86/6-31G(d) Etot=-2601.148371 Eb=-11.69

Mg1	0.672824	2.563592	0.381769
Mg2	-1.111009	2.367725	-2.240998
Mg3	-2.417876	1.960670	0.559379
Mg4	0.028954	-0.122611	-1.042293
Mg5	3.660125	2.038787	-0.168705
Mg6	4.325213	-1.031527	-0.531330
Mg7	-3.104829	-0.020120	-1.632356
Mg8	2.113529	-0.128248	1.362778
Mg9	-0.811905	0.637249	2.679252
Mg10	-3.167251	-0.923163	1.279087
Mg11	1.784259	-2.599182	-0.934396
Mg12	-1.677248	-2.669702	-1.144138
Mg13	-0.294785	-2.073470	1.431950

@mg13-isomer65 bp86/6-31G(d) Etot=-2601.148117 Eb=-11.68

Mg1	1.961255	-2.621218	-0.470943
Mg2	-3.382765	-1.115401	-0.446040
Mg3	-0.904216	-2.335849	0.916369
Mg4	-0.953340	-2.209756	-1.996126
Mg5	4.141932	-0.425792	-0.244000
Mg6	1.306542	0.048035	-1.750616
Mg7	-0.424041	-0.817615	3.492667
Mg8	-1.621308	0.961680	-1.737463
Mg9	1.450534	0.088942	1.269550
Mg10	-3.967975	2.224719	-0.113793
Mg11	3.507777	2.561078	0.042185
Mg12	-1.577413	0.935444	1.283742
Mg13	0.463017	2.705734	-0.245532

@mg13-isomer66 bp86/6-31G(d) Etot=-2601.148025 Eb=-11.67

Mg1	-0.377456	0.914633	1.133644
Mg2	-1.340239	-1.902335	1.464386
Mg3	-3.856102	-2.581001	-0.230978
Mg4	-2.241978	3.238981	0.069144
Mg5	-3.478229	0.498445	0.099719

Mg6	0.971690	3.636611	0.670003
Mg7	1.139193	-2.741080	-0.137946
Mg8	0.192869	1.789092	-1.688816
Mg9	1.844914	-0.681441	-2.342814
Mg10	2.684418	1.283066	0.115089
Mg11	3.869458	-1.464793	0.028098
Mg12	-1.150963	-1.047555	-1.489104
Mg13	1.742426	-0.942623	2.309576

@mg13-isomer67 bp86/6-31G(d) Etot=-2601.147751 Eb=-11.66

Mg1	-3.615741	-2.284322	-1.284464
Mg2	-2.074365	0.413174	-1.575898
Mg3	1.908345	-3.196425	-0.359229
Mg4	-1.119130	-2.061391	0.475647
Mg5	0.932435	-0.355979	-1.045477
Mg6	-3.616186	-0.137280	0.936545
Mg7	3.099983	1.676674	-1.766221
Mg8	0.160337	2.624757	-0.704887
Mg9	-2.743939	2.825395	0.328706
Mg10	3.856687	-0.824293	-0.079933
Mg11	-0.626850	0.938382	1.909914
Mg12	1.443425	-1.275994	2.016681
Mg13	2.394999	1.657304	1.148615

@mg13-isomer68 bp86/6-31G(d) Etot=-2601.147717 Eb=-11.66

Mg1	0.723866	3.841614	0.000139
Mg2	2.496403	1.500488	0.000034
Mg3	4.016649	-1.117031	-0.000036
Mg4	-0.345061	1.298949	1.491660
Mg5	-2.473060	3.181350	0.000013
Mg6	1.826343	-0.690522	-2.295562
Mg7	1.826364	-0.690584	2.295550
Mg8	1.424498	-2.736444	-0.000020
Mg9	-3.699586	-2.806844	-0.000039
Mg10	-1.098787	-1.684876	1.520835
Mg11	-0.344999	1.299118	-1.491783
Mg12	-1.098775	-1.684717	-1.520807
Mg13	-3.253856	0.289501	0.000015

@mg13-isomer69 bp86/6-31G(d) Etot=-2601.147425 Eb=-11.64

Mg1	2.920642	-2.988575	-0.084585
Mg2	0.321799	-1.805816	-1.299556
Mg3	3.381225	-0.017741	-1.166665
Mg4	2.882992	2.548197	0.569478
Mg5	-2.208999	2.585130	0.241604
Mg6	-1.172521	-0.228947	1.183426
Mg7	0.361019	4.299754	0.264763
Mg8	1.892512	-0.340641	1.364772
Mg9	-2.586491	-2.636437	-0.239158
Mg10	0.525607	1.417693	-0.903827
Mg11	-2.202905	0.190890	-1.720651
Mg12	0.116022	-3.077630	1.346264
Mg13	-4.230904	0.054123	0.444135

@mg13-isomer70 bp86/6-31G(d) Etot=-2601.147275 Eb=-11.64

Mg1	1.162131	0.640536	2.320862
Mg2	1.333593	-0.294155	-1.041589
Mg3	0.789071	-2.361555	1.391805
Mg4	-1.333552	-0.294179	1.041472
Mg5	-0.789085	-2.361505	-1.391878
Mg6	-3.174936	1.954761	-0.284080
Mg7	3.174900	1.954738	0.284168
Mg8	-4.291830	-0.124889	1.749985
Mg9	3.640692	-1.024577	1.154160

Mg10	-1.162155	0.640618	-2.320816
Mg11	-3.640730	-1.024516	-1.154204
Mg12	-0.000002	2.419511	0.000039
Mg13	4.291905	-0.124787	-1.749925

@mg13-isomer71 bp86/6-31G(d) Etot=-2601.147246 Eb=-11.64

Mg1	1.592331	2.672247	0.000289
Mg2	0.000023	1.700912	-2.536696
Mg3	-0.000112	-0.145635	-0.000215
Mg4	2.696665	0.183075	-1.513876
Mg5	2.696444	0.182606	1.513903
Mg6	-2.696726	0.183151	-1.513940
Mg7	-0.000070	1.700310	2.536978
Mg8	-1.604423	-2.744592	0.000060
Mg9	-2.696682	0.182717	1.513859
Mg10	-1.592285	2.672221	0.000228
Mg11	-4.442695	-1.921460	-0.000303
Mg12	4.442955	-1.921261	-0.000237
Mg13	1.604573	-2.744290	-0.000050

@mg13-isomer72 bp86/6-31G(d) Etot=-2601.146955 Eb=-11.62

Mg1	-0.670662	4.170934	-0.000064
Mg2	1.073377	1.541366	0.000132
Mg3	-1.641590	1.500250	1.607046
Mg4	-1.641354	1.500188	-1.607037
Mg5	0.878676	0.000057	-2.614106
Mg6	3.891303	0.000151	-1.530433
Mg7	-3.779883	-0.000108	-0.000162
Mg8	-1.641437	-1.500273	1.606909
Mg9	-1.641267	-1.500334	-1.607064
Mg10	3.891168	0.000156	1.530513
Mg11	0.878445	-0.000045	2.614219
Mg12	1.073576	-1.541343	0.000026
Mg13	-0.670352	-4.170998	0.000020

@mg13-isomer73 bp86/6-31G(d) Etot=-2601.146776 Eb=-11.61

Mg1	1.610701	-1.135154	2.183340
Mg2	-0.373481	1.289643	1.951553
Mg3	2.630162	1.525845	0.910203
Mg4	3.581042	-1.182123	-0.241453
Mg5	-1.281365	-1.640392	1.236912
Mg6	-2.635517	0.718593	-0.518976
Mg7	0.304325	2.842580	-0.722541
Mg8	-2.569657	3.609480	0.172858
Mg9	1.244575	-3.159670	-0.227658
Mg10	-4.225936	-1.793079	-0.070629
Mg11	2.832883	1.295699	-2.058291
Mg12	-1.628457	-2.163273	-1.736897
Mg13	0.510725	-0.208149	-0.878423

@mg13-isomer74 bp86/6-31G(d) Etot=-2601.146708 Eb=-11.61

Mg1	0.949038	-0.414614	2.668812
Mg2	-1.888327	-0.522436	1.477467
Mg3	2.854030	-2.411680	1.118515
Mg4	0.038485	1.836630	0.713772
Mg5	3.017731	0.530996	0.515412
Mg6	-3.091205	2.521194	0.485224
Mg7	2.531840	3.399021	-0.303072
Mg8	0.269378	-1.786718	-0.354335
Mg9	-4.492866	-0.224950	-0.307477
Mg10	2.938359	-1.628119	-1.818406
Mg11	-2.696219	-2.693993	-0.660593
Mg12	1.284619	1.062627	-2.012779
Mg13	-1.714863	0.332042	-1.522541

@mg13-isomer75 bp86/6-31G(d) Etot=-2601.146701 Eb=-11.61

Mg1	-1.099499	-1.347196	1.064041
Mg2	-1.703387	-2.070496	-1.746897
Mg3	-0.808356	1.905942	1.398008
Mg4	4.158876	-2.120704	0.050422
Mg5	1.308397	-2.276165	-0.875115
Mg6	-0.008907	-0.079384	3.611924
Mg7	-3.191656	0.792549	-0.406133
Mg8	1.742547	2.934176	-0.333746
Mg9	0.035582	0.524339	-1.456501
Mg10	-4.173240	-2.063777	0.009175
Mg11	-1.487260	3.193672	-1.192324
Mg12	3.306504	0.504368	-1.349175
Mg13	1.920399	0.102679	1.226323

@mg13-isomer76 bp86/6-31G(d) Etot=-2601.146604 Eb=-11.60

Mg1	0.357062	0.661831	1.509962
Mg2	4.232250	-2.092705	-0.891221
Mg3	-0.769156	1.646554	-1.493918
Mg4	1.886154	0.002248	-1.651520
Mg5	-2.801750	0.773280	0.683441
Mg6	1.882333	2.849610	-0.250121
Mg7	-1.205248	-1.857653	2.125640
Mg8	1.673585	-2.019745	0.834041
Mg9	-3.679200	-2.164122	0.216290
Mg10	-1.145755	3.274068	1.165569
Mg11	-3.320510	-0.149507	-2.153758
Mg12	3.693834	0.528490	0.812509
Mg13	-0.803598	-1.452350	-0.906915

@mg13-isomer77 bp86/6-31G(d) Etot=-2601.146483 Eb=-11.60

Mg1	1.858145	0.210699	-1.407809
Mg2	1.614533	-0.285006	1.838100
Mg3	-3.920719	0.133922	0.723475
Mg4	0.923613	2.660707	0.793609
Mg5	-2.625759	-2.352200	-0.562965
Mg6	-0.633145	-1.124610	-2.639370
Mg7	3.788547	1.618023	0.466488
Mg8	3.688171	-1.754389	-0.049629
Mg9	0.730505	-2.565242	-0.077569
Mg10	-0.706736	1.999826	-2.077605
Mg11	-0.890702	0.268913	0.258999
Mg12	-2.485138	2.875868	0.432959
Mg13	-1.341314	-1.686512	2.301316

@mg13-isomer78 bp86/6-31G(d) Etot=-2601.146335 Eb=-11.59

Mg1	-1.780627	-1.255376	-1.537325
Mg2	1.256125	-1.481257	-2.539190
Mg3	3.074838	-1.579946	-0.000025
Mg4	-3.024711	1.301662	0.000009
Mg5	-1.797436	4.018156	-0.000017
Mg6	-1.780615	-1.255390	1.537333
Mg7	2.755507	1.113609	-1.499531
Mg8	1.256140	-1.481373	2.539132
Mg9	2.755470	1.113568	1.499601
Mg10	0.421204	-2.973954	-0.000035
Mg11	-4.520549	-1.368254	0.000016
Mg12	0.166484	0.465379	-0.000017
Mg13	1.218170	3.383176	0.000049

@mg13-isomer79 bp86/6-31G(d) Etot=-2601.146278 Eb=-11.59

Mg1	4.275584	0.166353	-0.349794
Mg2	2.087034	2.395435	0.232032

Mg3	2.199070	-0.664636	1.652331
Mg4	-0.621340	3.990589	0.776256
Mg5	-0.546503	0.676565	1.026046
Mg6	2.959911	-2.861266	-0.249526
Mg7	1.290347	-0.306976	-1.243897
Mg8	-0.425561	2.370309	-1.648616
Mg9	-0.084829	-2.603071	0.467245
Mg10	-3.079071	2.031749	-0.061044
Mg11	-3.282212	-0.947487	1.153579
Mg12	-1.957677	-0.649271	-1.444454
Mg13	-2.814752	-3.598293	-0.310159

@mg13-isomer80 bp86/6-31G(d) Etot=-2601.146159 Eb=-11.58

Mg1	-0.074661	0.215063	1.542941
Mg2	4.487471	-0.264599	-0.000111
Mg3	-3.893599	-0.936869	0.000108
Mg4	-2.427108	-1.322617	2.634267
Mg5	-2.928706	1.531177	1.557517
Mg6	-0.074781	0.215053	-1.543053
Mg7	7.655599	-0.240457	0.000138
Mg8	1.908969	-1.753196	-0.000136
Mg9	-0.620352	2.767340	-0.000038
Mg10	-2.928829	1.531143	-1.557409
Mg11	2.414750	1.872843	-0.000085
Mg12	-2.427306	-1.322657	-2.634156
Mg13	-1.091447	-2.292224	0.000016

@mg13-isomer81 bp86/6-31G(d) Etot=-2601.146087 Eb=-11.58

Mg1	1.333936	-3.050514	0.378002
Mg2	-3.852073	2.355650	-0.401268
Mg3	-0.979540	-2.032873	-1.514921
Mg4	3.050211	-0.591174	1.012170
Mg5	-0.357280	-0.478690	0.980234
Mg6	1.739283	-0.659055	-1.808741
Mg7	4.285423	1.161553	-1.255519
Mg8	1.115361	1.248463	2.845657
Mg9	1.563174	1.994758	-0.212245
Mg10	-0.987436	1.085479	-1.829065
Mg11	-2.142328	-2.959826	1.203219
Mg12	-3.565110	-0.631588	-0.385331
Mg13	-1.203619	2.557818	0.987809

@mg13-isomer82 bp86/6-31G(d) Etot=-2601.145837 Eb=-11.57

Mg1	0.022737	2.147804	0.751239
Mg2	2.182549	0.062060	1.842171
Mg3	-1.405062	0.804830	-1.892353
Mg4	-3.012321	0.909836	0.812945
Mg5	-0.464585	-1.228405	0.846998
Mg6	-0.203949	-2.114274	-2.112020
Mg7	-3.058291	-1.774478	-0.823798
Mg8	3.246319	2.482223	0.286775
Mg9	4.441120	-0.519434	-0.093022
Mg10	1.558248	0.240113	-1.212799
Mg11	-2.410209	3.485837	-0.655287
Mg12	-3.123787	-1.784445	2.246515
Mg13	2.227231	-2.711666	0.002635

@mg13-isomer83 bp86/6-31G(d) Etot=-2601.145818 Eb=-11.57

Mg1	1.658548	1.107505	-0.782651
Mg2	-1.662877	1.054482	2.124496
Mg3	1.348988	1.515841	2.207666
Mg4	-0.383671	2.443908	-2.594143
Mg5	4.589543	-2.484120	-0.379936
Mg6	3.759232	-0.323924	1.513871

Mg7	-2.641950	1.556812	-0.735986
Mg8	-0.328960	3.256573	0.360529
Mg9	-2.667394	-1.282124	0.389476
Mg10	1.904463	-1.957251	-1.615232
Mg11	-5.155041	-3.266617	0.490463
Mg12	0.316324	-1.057991	0.955196
Mg13	-0.737203	-0.563095	-1.933749

@mg13-isomer84 bp86/6-31G(d) Etot=-2601.145594 Eb=-11.56

Mg1	-1.374191	-1.815105	1.886849
Mg2	0.609825	0.519473	1.715633
Mg3	3.660985	0.009631	0.420076
Mg4	0.965597	-1.974109	-0.190638
Mg5	-0.549813	3.133190	0.437497
Mg6	-2.070982	-1.431525	-0.963594
Mg7	-2.540472	1.053710	1.087860
Mg8	-4.405978	-1.354456	0.906882
Mg9	2.684835	2.944219	0.698926
Mg10	3.873604	-3.033963	0.213826
Mg11	-1.883761	1.616252	-1.852476
Mg12	-0.143750	-0.780609	-3.128458
Mg13	1.174100	1.113291	-1.232381

@mg13-isomer85 bp86/6-31G(d) Etot=-2601.145404 Eb=-11.55

Mg1	-4.033686	0.673586	0.891127
Mg2	-2.267391	3.071996	0.145442
Mg3	2.958018	-2.644940	0.495540
Mg4	0.644105	2.097990	-0.791090
Mg5	3.428474	-0.072635	-1.313850
Mg6	-1.028597	0.651360	1.697879
Mg7	-1.747641	-2.295462	-2.556053
Mg8	0.249302	-2.094016	2.116926
Mg9	-2.016479	0.613731	-1.561224
Mg10	0.449045	-1.119923	-0.833198
Mg11	-2.362575	-1.967737	0.437145
Mg12	2.092410	0.351342	1.386289
Mg13	3.635015	2.734709	-0.114933

@mg13-isomer86 bp86/6-31G(d) Etot=-2601.145313 Eb=-11.54

Mg1	-0.736691	4.171901	0.016834
Mg2	0.746066	1.525431	-0.926496
Mg3	3.610333	-0.000428	-1.621713
Mg4	5.015155	-0.000124	1.177065
Mg5	1.936584	-0.000231	1.548835
Mg6	-2.403658	1.525707	-0.833643
Mg7	-0.915690	0.000070	-2.980796
Mg8	0.745706	-1.525706	-0.926516
Mg9	-0.722927	1.520707	1.844184
Mg10	-2.403936	-1.525297	-0.833676
Mg11	-0.737577	-4.171761	0.017002
Mg12	-0.723241	-1.520587	1.844208
Mg13	-3.410124	0.000319	1.674711

@mg13-isomer87 bp86/6-31G(d) Etot=-2601.145254 Eb=-11.54

Mg1	0.257853	2.679491	0.734945
Mg2	0.434797	1.034631	-1.806791
Mg3	-1.238249	-0.071560	1.004752
Mg4	3.146693	-0.598361	-1.532337
Mg5	0.208350	0.906565	3.436549
Mg6	-2.028096	-0.755451	-1.837690
Mg7	2.041947	-0.028277	1.150755
Mg8	-4.322093	0.003629	0.096000
Mg9	3.239127	-2.896851	0.546536
Mg10	-2.746000	-2.759374	0.398110

Mg11	0.389296	-2.250476	-0.530077
Mg12	-2.395511	2.325770	-0.890520
Mg13	3.011886	2.410263	-0.770233
@mg13-isomer88 bp86/6-31G(d) Etot=-2601.144965 Eb=-11.53			
Mg1	3.294559	-0.319103	-1.736140
Mg2	0.295354	-0.619613	-2.568533
Mg3	5.003956	0.440056	0.597377
Mg4	0.674571	1.689291	-0.649030
Mg5	-2.053734	1.290864	-2.119519
Mg6	0.629652	-1.200882	0.417518
Mg7	-2.157131	-1.627384	-1.044371
Mg8	2.363373	0.915362	1.953490
Mg9	-0.418192	-4.332524	0.359891
Mg10	-1.761021	3.486546	0.096383
Mg11	-0.648598	1.175028	2.092934
Mg12	-3.284744	0.759891	0.625125
Mg13	-1.938045	-1.657532	1.974873
@mg13-isomer89 bp86/6-31G(d) Etot=-2601.144006 Eb=-11.48			
Mg1	3.957239	0.000024	-1.099606
Mg2	2.291665	-2.556990	-0.465378
Mg3	2.291704	2.556982	-0.465234
Mg4	0.753410	0.000044	-1.444581
Mg5	2.383951	-0.000116	1.391938
Mg6	-0.755605	-2.702178	-1.567166
Mg7	-0.433678	-1.645074	1.181008
Mg8	-0.755526	2.702336	-1.566988
Mg9	-0.433573	1.645052	1.181134
Mg10	-2.546007	0.000024	-0.748405
Mg11	-3.496481	-2.750345	-0.019019
Mg12	-3.496510	2.750356	-0.019054
Mg13	0.239412	-0.000115	3.641351
@mg13-isomer90 bp86/6-31G(d) Etot=-2601.143666 Eb=-11.46			
Mg1	-0.063554	-1.699552	2.589050
Mg2	-1.119947	1.013456	1.502447
Mg3	-3.750946	0.337097	-0.000004
Mg4	1.904893	0.341936	1.587617
Mg5	-1.730153	-1.873541	-0.000005
Mg6	1.412374	-2.273279	0.000036
Mg7	-6.914289	0.685610	0.000044
Mg8	-0.063514	-1.699665	-2.589009
Mg9	-1.119990	1.013436	-1.502570
Mg10	4.208687	2.093387	-0.000024
Mg11	4.412288	-1.049341	0.000007
Mg12	1.904822	0.341897	-1.587549
Mg13	0.919329	2.768558	-0.000040
@mg13-isomer91 bp86/6-31G(d) Etot=-2601.143545 Eb=-11.46			
Mg1	4.727671	0.238941	0.493050
Mg2	-2.156866	-4.213717	0.493107
Mg3	-0.100830	-1.929661	1.395347
Mg4	-2.897563	1.508533	-1.248272
Mg5	0.227086	3.157234	-0.277066
Mg6	0.000036	0.000026	-1.089242
Mg7	-2.570803	3.974749	0.493094
Mg8	-2.847789	-1.381935	-0.277165
Mg9	2.620658	-1.775301	-0.277073
Mg10	-1.620777	1.052108	1.395356
Mg11	1.721569	0.877537	1.395334
Mg12	0.142365	-3.263675	-1.248247
Mg13	2.755245	1.755160	-1.248222

@mg13-isomer92 bp86/6-31G(d) Etot=-2601.143091 Eb=-11.43

Mg1	-2.045430	0.194146	-1.726989
Mg2	-3.523822	2.599149	-0.481909
Mg3	-0.415719	2.452909	-0.079351
Mg4	2.333310	2.028769	-1.864247
Mg5	-0.618278	-2.721229	-1.423472
Mg6	2.363059	-2.863668	-0.064056
Mg7	4.065612	-0.286245	-0.346695
Mg8	0.893901	-0.237722	-0.519530
Mg9	-3.278846	-2.136296	-0.095366
Mg10	-2.428611	0.463230	1.334132
Mg11	-0.378394	-2.125932	1.567032
Mg12	2.701580	2.002428	1.065268
Mg13	0.331640	0.630461	2.635183

@mg13-isomer93 bp86/6-31G(d) Etot=-2601.142503 Eb=-11.41

Mg1	-2.724992	3.086883	0.211772
Mg2	-2.606245	1.248201	-2.291662
Mg3	-2.911114	-0.029163	0.449009
Mg4	-2.381972	-3.170728	0.590000
Mg5	-0.948439	1.530731	2.422091
Mg6	-0.076313	1.406777	-0.617204
Mg7	-0.965530	-1.425455	-1.587353
Mg8	-0.106731	-1.230393	1.455407
Mg9	4.746774	0.072242	0.127813
Mg10	2.081573	1.091152	1.546733
Mg11	0.811567	-3.782180	-0.191200
Mg12	3.003240	2.201283	-1.173160
Mg13	2.078182	-0.999350	-0.942244

@mg13-isomer94 bp86/6-31G(d) Etot=-2601.142488 Eb=-11.41

Mg1	3.427050	1.975721	0.286799
Mg2	2.269614	-2.951164	-0.538588
Mg3	1.444113	-0.359472	0.933380
Mg4	0.610318	2.543112	1.680035
Mg5	0.046404	-1.178504	-1.993700
Mg6	-3.252876	-1.687069	2.208435
Mg7	-1.731155	0.567290	0.975292
Mg8	0.672252	1.726009	-1.232962
Mg9	-2.135028	1.039552	-2.206990
Mg10	-2.022868	3.388522	-0.074095
Mg11	-0.663831	-2.609333	0.678832
Mg12	-3.112216	-1.526827	-0.851195
Mg13	4.448224	-0.927838	0.134758

@mg13-isomer95 bp86/6-31G(d) Etot=-2601.142113 Eb=-11.39

Mg1	3.885731	-0.536762	0.376670
Mg2	1.736359	-2.806010	0.722598
Mg3	1.134836	-0.167539	-1.004966
Mg4	2.552735	2.274645	0.496910
Mg5	3.600614	1.230653	-2.186428
Mg6	1.452542	0.048165	2.387298
Mg7	-0.588329	1.940145	0.940638
Mg8	-0.983003	-1.205714	1.224313
Mg9	-0.585014	-2.642224	-1.450299
Mg10	-3.736855	0.643650	0.948811
Mg11	-3.024303	3.198082	-0.558274
Mg12	-1.951092	0.272002	-1.493942
Mg13	-3.494222	-2.249093	-0.403330

@mg13-isomer96 bp86/6-31G(d) Etot=-2601.142074 Eb=-11.39

Mg1	1.145787	0.126842	1.096615
Mg2	0.602149	2.556149	-0.813301
Mg3	-1.805797	-1.047926	1.607023

Mg4	4.186455	-1.044417	0.493614
Mg5	-1.114269	2.221219	1.709100
Mg6	-3.026460	1.028094	-0.409709
Mg7	-3.512132	-2.080252	-0.595015
Mg8	-2.081346	3.982696	-0.519872
Mg9	3.455248	2.084106	0.249177
Mg10	2.297040	-0.121942	-1.650794
Mg11	-1.171158	-3.915689	0.128092
Mg12	1.668206	-2.846351	-0.082726
Mg13	-0.643724	-0.942529	-1.212205

@mg13-isomer97 bp86/6-31G(d) Etot=-2601.141927 Eb=-11.38

Mg1	-2.993472	-0.868372	0.000055
Mg2	-5.845216	-2.275867	-0.000036
Mg3	2.532719	-3.048282	-1.525636
Mg4	-0.030470	-1.376503	-0.000125
Mg5	1.238042	-0.353955	-2.623324
Mg6	-1.310766	1.066533	-1.633887
Mg7	2.532697	-3.048464	1.525572
Mg8	-1.310661	1.066420	1.634010
Mg9	1.238147	-0.354176	2.623215
Mg10	2.549227	0.282418	-0.000049
Mg11	1.238890	2.601594	-1.629118
Mg12	-1.078153	3.707190	0.000149
Mg13	1.239017	2.601465	1.629174

@mg13-isomer98 bp86/6-31G(d) Etot=-2601.141683 Eb=-11.37

Mg1	-1.844711	0.664456	1.539801
Mg2	-1.454279	-2.021775	-0.000042
Mg3	0.530753	2.138885	-2.635012
Mg4	6.239417	-2.479857	0.000000
Mg5	0.892392	-0.772824	1.541809
Mg6	3.513848	-0.858201	-0.000091
Mg7	0.530722	2.138780	2.635115
Mg8	-1.844775	0.664511	-1.539869
Mg9	-4.327582	-3.326801	0.000031
Mg10	-0.650242	3.102882	0.000040
Mg11	0.892339	-0.772758	-1.541822
Mg12	2.061584	1.763600	0.000051
Mg13	-4.539466	-0.240899	-0.000011

@mg13-isomer99 bp86/6-31G(d) Etot=-2601.141664 Eb=-11.37

Mg1	0.331792	-4.300109	0.565373
Mg2	1.429036	-1.135170	0.443756
Mg3	-0.915926	-1.444521	2.312551
Mg4	3.942846	-0.137539	-1.466164
Mg5	-1.422902	-1.681138	-0.731503
Mg6	0.832498	-0.670109	-2.567984
Mg7	0.348026	1.324278	2.057746
Mg8	3.547591	1.051897	1.466744
Mg9	1.309911	1.794161	-0.812654
Mg10	-2.627700	0.920356	1.242337
Mg11	-4.216861	-0.380061	-0.954337
Mg12	-1.558215	1.137198	-1.797753
Mg13	-1.000094	3.520759	0.241888

@mg13-isomer100 bp86/6-31G(d) Etot=-2601.141584 Eb=-11.36

Mg1	1.381342	-0.264493	-2.282297
Mg2	0.773943	1.833532	-0.099294
Mg3	1.218044	-0.238993	2.353982
Mg4	-1.531037	0.018427	-1.300199
Mg5	-1.032645	-2.069450	1.199665
Mg6	-1.911665	2.978587	-0.750687
Mg7	1.879411	-2.288033	0.187665

Mg8	3.374623	0.312456	0.123747
Mg9	-4.513249	1.554483	-0.174374
Mg10	-1.569869	0.867517	1.639449
Mg11	-3.962041	-1.265886	0.697052
Mg12	6.379030	1.271944	0.171695
Mg13	-0.485888	-2.710092	-1.766403
@mg13-isomer101 bp86/6-31G(d) Etot=-2601.141492 Eb=-11.36			
Mg1	4.327497	-0.000202	1.192039
Mg2	1.570151	1.554065	0.688485
Mg3	0.000540	-0.000024	2.846718
Mg4	-0.000102	4.172200	-0.213670
Mg5	1.570170	-1.554314	0.688531
Mg6	2.862034	0.000104	-1.745745
Mg7	-1.569938	1.553933	0.688942
Mg8	-1.570055	-1.554308	0.689043
Mg9	-0.000150	1.492283	-2.033410
Mg10	-4.327652	-0.000113	1.192062
Mg11	-2.862186	0.000128	-1.745404
Mg12	-0.000197	-1.491722	-2.033203
Mg13	-0.000110	-4.172030	-0.214387
@mg13-isomer102 bp86/6-31G(d) Etot=-2601.140844 Eb=-11.33			
Mg1	1.756477	-2.194112	0.775450
Mg2	0.809095	-1.282955	-1.941890
Mg3	3.494152	0.015587	-0.794247
Mg4	-1.354280	-1.780305	0.243630
Mg5	-1.771101	0.530486	-1.804903
Mg6	1.861729	0.926704	1.597713
Mg7	3.514424	3.234799	0.026320
Mg8	0.975355	1.777956	-1.233527
Mg9	-4.163549	-0.221173	0.330459
Mg10	-0.118313	-0.920987	2.948294
Mg11	-3.825242	2.809320	-0.348617
Mg12	-1.223898	1.272336	1.074983
Mg13	0.045150	-4.167656	-0.873664
@mg13-isomer103 bp86/6-31G(d) Etot=-2601.140795 Eb=-11.32			
Mg1	4.462464	0.334387	-1.061983
Mg2	-3.293352	-0.070947	0.266023
Mg3	2.746112	2.060320	0.817667
Mg4	1.116558	0.414161	3.055376
Mg5	-3.492786	3.052894	0.241637
Mg6	1.516576	1.236631	-1.864664
Mg7	-0.654514	-1.582314	1.560966
Mg8	0.737296	-3.655798	-0.408924
Mg9	-2.672023	-3.070007	-0.359661
Mg10	2.175299	-1.117123	0.287925
Mg11	-0.564309	-1.025011	-1.471328
Mg12	-1.564876	1.896754	-1.891762
Mg13	-0.512446	1.526053	0.828728
@mg13-isomer104 bp86/6-31G(d) Etot=-2601.140456 Eb=-11.31			
Mg1	4.271026	0.060415	-0.685296
Mg2	0.941602	1.219816	-1.032278
Mg3	-1.976995	1.087197	-2.132006
Mg4	-0.898835	3.580482	-0.429545
Mg5	2.086242	-1.297522	-2.250650
Mg6	3.153535	1.456022	1.733544
Mg7	-0.718126	-1.570603	-1.284795
Mg8	0.039485	1.502329	1.935110
Mg9	1.337948	-1.085473	0.979638
Mg10	-3.624649	-1.073732	-0.553901
Mg11	-2.864331	1.411523	0.930728

Mg12	-0.128551	-4.073831	0.932499
Mg13	-1.618352	-1.216624	1.856953
@mg13-isomer105 bp86/6-31G(d) Etot=-2601.140318 Eb=-11.30			
Mg1	-0.338119	-4.045835	0.703636
Mg2	-3.077609	-2.844976	-0.351015
Mg3	2.577458	-0.334860	-1.807363
Mg4	0.471594	3.894110	0.166826
Mg5	-2.397302	3.370306	-0.883353
Mg6	0.013278	0.957763	-0.525449
Mg7	-0.256033	-2.014878	-1.465403
Mg8	4.659670	-0.511199	0.340808
Mg9	-1.805738	2.064560	1.672924
Mg10	2.779961	1.891965	0.471920
Mg11	1.834602	-1.657642	0.809550
Mg12	-1.278478	-1.104228	1.389548
Mg13	-3.183286	0.334915	-0.522626
@mg13-isomer106 bp86/6-31G(d) Etot=-2601.140292 Eb=-11.30			
Mg1	-2.013271	-2.399921	-0.656979
Mg2	0.000045	0.167816	-0.529706
Mg3	-2.513665	-0.045115	1.345477
Mg4	3.021837	0.441695	-1.531376
Mg5	4.358832	2.318153	0.442870
Mg6	-1.486704	2.997943	-0.105962
Mg7	0.000057	-2.152388	1.666216
Mg8	0.000050	-4.640761	-0.124462
Mg9	-3.021862	0.441565	-1.531376
Mg10	-4.358968	2.318002	0.442852
Mg11	1.486574	2.998047	-0.105901
Mg12	2.013322	-2.399891	-0.657104
Mg13	2.513754	-0.045145	1.345451
@mg13-isomer107 bp86/6-31G(d) Etot=-2601.140102 Eb=-11.29			
Mg1	-1.529445	-1.286678	-1.238998
Mg2	1.288391	2.085500	1.723427
Mg3	-2.124371	-1.544341	1.996273
Mg4	3.874450	-0.471013	-1.425385
Mg5	1.288380	-2.085431	-1.723527
Mg6	-1.529461	1.286682	1.239184
Mg7	-0.358409	-3.821550	0.422362
Mg8	-2.124452	1.544232	-1.996321
Mg9	-3.949652	0.000009	0.000082
Mg10	-0.358517	3.821462	-0.422444
Mg11	3.874534	0.471049	1.425479
Mg12	0.824286	-0.940275	1.236666
Mg13	0.824267	0.940354	-1.236799
@mg13-isomer108 bp86/6-31G(d) Etot=-2601.139941 Eb=-11.28			
Mg1	1.413675	-3.815980	-0.710637
Mg2	-0.760395	-1.554070	-0.164490
Mg3	-3.010507	-1.414540	2.010983
Mg4	-3.776380	-1.002051	-1.028640
Mg5	2.218570	-1.252607	0.823056
Mg6	1.334786	-0.786813	-2.212778
Mg7	0.000084	-0.000282	2.563678
Mg8	-1.334858	0.787192	-2.212647
Mg9	-2.218408	1.252400	0.823394
Mg10	3.776359	1.002338	-1.028605
Mg11	0.760432	1.554181	-0.164291
Mg12	3.010610	1.414130	2.011116
Mg13	-1.413968	3.816102	-0.710139
@mg13-isomer109 bp86/6-31G(d) Etot=-2601.139775 Eb=-11.27			

Mg1	1.845614	1.741785	0.000492
Mg2	-1.148977	-1.066328	1.246471
Mg3	-1.845640	1.741778	-0.000662
Mg4	-1.827087	-0.806014	-1.752580
Mg5	4.120456	-0.297372	-0.454793
Mg6	1.148955	-1.066463	-1.246266
Mg7	1.827099	-0.805819	1.752684
Mg8	0.023669	1.676227	-2.408622
Mg9	-0.023681	1.676524	2.408420
Mg10	-0.000066	4.050465	-0.000045
Mg11	-4.120412	-0.297404	0.454882
Mg12	-3.347171	-3.273723	-0.047760
Mg13	3.347240	-3.273657	0.047781

@mg13-isomer110 bp86/6-31G(d) Etot=-2601.139524 Eb=-11.26

Mg1	-1.198428	-1.706469	1.531683
Mg2	4.437462	-2.022049	-0.000006
Mg3	-0.143372	-4.256140	0.000040
Mg4	1.470399	-1.610367	-0.000005
Mg5	0.589011	1.021781	1.514301
Mg6	3.418629	0.954336	-0.000033
Mg7	-2.595320	1.248650	1.536572
Mg8	-3.812650	-1.222110	0.000030
Mg9	-1.198481	-1.706566	-1.531720
Mg10	-1.000536	3.401270	-0.000005
Mg11	0.588893	1.021700	-1.514241
Mg12	2.039774	3.627339	-0.000062
Mg13	-2.595380	1.248624	-1.536555

@mg13-isomer111 bp86/6-31G(d) Etot=-2601.139451 Eb=-11.26

Mg1	2.107537	1.254713	0.939248
Mg2	-0.060868	-1.075289	0.904830
Mg3	5.126286	-3.671477	-0.039070
Mg4	2.762200	-1.542164	-0.026246
Mg5	-4.101444	-2.980913	-1.164672
Mg6	-1.969696	-0.782992	-1.638796
Mg7	-1.166024	2.174609	-1.869623
Mg8	-0.114623	1.178790	2.993152
Mg9	1.759613	3.066135	-1.588572
Mg10	0.978213	0.065417	-1.854631
Mg11	-0.065909	3.348925	0.871967
Mg12	-3.043098	-2.098544	1.633079
Mg13	-2.212188	1.062791	0.839333

@mg13-isomer112 bp86/6-31G(d) Etot=-2601.139411 Eb=-11.26

Mg1	1.902670	-0.934457	-0.615327
Mg2	-1.106151	-1.100291	-1.392885
Mg3	-0.261830	1.483996	0.569657
Mg4	4.768267	0.093193	0.358768
Mg5	-2.510351	1.704518	-1.495855
Mg6	0.550006	-3.709193	-0.641965
Mg7	-2.975209	0.007122	1.039376
Mg8	0.487056	1.139997	-2.585091
Mg9	-2.945078	3.227240	1.102499
Mg10	-2.615280	-3.139891	0.353175
Mg11	2.196595	0.513372	2.141044
Mg12	2.722249	2.251046	-0.431352
Mg13	-0.212945	-1.536651	1.597955

@mg13-isomer113 bp86/6-31G(d) Etot=-2601.138655 Eb=-11.22

Mg1	-2.378108	-0.469727	-1.822617
Mg2	0.465972	0.549087	-0.894839
Mg3	-4.818392	0.797776	-0.350358
Mg4	3.037172	1.125538	0.906423

Mg5	0.730792	-0.697206	2.264287
Mg6	-0.677833	-2.370902	0.040445
Mg7	2.446560	-1.775856	-0.166486
Mg8	-3.969139	-2.129215	0.308073
Mg9	-1.993972	0.198920	1.227749
Mg10	3.394654	0.472408	-2.093812
Mg11	0.133586	2.376273	1.606305
Mg12	5.519531	-0.545174	-0.128587
Mg13	-1.890822	2.468079	-0.896585

@mg13-isomer114 bp86/6-31G(d) Etot=-2601.138537 Eb=-11.22

Mg1	-3.885395	0.479038	0.763337
Mg2	0.839163	-0.405400	2.626270
Mg3	-1.334684	-1.278013	0.681414
Mg4	-0.855054	1.730391	1.041446
Mg5	1.058740	-3.128772	0.825901
Mg6	4.334647	1.686757	-0.903384
Mg7	-3.385378	3.286381	-0.412147
Mg8	-1.602905	-4.111770	-0.720825
Mg9	0.395610	-1.650698	-1.858451
Mg10	-1.724355	0.656591	-1.706889
Mg11	1.234273	1.382038	-1.611320
Mg12	2.722257	-0.753414	0.048739
Mg13	2.203081	2.106872	1.225908

@mg13-isomer115 bp86/6-31G(d) Etot=-2601.138393 Eb=-11.21

Mg1	-2.002825	1.709640	-1.651629
Mg2	-0.438950	-0.870475	-0.975289
Mg3	-4.533738	2.021973	0.022506
Mg4	2.895276	-0.532206	-0.317117
Mg5	3.161028	1.441773	1.932033
Mg6	0.723371	-0.545975	2.129280
Mg7	-1.844028	0.816337	1.306004
Mg8	0.765007	1.992960	-0.093117
Mg9	-1.767934	-2.415170	1.508746
Mg10	1.214498	-3.084757	0.326678
Mg11	1.748615	-2.169556	-2.608821
Mg12	-3.664257	-0.906484	-0.656215
Mg13	3.743937	2.541941	-0.923060

@mg13-isomer116 bp86/6-31G(d) Etot=-2601.138086 Eb=-11.19

Mg1	-3.112627	3.052513	-0.705198
Mg2	-3.580041	0.046151	-0.360380
Mg3	-0.884003	1.507989	0.842919
Mg4	-1.245637	1.223375	-2.282692
Mg5	-2.175965	-1.231589	2.101729
Mg6	-3.372591	-2.957587	-0.171397
Mg7	1.932679	2.180509	2.171111
Mg8	-0.656461	-1.584535	-0.746785
Mg9	1.519334	0.807245	-0.994902
Mg10	0.914005	-0.723029	1.821057
Mg11	2.460966	-2.216387	-0.635663
Mg12	4.299267	-0.222103	-2.025909
Mg13	3.901075	0.117449	0.986110

@mg13-isomer117 bp86/6-31G(d) Etot=-2601.137543 Eb=-11.17

Mg1	-1.546566	0.701166	1.671942
Mg2	1.118349	2.163884	1.792390
Mg3	1.016554	-0.853398	2.309160
Mg4	-1.313122	3.642684	0.548559
Mg5	1.008885	2.741531	-1.219496
Mg6	5.005475	-1.712224	-0.417148
Mg7	2.403510	-3.220677	0.461233
Mg8	2.492144	0.194243	-0.217880

Mg9	-5.890694	-2.679871	-0.212768
Mg10	-0.250913	-1.389836	-0.386551
Mg11	-3.224269	-0.982604	-0.130115
Mg12	-1.660366	1.239244	-1.386745
Mg13	0.841014	0.155856	-2.812581

@mg13-isomer118 bp86/6-31G(d) Etot=-2601.137542 Eb=-11.17

Mg1	-0.690725	-2.083982	0.011317
Mg2	5.554751	-0.191096	-0.003111
Mg3	-2.237756	2.834294	-0.012431
Mg4	-2.137752	0.200441	1.562163
Mg5	-2.136346	0.186100	-1.563365
Mg6	3.144253	1.092370	-1.560376
Mg7	2.379204	-1.444104	0.008155
Mg8	-3.956162	-2.074094	0.006548
Mg9	0.392086	1.210276	-0.002586
Mg10	0.679184	-0.869211	-2.520245
Mg11	3.147273	1.107266	1.549116
Mg12	-4.817152	0.874110	-0.005851
Mg13	0.679141	-0.842369	2.530666

@mg13-isomer119 bp86/6-31G(d) Etot=-2601.137040 Eb=-11.14

Mg1	0.272851	1.416979	-1.268986
Mg2	-1.348499	-0.822516	-2.466767
Mg3	-0.978989	-1.371221	0.644535
Mg4	-2.926313	1.062662	-0.306754
Mg5	1.448608	-1.488852	-1.443088
Mg6	3.484767	1.424629	-0.683057
Mg7	1.519498	3.090544	0.939058
Mg8	-3.810504	-1.852059	-0.667153
Mg9	1.726505	0.082882	1.488719
Mg10	-1.512708	3.657927	0.225892
Mg11	4.094295	-1.538820	0.198033
Mg12	-3.595937	-0.642866	2.147709
Mg13	1.626426	-3.019289	1.191857

@mg13-isomer120 bp86/6-31G(d) Etot=-2601.136995 Eb=-11.14

Mg1	0.578859	0.694897	1.388848
Mg2	1.195435	2.347538	-1.102081
Mg3	3.820069	-0.689753	1.367363
Mg4	1.195544	-2.347537	1.102053
Mg5	0.578798	-0.694907	-1.388904
Mg6	-1.768962	1.517470	-0.659016
Mg7	-1.768847	-1.517501	0.659115
Mg8	3.271842	2.342300	1.175310
Mg9	-3.845002	0.582017	1.395637
Mg10	3.271893	-2.342238	-1.175345
Mg11	-3.844958	-0.582190	-1.395565
Mg12	3.819986	0.689816	-1.367361
Mg13	-6.504657	0.000088	-0.000054

@mg13-isomer121 bp86/6-31G(d) Etot=-2601.136969 Eb=-11.14

Mg1	2.718298	0.002630	-2.660802
Mg2	2.431549	1.522565	0.118719
Mg3	0.615586	4.178341	-0.111536
Mg4	2.433455	-1.519655	0.117541
Mg5	1.569569	-0.000107	2.648589
Mg6	0.100659	1.534073	-1.892726
Mg7	-0.580012	1.545199	1.149001
Mg8	0.102595	-1.532849	-1.893936
Mg9	0.620967	-4.177719	-0.114542
Mg10	-2.347388	-0.001328	-0.851438
Mg11	-5.449586	-0.001561	-1.625041
Mg12	-1.637704	-0.002594	3.968337

Mg13	-0.577987	-1.546995	1.147834	
@mg13-isomer122 bp86/6-31G(d) Etot=-2601.136417 Eb=-11.11				
Mg1	0.706680	1.556641	-1.062095	
Mg2	-1.288401	0.000249	-2.847800	
Mg3	-2.345754	1.556000	-0.432584	
Mg4	-2.346370	-1.555149	-0.432642	
Mg5	-0.686466	4.308787	-1.053961	
Mg6	-0.780289	2.885112	1.798073	
Mg7	-0.688109	-4.308562	-1.053944	
Mg8	0.706061	-1.556921	-1.062035	
Mg9	-2.316173	0.000408	2.273338	
Mg10	3.036424	-0.000593	0.130426	
Mg11	-0.781394	-2.884829	1.798049	
Mg12	0.579623	-0.000095	1.784689	
Mg13	6.204167	-0.001048	0.160485	
@mg13-isomer123 bp86/6-31G(d) Etot=-2601.136390 Eb=-11.11				
Mg1	-1.025954	1.439953	-1.372678	
Mg2	-3.294283	0.910468	0.672476	
Mg3	1.654705	2.505127	-0.127034	
Mg4	-0.038452	0.486448	1.742983	
Mg5	3.182744	0.236941	1.336874	
Mg6	1.243368	-0.714764	-1.141350	
Mg7	3.811022	-2.300379	-0.380919	
Mg8	3.919647	0.773189	-1.576485	
Mg9	-1.430135	-1.769807	-0.049466	
Mg10	1.213437	-2.323457	1.503276	
Mg11	-3.509317	-0.474945	-2.078042	
Mg12	-1.306763	3.303454	1.024991	
Mg13	-4.420020	-2.072228	0.445375	
@mg13-isomer124 bp86/6-31G(d) Etot=-2601.136301 Eb=-11.11				
Mg1	2.015588	1.690806	-1.287446	
Mg2	-3.580887	0.043594	-0.049256	
Mg3	1.989684	1.076679	1.715201	
Mg4	-0.904954	-1.498724	-0.428093	
Mg5	4.766674	0.554219	0.100008	
Mg6	0.638692	-1.649409	2.199228	
Mg7	2.207077	-1.292015	-0.374756	
Mg8	-6.824570	0.041545	0.067440	
Mg9	-1.047152	0.875949	1.665220	
Mg10	0.331010	3.543470	0.578585	
Mg11	0.814055	-4.352820	0.056927	
Mg12	-1.057146	1.489732	-1.343739	
Mg13	0.651928	-0.523027	-2.899320	
@mg13-isomer125 bp86/6-31G(d) Etot=-2601.136013 Eb=-11.09				
Mg1	-3.408284	2.846352	0.092207	
Mg2	-0.697414	3.626255	-1.180701	
Mg3	4.169266	1.528358	0.092196	
Mg4	-0.531201	1.848084	1.231621	
Mg5	-2.791854	-2.417075	-1.180512	
Mg6	3.489136	-1.209280	-1.180567	
Mg7	-0.000024	0.000131	3.627988	
Mg8	1.865991	-0.463879	1.231660	
Mg9	0.375334	-1.775776	-1.352604	
Mg10	-1.725489	0.562781	-1.352592	
Mg11	1.350209	1.212933	-1.352598	
Mg12	-0.760984	-4.374866	0.092256	
Mg13	-1.334686	-1.384019	1.231647	
@mg13-isomer126 bp86/6-31G(d) Etot=-2601.135929 Eb=-11.09				
Mg1	1.016610	2.221945	0.692326	

Mg2	-0.344091	1.699086	-2.014749
Mg3	-0.059374	-0.999254	-0.143752
Mg4	-2.715327	-1.213464	1.351318
Mg5	2.449486	-0.481425	1.563504
Mg6	4.996204	-0.989327	-0.319000
Mg7	-0.347310	0.323444	2.787361
Mg8	2.431708	0.308220	-1.459940
Mg9	2.602219	-2.888238	-0.472196
Mg10	-2.147917	1.608120	0.499692
Mg11	-4.252245	-3.297797	-0.508946
Mg12	-2.659304	-0.594104	-1.638077
Mg13	-0.970659	4.302793	-0.337542

@mg13-isomer127 bp86/6-31G(d) Etot=-2601.135753 Eb=-11.08

Mg1	-0.132460	1.253915	-1.277160
Mg2	-1.906751	-1.359107	-1.536233
Mg3	-3.352594	1.488458	-0.773569
Mg4	3.054155	0.622820	-0.910229
Mg5	-1.228991	3.360574	0.708219
Mg6	0.876076	-1.757108	-0.049593
Mg7	-1.514457	-0.021069	1.201856
Mg8	1.351234	1.303750	1.510156
Mg9	-1.732456	-3.363454	0.776786
Mg10	3.496711	-1.095768	1.511347
Mg11	-4.225485	-1.453979	0.337337
Mg12	1.653713	3.655514	-0.376553
Mg13	3.661304	-2.634546	-1.122364

@mg13-isomer128 bp86/6-31G(d) Etot=-2601.135723 Eb=-11.08

Mg1	5.520367	-0.480290	0.572743
Mg2	2.622534	-1.674104	0.198229
Mg3	3.958036	0.302837	-1.880561
Mg4	-0.129321	-0.858041	1.792627
Mg5	-0.378972	-2.468183	-0.729640
Mg6	3.088128	1.349810	0.909089
Mg7	-2.983842	-2.026775	0.872124
Mg8	0.719021	0.460477	-1.083315
Mg9	-5.314827	-0.145305	-0.274885
Mg10	-1.599313	2.541978	-1.238323
Mg11	-2.547599	-0.380662	-1.684099
Mg12	-2.924542	1.149155	1.162555
Mg13	-0.029670	2.229102	1.383457

@mg13-isomer129 bp86/6-31G(d) Etot=-2601.135532 Eb=-11.07

Mg1	1.143402	0.461655	-1.545718
Mg2	-0.595478	2.307871	0.311713
Mg3	-1.869549	-0.157680	-1.253867
Mg4	-2.527013	-2.386486	0.915875
Mg5	-0.005567	-0.596411	1.281084
Mg6	4.469570	0.631014	-1.541755
Mg7	5.377571	0.057774	1.243010
Mg8	-4.887883	-0.553746	-0.331785
Mg9	2.533802	1.423812	1.010266
Mg10	2.976293	-1.548741	0.067613
Mg11	-0.000917	-2.579567	-1.098711
Mg12	-2.955008	0.623949	1.705746
Mg13	-3.659223	2.316555	-0.763470

@mg13-isomer130 bp86/6-31G(d) Etot=-2601.135417 Eb=-11.06

Mg1	-4.608986	-0.487347	-0.000104
Mg2	-2.192649	0.577203	1.600524
Mg3	-1.406509	3.391157	0.000022
Mg4	-2.192536	0.577238	-1.600524
Mg5	0.727602	1.856903	1.626453

Mg6	0.574508	-1.202988	1.628903
Mg7	-1.966785	-2.081354	0.000013
Mg8	0.727658	1.856910	-1.626339
Mg9	3.084992	0.250827	3.008481
Mg10	0.574534	-1.203020	-1.628979
Mg11	3.085062	0.250938	-3.008466
Mg12	0.659997	-4.047024	0.000014
Mg13	2.933112	0.260557	0.000002

@mg13-isomer131 bp86/6-31G(d) Etot=-2601.135129 Eb=-11.05

Mg1	3.361045	-0.123927	-2.068368
Mg2	4.777542	-1.762717	0.111335
Mg3	3.139134	0.860333	0.819913
Mg4	1.806149	-2.095543	-0.011913
Mg5	-3.200336	-0.450160	1.728075
Mg6	0.410257	0.556534	-0.955753
Mg7	0.073081	-0.102803	2.119325
Mg8	1.057868	2.796913	1.728682
Mg9	-4.286237	-2.437216	-0.452466
Mg10	-1.212451	-2.204838	0.135744
Mg11	-1.787530	2.227877	0.620511
Mg12	-2.808432	0.133197	-1.433888
Mg13	-1.330091	2.602351	-2.341197

@mg13-isomer132 bp86/6-31G(d) Etot=-2601.135110 Eb=-11.05

Mg1	0.648025	-0.794130	-0.732755
Mg2	0.662895	1.416115	1.744972
Mg3	1.975716	2.143131	-0.930478
Mg4	-1.736388	-0.690723	1.253929
Mg5	3.325022	-0.126956	0.833224
Mg6	-1.176702	1.829184	-0.836451
Mg7	-2.312728	-1.016353	-1.782920
Mg8	3.360586	-0.662115	-2.119596
Mg9	-4.387877	-2.381960	0.091835
Mg10	2.820239	-3.093679	-0.076150
Mg11	-0.008542	4.276726	0.520464
Mg12	1.014796	-1.704336	2.252559
Mg13	-4.185042	0.805098	-0.218634

@mg13-isomer133 bp86/6-31G(d) Etot=-2601.134535 Eb=-11.02

Mg1	-2.906950	-1.783893	0.236526
Mg2	0.180837	1.098232	1.428242
Mg3	0.180747	0.688079	-1.665158
Mg4	0.180846	-1.786015	0.236711
Mg5	-2.907213	1.096569	1.426613
Mg6	2.757284	0.000037	-0.000247
Mg7	5.914981	0.000237	-0.000594
Mg8	-1.374040	-1.842566	-2.397005
Mg9	-1.374064	2.997336	-0.397344
Mg10	9.256980	-0.000316	0.000543
Mg11	-1.373745	-1.154360	2.794345
Mg12	-5.628336	-0.000382	0.000205
Mg13	-2.907328	0.687042	-1.662836

@mg13-isomer134 bp86/6-31G(d) Etot=-2601.133448 Eb=-10.97

Mg1	0.830994	0.257228	-1.494443
Mg2	2.327122	0.706818	1.347002
Mg3	4.125418	0.168691	-1.180781
Mg4	4.807481	-1.190838	1.400453
Mg5	-0.774164	-2.326491	-1.487487
Mg6	-0.586824	-0.811584	1.154695
Mg7	-0.351749	2.279327	0.666224
Mg8	-3.281418	0.987457	1.712079
Mg9	-3.608328	-1.810494	0.346667

Mg10	-5.559126	0.469559	-0.388841
Mg11	2.085837	-2.143030	0.087553
Mg12	2.344026	2.877896	-0.972191
Mg13	-2.359269	0.535462	-1.190930

@mg13-isomer135 bp86/6-31G(d) Etot=-2601.133258 Eb=-10.96

Mg1	-0.610748	0.622805	-1.990044
Mg2	-2.899196	-1.398727	-0.945341
Mg3	-2.086435	1.265306	0.994178
Mg4	-0.234409	-2.343849	-2.234893
Mg5	2.324977	-0.692803	-1.122774
Mg6	-2.989029	-1.431086	2.149118
Mg7	-5.128448	0.233191	0.565990
Mg8	5.329178	-1.134938	0.322553
Mg9	4.173854	1.680507	0.248781
Mg10	-0.185187	-1.372892	0.661451
Mg11	2.698883	-0.542404	1.860283
Mg12	-1.330925	3.353245	-1.037320
Mg13	0.937484	1.761643	0.528019

@mg13-isomer136 bp86/6-31G(d) Etot=-2601.133126 Eb=-10.95

Mg1	-2.067772	1.034717	1.304504
Mg2	-1.419305	2.895291	-1.101163
Mg3	0.118347	-1.350776	1.261393
Mg4	-0.762361	0.050312	-1.573279
Mg5	-4.002628	0.741774	-1.214738
Mg6	-2.803733	-1.907838	0.118252
Mg7	3.288809	-0.224106	1.884648
Mg8	0.930174	1.678166	0.612510
Mg9	2.355771	-0.833079	-0.957698
Mg10	5.537392	-0.758840	-0.238631
Mg11	-0.253565	-2.902982	-1.363757
Mg12	4.027828	1.835606	-0.223461
Mg13	-4.948956	-0.258246	1.491420

@mg13-isomer137 bp86/6-31G(d) Etot=-2601.132656 Eb=-10.93

Mg1	0.136902	0.584667	-1.658722
Mg2	3.633187	1.352750	-1.151427
Mg3	-0.704775	-0.551370	1.189825
Mg4	-2.733642	-2.794758	1.006209
Mg5	2.319473	-1.180601	-0.048972
Mg6	-1.774213	2.206145	0.206491
Mg7	5.612954	-0.862142	-0.461836
Mg8	-4.667771	1.865794	-0.913696
Mg9	-2.900791	-0.589990	-1.244681
Mg10	-0.488717	-2.515903	-1.221607
Mg11	4.198878	0.597332	1.767142
Mg12	-3.916042	0.134015	1.552179
Mg13	1.284556	1.754062	0.979095

@mg13-isomer138 bp86/6-31G(d) Etot=-2601.132633 Eb=-10.93

Mg1	-0.018908	-0.723519	-0.644183
Mg2	-2.220775	1.646349	-0.877162
Mg3	0.924442	2.397825	-1.027923
Mg4	-1.199934	4.241330	0.354763
Mg5	2.462300	0.530469	0.930344
Mg6	2.702063	-0.107003	-2.025842
Mg7	-2.504569	-0.725441	1.130009
Mg8	0.345435	-1.304783	2.411277
Mg9	5.041764	-1.046720	-0.164670
Mg10	-0.311294	1.631848	1.759503
Mg11	2.447026	-2.670514	0.121569
Mg12	-2.769774	-1.175551	-1.861190
Mg13	-4.897776	-2.694288	-0.106496

@mg13-isomer139 bp86/6-31G(d) Etot=-2601.132156 Eb=-10.91

Mg1	4.371151	1.361383	-1.269069
Mg2	-0.554038	-0.765097	-1.692794
Mg3	-4.870905	0.782807	0.289088
Mg4	2.383525	-1.173502	-0.455538
Mg5	5.420095	-0.831607	0.502346
Mg6	0.003989	-0.139871	1.380232
Mg7	3.220328	1.088970	1.493941
Mg8	-0.162335	-3.096169	0.324654
Mg9	-3.583866	-0.119901	-2.383726
Mg10	1.171942	1.732770	-0.954856
Mg11	-2.764934	-1.401098	0.472627
Mg12	-1.917830	1.700111	-0.337458
Mg13	-2.717123	0.861204	2.630553

@mg13-isomer140 bp86/6-31G(d) Etot=-2601.131588 Eb=-10.88

Mg1	-0.866353	3.274596	-2.851133
Mg2	3.062986	-0.000217	0.186993
Mg3	0.802814	-0.000170	2.243414
Mg4	-2.384012	1.595604	-0.182980
Mg5	-2.384224	-1.595261	-0.183090
Mg6	-0.771468	2.744166	2.302463
Mg7	6.215639	-0.000211	-0.188653
Mg8	-0.771888	-2.744249	2.302270
Mg9	-1.046004	0.000131	-2.438373
Mg10	-2.237749	0.000061	2.463289
Mg11	-0.866842	-3.274338	-2.851318
Mg12	0.623450	-1.663971	-0.401496
Mg13	0.623652	1.663858	-0.401386

@mg13-isomer141 bp86/6-31G(d) Etot=-2601.130614 Eb=-10.83

Mg1	1.130809	-0.023755	-1.702357
Mg2	3.688962	0.704944	-0.166193
Mg3	0.260252	-3.148910	-1.120895
Mg4	0.945287	1.306313	1.171825
Mg5	6.386529	2.391157	-0.125380
Mg6	-1.359236	1.647017	-0.933749
Mg7	-4.068784	3.054444	0.102954
Mg8	-0.013795	-3.579087	1.899415
Mg9	-1.633697	-1.047575	-2.489193
Mg10	-2.164194	1.474511	2.013080
Mg11	2.103835	-1.657176	0.905737
Mg12	-4.089904	0.002576	-0.210370
Mg13	-1.186064	-1.124458	0.655125

@mg13-isomer142 bp86/6-31G(d) Etot=-2601.129799 Eb=-10.79

Mg1	-4.055309	-2.015635	-1.153320
Mg2	-0.000003	1.325518	-0.000058
Mg3	-2.986705	0.878480	-1.321182
Mg4	2.707578	2.434885	-1.369504
Mg5	5.148437	0.266020	-0.661558
Mg6	2.986656	0.878497	1.321176
Mg7	2.156666	-0.617993	-1.233154
Mg8	-2.707520	2.434887	1.369524
Mg9	-0.864473	-1.608539	-1.330927
Mg10	4.055293	-2.015650	1.153359
Mg11	-2.156649	-0.617986	1.233140
Mg12	0.864459	-1.608528	1.330900
Mg13	-5.148432	0.266044	0.661604

@mg13-isomer143 bp86/6-31G(d) Etot=-2601.129781 Eb=-10.79

Mg1	3.931435	1.760928	1.042286
Mg2	0.680671	1.330613	-0.000820

Mg3	-4.706282	1.158773	-0.219186
Mg4	2.632606	-1.019652	1.064029
Mg5	-2.169692	-3.024670	-0.791250
Mg6	-3.745570	-1.270647	1.395460
Mg7	-1.817835	2.899033	-1.167344
Mg8	-2.117648	1.451825	1.532573
Mg9	-0.631594	-1.353592	1.307974
Mg10	5.770545	-0.587662	0.240065
Mg11	3.454316	0.248546	-1.585735
Mg12	-1.970033	-0.040383	-1.340257
Mg13	0.689081	-1.553111	-1.477795

@mg13-isomer144 bp86/6-31G(d) Etot=-2601.129636 Eb=-10.79

Mg1	-0.902805	-1.484886	0.356368
Mg2	-3.724420	0.261133	-0.492765
Mg3	-1.711819	1.388002	1.797779
Mg4	2.255766	-2.031633	0.862545
Mg5	-0.866801	1.748435	-1.165515
Mg6	-3.539708	-2.736567	-0.530620
Mg7	-3.389038	3.260094	-0.071808
Mg8	1.237307	0.996353	1.063452
Mg9	1.380029	-0.399318	-1.701236
Mg10	-0.228888	-0.991059	3.175046
Mg11	4.007250	0.335678	-0.024279
Mg12	7.079143	0.767949	-0.792492
Mg13	-1.596015	-1.114180	-2.476476

@mg13-isomer145 bp86/6-31G(d) Etot=-2601.129491 Eb=-10.78

Mg1	-0.618604	-1.046476	1.553025
Mg2	4.134931	1.602403	0.399297
Mg3	0.942544	1.188869	-0.159390
Mg4	-5.131459	-0.504620	-1.015995
Mg5	3.461809	-0.422874	-1.756550
Mg6	5.575666	-1.010268	0.402555
Mg7	0.333840	-1.788587	-1.237025
Mg8	-2.072418	0.434924	-1.074838
Mg9	-3.784525	-0.240710	1.668699
Mg10	-1.159507	3.287189	-1.189541
Mg11	-1.505937	2.093455	1.621277
Mg12	-2.694716	-2.438964	-0.318412
Mg13	2.518375	-1.154342	1.106898

@mg13-isomer146 bp86/6-31G(d) Etot=-2601.128746 Eb=-10.74

Mg1	0.373388	1.448168	1.520517
Mg2	-0.867829	2.042663	-1.226757
Mg3	3.573088	1.247205	1.574588
Mg4	-2.801486	1.058415	1.138318
Mg5	1.802170	0.473623	-1.085854
Mg6	4.258327	-1.294831	0.011185
Mg7	-3.569669	0.227080	-1.757593
Mg8	-5.845947	0.491755	0.261490
Mg9	-0.837596	-1.012241	-0.207051
Mg10	4.707922	1.452640	-1.277284
Mg11	1.559444	-2.758655	-1.112941
Mg12	-3.899876	-1.822257	0.491210
Mg13	1.548064	-1.553565	1.670173

@mg13-isomer147 bp86/6-31G(d) Etot=-2601.128080 Eb=-10.71

Mg1	3.805395	2.404908	-1.143974
Mg2	-2.439328	2.760032	-0.533081
Mg3	-0.115137	-1.833057	-2.252924
Mg4	3.469377	1.061982	1.659283
Mg5	2.484884	-3.413886	-0.920369
Mg6	2.061692	-0.360846	-0.631155

Mg7	0.443238	0.264002	2.458218
Mg8	-4.158629	0.386472	0.469570
Mg9	-1.115484	0.059278	-0.045163
Mg10	0.807360	2.422132	0.043495
Mg11	0.009429	-2.602087	0.851976
Mg12	-2.938052	0.195058	-2.401546
Mg13	-2.314747	-1.343987	2.445669

@mg13-isomer148 bp86/6-31G(d) Etot=-2601.128067 Eb=-10.71

Mg1	-0.620670	0.949263	1.537259
Mg2	-3.731140	1.804767	1.465200
Mg3	2.294985	-0.351680	1.135309
Mg4	-0.516268	-2.324575	1.596962
Mg5	-0.017182	-0.842196	-1.087609
Mg6	-3.112383	-1.009160	0.555730
Mg7	1.231076	1.906517	-0.770764
Mg8	4.325105	1.881096	0.075680
Mg9	3.481566	-0.371868	-1.749146
Mg10	-1.900418	-3.273972	-1.095574
Mg11	-4.955145	0.730500	-1.142958
Mg12	-1.937650	1.749012	-1.102706
Mg13	5.458124	-0.847704	0.582615

@mg13-isomer149 bp86/6-31G(d) Etot=-2601.128045 Eb=-10.71

Mg1	2.844119	0.251752	-1.407256
Mg2	-1.700178	0.541143	1.065531
Mg3	-4.484173	-0.765954	0.260577
Mg4	1.293322	1.373094	1.002318
Mg5	-3.419574	1.432630	-1.575863
Mg6	5.836961	-0.569021	-0.715766
Mg7	-2.203493	-2.758580	1.212134
Mg8	0.402772	-1.490169	0.065997
Mg9	3.550110	-1.148863	1.259563
Mg10	4.600560	1.656262	0.872744
Mg11	-2.183718	-1.725285	-1.632963
Mg12	-4.244943	2.185238	1.277901
Mg13	-0.291765	1.017752	-1.684917

@mg13-isomer150 bp86/6-31G(d) Etot=-2601.127448 Eb=-10.68

Mg1	-1.725190	0.837276	1.133797
Mg2	-0.183359	1.901879	3.515724
Mg3	1.326845	-0.062882	1.818530
Mg4	0.638983	2.960643	0.796572
Mg5	-3.006422	-0.265851	-1.434047
Mg6	1.590514	3.799479	-1.999380
Mg7	2.730405	-1.881598	-0.102652
Mg8	-2.519462	-2.282777	1.085496
Mg9	-0.794614	1.831280	-1.840292
Mg10	-0.137844	-1.219641	-0.802855
Mg11	-5.077187	-2.411916	-0.764245
Mg12	2.198140	0.916854	-1.117409
Mg13	4.959192	-4.122746	-0.289239

@mg13-isomer151 bp86/6-31G(d) Etot=-2601.126993 Eb=-10.66

Mg1	1.104002	-0.202508	-1.761380
Mg2	-1.007970	-1.782341	0.587571
Mg3	-2.657822	0.620694	1.759327
Mg4	-2.001719	0.525720	-1.265508
Mg5	0.263691	1.397477	0.838739
Mg6	2.206735	-1.080252	1.169779
Mg7	5.494475	3.479377	-0.121346
Mg8	3.143710	1.369064	-0.275527
Mg9	1.206837	-3.399510	-0.814812
Mg10	-4.985013	1.456640	-0.124137

Mg11	-2.484559	3.363526	0.322805
Mg12	0.809740	-3.592984	2.225171
Mg13	-1.092107	-2.154902	-2.540682

@mg13-isomer152 bp86/6-31G(d) Etot=-2601.126070 Eb=-10.61

Mg1	-0.916144	-1.330692	0.884406
Mg2	-0.511360	1.995804	0.590675
Mg3	-2.896343	3.100024	-1.086068
Mg4	-0.667950	-2.320797	-2.108121
Mg5	-3.464472	-1.974543	-0.754314
Mg6	1.644424	0.125057	2.031569
Mg7	2.799414	2.442138	0.348457
Mg8	4.222445	-0.337601	0.457904
Mg9	7.204604	-1.079243	-0.466185
Mg10	1.294618	-0.161489	-1.011077
Mg11	-3.454933	0.831596	0.790405
Mg12	-3.572975	-1.829585	2.307013
Mg13	-1.681327	0.539331	-1.984663

@mg13-isomer153 bp86/6-31G(d) Etot=-2601.125025 Eb=-10.56

Mg1	-5.259968	-0.740910	-0.033218
Mg2	-0.267908	-0.000964	1.535741
Mg3	3.140628	-0.860770	1.267785
Mg4	3.271837	-2.918770	-1.228122
Mg5	-2.142486	-1.042373	-0.695096
Mg6	-0.848798	1.695803	-1.135024
Mg7	4.850694	1.784040	1.252152
Mg8	-3.275497	1.230463	0.981646
Mg9	4.438013	0.020641	-1.220788
Mg10	-3.906549	1.226305	-2.091059
Mg11	1.954235	1.901346	0.266784
Mg12	1.095459	-0.742248	-1.196085
Mg13	-3.049660	-1.552564	2.295282

@mg13-isomer154 bp86/6-31G(d) Etot=-2601.124618 Eb=-10.54

Mg1	-3.255131	0.290138	-1.834895
Mg2	0.029461	-1.369607	1.836140
Mg3	-4.661897	2.574263	-0.282488
Mg4	-4.893747	-0.355127	0.583639
Mg5	5.467729	-0.022903	-0.982100
Mg6	4.300140	1.809350	1.117068
Mg7	2.783713	-1.131336	0.289643
Mg8	0.610508	-3.404007	-0.321994
Mg9	1.109792	1.560498	1.230063
Mg10	-1.989112	1.137521	0.885717
Mg11	-2.331471	-2.184375	-0.018139
Mg12	2.835850	1.500696	-1.474928
Mg13	-0.005836	-0.405111	-1.027725

@mg13-isomer155 bp86/6-31G(d) Etot=-2601.124435 Eb=-10.53

Mg1	-0.485729	-1.079530	-0.974062
Mg2	-1.570652	1.649611	0.387806
Mg3	0.561211	-0.107176	1.791409
Mg4	3.740265	1.007681	1.408655
Mg5	1.335622	1.488188	-0.717314
Mg6	-3.999978	2.461085	-1.287728
Mg7	-2.476076	-3.387590	-0.878377
Mg8	4.561332	1.068106	-1.594439
Mg9	-2.331387	-1.542035	1.557508
Mg10	-3.758578	-0.582685	-1.073576
Mg11	2.840073	-1.251890	-0.431878
Mg12	-4.396801	1.052980	1.469286
Mg13	5.980697	-0.776745	0.342710

@mg13-isomer156 bp86/6-31G(d) Etot=-2601.124293 Eb=-10.53

Mg1	-1.145343	0.957743	-0.828213
Mg2	-4.004658	-0.030081	-0.836598
Mg3	-3.586184	3.177984	-0.917112
Mg4	0.222459	0.662720	2.136720
Mg5	0.992507	-1.462809	-0.275685
Mg6	1.868816	1.654211	-0.493605
Mg7	3.914740	-0.636429	-1.527527
Mg8	4.957219	2.024216	-0.365935
Mg9	-1.703767	-2.252110	-1.681556
Mg10	-2.823987	1.596552	1.630723
Mg11	-1.871059	-1.528725	1.204053
Mg12	3.444883	-0.067739	1.465854
Mg13	-0.265626	-4.095532	0.488882

@mg13-isomer157 bp86/6-31G(d) Etot=-2601.122623 Eb=-10.45

Mg1	3.825232	0.689422	-0.251156
Mg2	2.283401	-1.956240	-0.126157
Mg3	-0.589624	-2.102206	-1.588103
Mg4	1.179059	2.063164	0.397669
Mg5	-3.051522	-2.676669	0.389722
Mg6	-3.953811	0.152363	0.553575
Mg7	1.507501	0.314034	-2.111078
Mg8	-1.809750	2.249431	1.496780
Mg9	-3.950386	3.136508	-0.433335
Mg10	-0.681407	-0.643083	1.100452
Mg11	-1.461409	1.242339	-1.294914
Mg12	6.704047	1.186224	0.933707
Mg13	-0.001329	-3.655287	0.932836

@mg13-isomer158 bp86/6-31G(d) Etot=-2601.119357 Eb=-10.29

Mg1	0.066917	3.138533	-0.430680
Mg2	2.633490	1.608016	-0.129613
Mg3	4.617518	-0.668497	0.071918
Mg4	-2.749174	1.860676	-1.385217
Mg5	-0.046036	0.016333	-1.486561
Mg6	7.787087	-0.823583	-0.053300
Mg7	1.865006	-1.685607	0.270173
Mg8	-2.382942	2.730857	1.500080
Mg9	-3.588159	-0.081868	0.916679
Mg10	-3.018566	-1.273619	-1.765181
Mg11	0.002885	0.643721	1.513916
Mg12	-1.127088	-2.219055	0.536652
Mg13	-4.060939	-3.245906	0.441134

@mg13-isomer159 bp86/6-31G(d) Etot=-2601.118660 Eb=-10.26

Mg1	0.420395	-0.320991	1.518945
Mg2	-1.608458	2.377458	1.344009
Mg3	-2.794847	-0.836835	1.106655
Mg4	-1.069461	0.515332	-1.138652
Mg5	-3.680485	-1.390537	-1.850351
Mg6	1.359422	2.289877	0.098316
Mg7	4.277974	1.749797	-1.270463
Mg8	3.641337	0.219185	1.326901
Mg9	-4.184921	1.326111	-0.496641
Mg10	2.600680	-2.724965	1.059187
Mg11	4.903941	-1.552611	-0.796800
Mg12	1.979969	-0.479028	-1.167351
Mg13	-5.845545	-1.172794	0.266245

@mg13-isomer160 bp86/6-31G(d) Etot=-2601.118277 Eb=-10.24

Mg1	-2.120756	0.587692	0.776149
Mg2	-0.220847	-1.058948	-1.220404
Mg3	-0.236283	-2.097636	1.570796

Mg4	1.071818	0.735960	1.082615
Mg5	-2.883908	-2.410695	0.018627
Mg6	-3.651339	0.080000	-1.856446
Mg7	2.530706	3.358417	0.308069
Mg8	-5.229473	-0.266280	0.668838
Mg9	2.544124	-1.912717	0.239031
Mg10	-4.443206	2.572750	-0.183080
Mg11	2.937265	0.774654	-1.510822
Mg12	4.384997	0.934190	1.041204
Mg13	5.316902	-1.297389	-0.934577

@mg13-isomer161 bp86/6-31G(d) Etot=-2601.117815 Eb=-10.22

Mg1	1.247955	1.784034	1.273443
Mg2	2.529043	-1.244259	1.340265
Mg3	4.386047	1.246888	1.726224
Mg4	2.723412	0.657430	-1.099867
Mg5	-1.906680	1.366170	0.863894
Mg6	5.176317	-1.211972	-0.083548
Mg7	2.524552	-2.449198	-1.490098
Mg8	-3.079882	-1.460325	0.301856
Mg9	-2.618176	0.593416	-1.990585
Mg10	0.095281	2.284602	-1.518378
Mg11	-5.031335	0.930418	-0.062047
Mg12	-6.012299	-1.698990	1.361220
Mg13	-0.034236	-0.798215	-0.622379

@mg13-isomer162 bp86/6-31G(d) Etot=-2601.114070 Eb=-10.03

Mg1	-0.548543	1.372151	0.295342
Mg2	-3.449556	2.775672	-0.228213
Mg3	2.635299	1.502180	-1.148177
Mg4	4.968942	0.073042	0.232519
Mg5	0.317934	-0.761240	-1.794462
Mg6	-2.754244	-0.190580	-1.168494
Mg7	-4.287037	-2.323153	0.726766
Mg8	-1.103256	-1.726642	0.866436
Mg9	7.689990	0.457594	1.835348
Mg10	-3.394530	0.452996	1.799391
Mg11	3.594938	-1.216804	-2.067325
Mg12	2.002677	-0.795224	0.754015
Mg13	-5.672612	0.380008	-0.103146

@mg13-isomer163 bp86/6-31G(d) Etot=-2601.109823 Eb=-9.83

Mg1	-1.185901	0.543332	-1.453378
Mg2	-3.879159	2.218442	-1.393885
Mg3	1.173944	-1.639323	-0.413771
Mg4	3.596972	-0.000321	-0.000226
Mg5	6.672047	-0.000150	-0.000018
Mg6	9.983393	0.000214	0.000270
Mg7	-4.440231	0.856101	1.281450
Mg8	1.174258	1.639130	0.413412
Mg9	-1.794660	2.465461	0.854672
Mg10	-1.185850	-0.543261	1.453155
Mg11	-3.879064	-2.218366	1.394173
Mg12	-1.795042	-2.465327	-0.854886
Mg13	-4.440706	-0.855932	-1.280969

@mg13-isomer164 bp86/6-31G(d) Etot=-2601.108000 Eb=-9.74

Mg1	2.114945	-0.884676	1.126933
Mg2	0.483242	1.479274	-0.130702
Mg3	5.020322	-1.491294	-0.769087
Mg4	3.683349	1.378816	-0.209597
Mg5	1.793634	-0.684517	-1.854896
Mg6	-2.601103	1.441255	-0.089956
Mg7	-5.379175	1.011107	1.604630

Mg8	-0.793330	-1.345701	-0.173121
Mg9	-3.886129	-1.341362	0.010284
Mg10	-5.588968	1.002912	-1.354143
Mg11	5.361970	-0.326500	1.967783
Mg12	6.783953	0.971355	-0.368402
Mg13	-6.992710	-1.210670	0.240274

@mg13-isomer165 bp86/6-31G(d) Etot=-2601.083032 Eb=-8.54

Mg1	-1.426775	-0.363290	-0.007378
Mg2	0.495363	-2.796239	-0.471822
Mg3	-4.467717	0.012418	-0.075350
Mg4	0.576520	-1.178736	2.149829
Mg5	3.262435	2.496043	-0.203984
Mg6	-7.645372	0.521275	-0.129790
Mg7	-10.973630	0.922051	-0.142916
Mg8	1.449536	0.155631	-0.703806
Mg9	3.297779	0.431534	2.045713
Mg10	3.310532	-2.723329	0.849024
Mg11	3.071562	-2.570929	-2.200990
Mg12	4.486321	5.422820	-0.445590
Mg13	4.563445	-0.329248	-0.662938

@mg14-isomer01 bp86/6-31G(d) Etot=-2801.257306 Eb=-12.62

Mg1	-1.850545	1.576478	2.072646
Mg2	3.386055	-0.800910	-1.133842
Mg3	-2.914137	-0.556025	-1.926258
Mg4	1.663531	-2.970421	0.169218
Mg5	-3.360022	-0.897253	1.073350
Mg6	2.929120	-0.656987	1.890462
Mg7	1.032200	1.743720	1.082327
Mg8	-3.982117	1.820057	-0.102090
Mg9	3.979527	1.828988	0.224290
Mg10	-1.084616	1.898189	-1.048636
Mg11	1.850830	1.723737	-1.980222
Mg12	0.189076	-0.788881	-1.606136
Mg13	-0.198506	-0.960291	1.644930
Mg14	-1.640396	-2.960402	-0.360037

@mg14-isomer02 bp86/6-31G(d) Etot=-2801.257106 Eb=-12.61

Mg1	3.290426	2.523828	0.140180
Mg2	0.457469	-1.384144	1.898501
Mg3	-2.733108	-1.578180	-2.237270
Mg4	2.664205	-2.852339	0.098823
Mg5	0.218348	-1.226944	-1.189094
Mg6	3.713446	-0.261740	-1.276616
Mg7	0.260748	1.515339	0.791714
Mg8	-1.639662	1.216118	-1.684484
Mg9	3.285011	-0.158445	1.702322
Mg10	-2.644959	2.760725	0.814311
Mg11	-2.084886	0.243314	2.420580
Mg12	-3.957114	0.076975	0.028789
Mg13	1.314485	1.506971	-2.077805
Mg14	-2.144409	-2.381478	0.570048

@mg14-isomer03 bp86/6-31G(d) Etot=-2801.256413 Eb=-12.58

Mg1	-1.334441	-2.386780	0.843251
Mg2	0.896238	-0.648873	1.967560
Mg3	2.970744	2.463897	0.233305
Mg4	-1.951898	0.292086	2.513166
Mg5	0.307331	-0.992779	-1.257370
Mg6	2.505106	-2.716505	0.102886
Mg7	-2.526228	-2.101599	-1.922990
Mg8	1.019118	1.725759	-2.181366
Mg9	-3.836728	-0.539782	0.267804

Mg10	-2.032932	0.929705	-1.808297
Mg11	-3.204293	2.425055	0.676964
Mg12	-0.160745	1.927553	0.558451
Mg13	3.454195	-0.136244	-1.481876
Mg14	3.894534	-0.241494	1.488512

@mg14-isomer04 bp86/6-31G(d) Etot=-2801.256387 Eb=-12.58

Mg1	2.375080	-2.644681	-0.209682
Mg2	-3.760695	-0.698641	-0.409963
Mg3	2.842542	2.384152	-0.255347
Mg4	-1.869725	0.388953	-2.526856
Mg5	4.033556	-0.267958	-1.406265
Mg6	-1.034781	-2.290053	-0.976612
Mg7	-2.479671	-2.319999	1.721229
Mg8	3.402994	-0.140765	1.518684
Mg9	-3.348677	2.322949	-0.598916
Mg10	0.293527	-0.978819	1.352506
Mg11	-2.162902	0.759345	1.860072
Mg12	0.980792	1.721642	2.267198
Mg13	1.036877	-0.292566	-1.936003
Mg14	-0.308915	2.056440	-0.400045

@mg14-isomer05 bp86/6-31G(d) Etot=-2801.256272 Eb=-12.57

Mg1	1.511168	-0.637292	1.536134
Mg2	-1.508569	-0.626363	-1.538839
Mg3	-0.009437	4.205175	0.015005
Mg4	-4.177318	-0.247456	0.011994
Mg5	2.255941	2.090431	-0.003207
Mg6	-1.484247	-0.633365	1.526361
Mg7	-0.003172	-3.086007	0.000138
Mg8	4.183402	-0.241262	-0.019822
Mg9	-3.020368	-3.084760	-0.001854
Mg10	1.484059	-0.617476	-1.519857
Mg11	3.028547	-3.086511	-0.006748
Mg12	-0.014227	1.956006	-2.104850
Mg13	0.008644	1.935478	2.099071
Mg14	-2.254424	2.073401	0.006476

@mg14-isomer06 bp86/6-31G(d) Etot=-2801.255308 Eb=-12.53

Mg1	-1.152717	-0.546626	-1.223339
Mg2	1.152751	-0.546579	1.223370
Mg3	-3.133673	-2.825382	-0.281210
Mg4	1.647279	-1.367346	-1.952476
Mg5	0.000071	-3.237321	0.000000
Mg6	3.133789	-2.825253	0.281201
Mg7	-2.098724	2.393694	-1.392857
Mg8	-0.000092	4.256822	0.000001
Mg9	-3.726561	0.248176	0.187766
Mg10	1.010489	1.587582	-1.285110
Mg11	-1.010556	1.587537	1.285107
Mg12	2.098626	2.393787	1.392853
Mg13	-1.647220	-1.367420	1.952469
Mg14	3.726538	0.248330	-0.187773

@mg14-isomer07 bp86/6-31G(d) Etot=-2801.255114 Eb=-12.52

Mg1	-3.183785	0.406526	-1.728827
Mg2	-0.836667	-2.085197	1.392800
Mg3	3.763188	1.549586	0.878320
Mg4	1.616042	-3.089469	-0.572154
Mg5	2.446538	1.050205	-1.820437
Mg6	-2.686859	-2.517795	-1.021357
Mg7	-2.405207	2.430649	0.542954
Mg8	0.757509	2.254340	0.589702
Mg9	-3.469845	-0.357589	1.174007

Mg10	-0.590187	2.062081	-2.157533
Mg11	-0.998587	0.690271	2.611264
Mg12	1.797964	-0.588878	1.668280
Mg13	-0.187538	-0.580488	-1.068544
Mg14	3.977434	-1.224243	-0.488475

@mg14-isomer08 bp86/6-31G(d) Etot=-2801.254596 Eb=-12.50

Mg1	0.018935	-1.703563	1.869034
Mg2	-2.846646	2.698235	0.922872
Mg3	-3.883150	0.148884	-0.482708
Mg4	-2.646496	-0.140204	2.238674
Mg5	-0.115908	1.289413	1.254863
Mg6	2.818956	-0.234936	1.614773
Mg7	4.152623	2.241941	0.312796
Mg8	0.359722	-0.895987	-1.087887
Mg9	-1.352611	1.638404	-1.546505
Mg10	1.629150	1.906031	-1.281684
Mg11	3.811326	-0.410919	-1.250337
Mg12	2.531884	-2.991224	0.097221
Mg13	-2.280962	-2.433570	0.031636
Mg14	-2.196823	-1.112505	-2.692748

@mg14-isomer09 bp86/6-31G(d) Etot=-2801.254551 Eb=-12.50

Mg1	-3.483428	-0.994255	0.489235
Mg2	0.365656	-0.501204	-1.142520
Mg3	-0.658178	-1.275459	1.723929
Mg4	2.282071	-0.286110	1.609225
Mg5	-2.644110	0.950017	2.651559
Mg6	3.743363	-0.882708	-0.962917
Mg7	-2.540166	-0.330468	-2.276652
Mg8	-3.230805	1.980335	-0.189561
Mg9	1.840340	-3.144030	0.049573
Mg10	-0.779573	2.188130	-1.929360
Mg11	2.303190	1.901946	-1.088214
Mg12	-0.221160	1.731119	1.006189
Mg13	-1.506648	-2.892543	-0.773404
Mg14	4.529448	1.555230	0.832918

@mg14-isomer10 bp86/6-31G(d) Etot=-2801.254308 Eb=-12.49

Mg1	0.866136	1.462691	2.528947
Mg2	0.422629	-1.434458	-1.459815
Mg3	-4.176226	-0.899899	0.084443
Mg4	2.728399	-2.733996	0.161839
Mg5	-2.236526	0.373529	2.113268
Mg6	3.345116	-0.028915	1.554799
Mg7	2.577965	2.478825	-0.108398
Mg8	-3.541538	2.076294	-0.144903
Mg9	3.372802	-0.159019	-1.487153
Mg10	-0.465846	1.767861	-0.091036
Mg11	0.918982	1.240654	-2.648806
Mg12	-2.205902	0.053336	-2.097882
Mg13	0.345240	-1.269788	1.533165
Mg14	-1.951231	-2.927114	0.061532

@mg14-isomer11 bp86/6-31G(d) Etot=-2801.254243 Eb=-12.48

Mg1	-1.794201	1.137999	2.741262
Mg2	0.119002	-0.802123	-1.425332
Mg3	2.251300	1.413918	-1.886997
Mg4	-3.046573	-0.227400	-1.977666
Mg5	0.378504	1.735542	0.692010
Mg6	-3.495903	-0.677221	0.989003
Mg7	-0.459880	-1.323563	1.571922
Mg8	3.656986	1.935073	0.721779
Mg9	-2.035072	-2.837736	-0.674483

Mg10	2.435238	-0.540084	1.975717
Mg11	1.792904	-3.056745	-0.099900
Mg12	3.918267	-0.875044	-0.680905
Mg13	-2.906721	2.220891	0.158156
Mg14	-0.813852	1.896493	-2.104565

@mg14-isomer12 bp86/6-31G(d) Etot=-2801.253784 Eb=-12.46

Mg1	-1.239624	-2.304875	0.909523
Mg2	0.329666	-0.886865	-1.317673
Mg3	-2.898750	2.604611	0.917678
Mg4	3.262144	1.629020	1.606858
Mg5	-1.443366	0.411622	2.488157
Mg6	3.840611	-1.041648	0.100608
Mg7	1.816080	-3.360261	-0.178632
Mg8	-3.774245	-0.417107	0.651690
Mg9	3.206987	1.541702	-1.378339
Mg10	-2.739221	-2.078487	-1.692681
Mg11	0.438781	1.764043	-2.664922
Mg12	-2.259607	0.929329	-1.601573
Mg13	1.256474	-0.726275	1.769829
Mg14	0.204071	1.935191	0.389477

@mg14-isomer13 bp86/6-31G(d) Etot=-2801.253639 Eb=-12.46

Mg1	1.742918	-0.397585	2.432228
Mg2	2.520211	2.433104	1.561008
Mg3	-3.309569	-0.035976	-1.424515
Mg4	3.020371	-1.093399	-2.332176
Mg5	-0.677138	-1.881541	1.291972
Mg6	3.946824	-0.025938	0.385359
Mg7	-0.344840	1.218444	0.995954
Mg8	-3.269443	-2.838689	-0.110361
Mg9	1.953940	1.594358	-1.291585
Mg10	-3.401677	-0.181203	1.590107
Mg11	-0.986862	2.007193	-1.843592
Mg12	-3.303403	2.621511	0.189885
Mg13	2.094747	-2.562135	0.121826
Mg14	0.013921	-0.858144	-1.566110

@mg14-isomer14 bp86/6-31G(d) Etot=-2801.253480 Eb=-12.45

Mg1	0.852813	-1.179732	-1.738379
Mg2	-1.525049	0.402551	1.853901
Mg3	0.572544	2.264130	0.723186
Mg4	-3.775443	0.686263	-0.399917
Mg5	2.314767	1.529556	-1.835373
Mg6	-2.314168	-1.525112	-1.837564
Mg7	-0.571238	-2.267644	0.720957
Mg8	3.775622	-0.685186	-0.402774
Mg9	-3.566656	-1.881266	1.049807
Mg10	2.297937	-3.185299	0.343525
Mg11	1.525743	-0.408950	1.856481
Mg12	3.564892	1.878303	1.053915
Mg13	-0.855823	1.189403	-1.740454
Mg14	-2.295942	3.182983	0.352688

@mg14-isomer15 bp86/6-31G(d) Etot=-2801.252357 Eb=-12.40

Mg1	-1.666103	0.037144	1.815925
Mg2	3.089708	-1.620450	-1.550899
Mg3	-3.914727	1.505634	0.319923
Mg4	3.060956	1.546445	-1.648450
Mg5	-3.951766	-1.487507	0.429344
Mg6	2.661876	2.678787	1.165605
Mg7	4.108313	0.044615	0.787185
Mg8	-6.553267	0.019409	-0.211931
Mg9	2.708801	-2.583726	1.328208

Mg10	-2.208485	-0.085268	-1.612241
Mg11	1.360643	0.069372	2.263195
Mg12	0.289494	-1.568715	-0.122727
Mg13	0.263768	1.539826	-0.223962
Mg14	0.750789	-0.095568	-2.739174

@mg14-isomer16 bp86/6-31G(d) Etot=-2801.251831 Eb=-12.37

Mg1	3.077999	-1.559227	-0.780588
Mg2	-0.372100	0.003993	-0.063000
Mg3	0.158886	2.557107	-1.273958
Mg4	-2.911570	1.569496	-1.410834
Mg5	3.058336	1.557062	-0.807585
Mg6	-2.895604	-1.577284	-1.410965
Mg7	0.176124	-2.573290	-1.226486
Mg8	3.693244	0.023925	1.778683
Mg9	-4.052787	-0.007470	1.013970
Mg10	1.260658	-1.763760	1.807660
Mg11	-1.875930	-2.045280	1.662488
Mg12	1.251728	1.796827	1.783302
Mg13	1.320541	-0.024920	-2.742857
Mg14	-1.889524	2.042823	1.670170

@mg14-isomer17 bp86/6-31G(d) Etot=-2801.251769 Eb=-12.37

Mg1	-1.684443	-0.187008	-2.458529
Mg2	0.196882	-2.404717	-1.269496
Mg3	1.645352	0.660414	2.193127
Mg4	-2.818762	-2.137048	-0.337036
Mg5	0.783553	0.509764	-0.885110
Mg6	3.203096	-1.366682	-1.855533
Mg7	-1.404846	2.744883	-1.359410
Mg8	1.921583	3.186074	0.050237
Mg9	-3.679311	0.939705	-0.504200
Mg10	-1.159706	1.445491	1.380191
Mg11	-3.358215	-0.578339	2.165315
Mg12	-0.408571	-1.559694	1.604165
Mg13	3.937339	0.769362	0.221881
Mg14	2.826049	-2.022206	1.054397

@mg14-isomer18 bp86/6-31G(d) Etot=-2801.251277 Eb=-12.35

Mg1	-2.375454	0.768440	1.614625
Mg2	0.720897	-0.047494	-1.559310
Mg3	4.105869	0.301869	1.498122
Mg4	-0.163991	-2.619536	0.000426
Mg5	0.722133	-0.045762	1.558783
Mg6	-3.167267	-1.742721	0.000501
Mg7	-3.498691	3.141397	-0.000265
Mg8	2.712284	2.555322	0.000286
Mg9	-1.598272	-1.865753	-2.627316
Mg10	-0.338202	2.453083	-0.001302
Mg11	-2.377716	0.766975	-1.613833
Mg12	4.105296	0.302915	-1.498699
Mg13	-1.598162	-1.864805	2.628331
Mg14	2.751277	-2.103930	-0.000348

@mg14-isomer19 bp86/6-31G(d) Etot=-2801.250876 Eb=-12.33

Mg1	0.841640	-0.383329	-1.326559
Mg2	1.090057	0.295523	1.720485
Mg3	-3.207967	-2.353979	0.831049
Mg4	2.906797	-2.334489	0.414499
Mg5	-1.780621	-1.933730	-1.827059
Mg6	3.986245	0.020489	-1.510419
Mg7	2.545770	2.528249	-0.236460
Mg8	-3.355334	0.387392	-0.634994
Mg9	4.215636	0.375443	1.403921

Mg10	-0.595887	2.114130	-0.143935
Mg11	-3.221461	2.733973	1.256757
Mg12	-1.870450	0.078333	2.072941
Mg13	-1.386905	0.862364	-2.890339
Mg14	-0.167519	-2.390369	0.870114

@mg14-isomer20 bp86/6-31G(d) Etot=-2801.250674 Eb=-12.32

Mg1	-1.052320	-2.467506	0.562392
Mg2	1.950612	1.446504	-0.962093
Mg3	-2.491502	0.230757	1.709512
Mg4	3.877250	-0.234540	1.061135
Mg5	-4.122824	-2.262311	0.791419
Mg6	2.155600	-2.681871	0.323154
Mg7	0.361985	-1.069741	-1.794308
Mg8	-3.258285	2.326801	-0.425793
Mg9	3.573988	-1.062674	-1.859342
Mg10	-2.773657	-0.501932	-1.323235
Mg11	-0.891104	1.698059	-2.324064
Mg12	-0.415857	2.496345	0.697814
Mg13	0.653343	-0.213800	1.677015
Mg14	2.432771	2.295909	1.866394

@mg14-isomer21 bp86/6-31G(d) Etot=-2801.250613 Eb=-12.32

Mg1	1.221981	0.854023	-1.883352
Mg2	0.833757	0.202624	1.007160
Mg3	-4.035524	0.582355	-0.541253
Mg4	1.306705	3.753023	0.089503
Mg5	-1.375348	2.196873	-0.528484
Mg6	3.606736	1.872668	-0.154935
Mg7	2.255840	-3.849841	0.547488
Mg8	-2.707529	-2.216074	-0.294436
Mg9	3.378396	-1.160081	-0.316260
Mg10	0.336766	-2.047298	-1.111216
Mg11	-0.455344	-2.722083	1.679665
Mg12	-2.057949	-0.028913	1.739306
Mg13	-1.677716	-0.106440	-2.483447
Mg14	-0.630771	2.669163	2.250262

@mg14-isomer22 bp86/6-31G(d) Etot=-2801.250541 Eb=-12.32

Mg1	2.150244	-0.586787	1.948709
Mg2	-2.994679	1.926107	-0.994270
Mg3	1.813564	-0.099373	-1.534645
Mg4	-2.505265	-3.255614	-1.272451
Mg5	4.377185	0.307923	0.171188
Mg6	-0.039962	-2.096725	0.197585
Mg7	-0.945594	-0.602920	2.756735
Mg8	2.597018	2.766332	-0.128007
Mg9	-3.145421	-0.835533	0.345424
Mg10	-0.125727	1.356720	0.784057
Mg11	-3.042305	1.672344	2.045230
Mg12	-0.033265	2.377264	-1.945704
Mg13	3.214353	-2.489901	-0.257110
Mg14	-1.320146	-0.439836	-2.116742

@mg14-isomer23 bp86/6-31G(d) Etot=-2801.250126 Eb=-12.30

Mg1	-1.896184	0.016373	-2.825107
Mg2	0.642069	-0.032094	1.554024
Mg3	-1.802200	2.025908	1.813604
Mg4	3.425686	1.526089	0.333609
Mg5	-1.677274	2.566189	-1.269559
Mg6	4.198129	-0.814426	-1.523025
Mg7	1.912028	-2.408703	-0.322741
Mg8	-3.913444	-2.701383	0.175290
Mg9	4.097533	-1.240908	1.460378

Mg10	-3.423411	0.388780	-0.186794
Mg11	-1.018445	-1.766346	-0.468602
Mg12	-2.197362	-0.927360	2.257203
Mg13	0.815168	0.463582	-1.506171
Mg14	0.837708	2.904300	0.507892

@mg14-isomer24 bp86/6-31G(d) Etot=-2801.249375 Eb=-12.26

Mg1	-3.784615	0.376645	0.063921
Mg2	0.086750	-1.066898	-1.045694
Mg3	4.047032	-0.344947	-0.761735
Mg4	1.996903	-0.203292	1.600282
Mg5	1.775246	1.266095	-2.017324
Mg6	-2.549434	2.828848	1.157965
Mg7	-2.759420	-2.380036	0.459285
Mg8	-1.318735	1.477734	-1.698769
Mg9	-1.341710	0.106274	1.968973
Mg10	-2.716560	-1.152366	-2.368685
Mg11	0.061994	-2.547835	1.555205
Mg12	2.666367	-2.938482	-0.064579
Mg13	0.372381	2.324990	0.622417
Mg14	3.463802	2.253271	0.528738

@mg14-isomer25 bp86/6-31G(d) Etot=-2801.247950 Eb=-12.20

Mg1	-1.273752	1.200021	2.089299
Mg2	1.514352	-1.693230	-1.656266
Mg3	3.366979	-1.298678	0.681334
Mg4	-3.342446	1.801994	-0.169254
Mg5	1.627861	1.249507	1.208653
Mg6	-0.633459	3.405614	0.021900
Mg7	-3.151934	-1.053930	0.902777
Mg8	0.061144	-1.506824	1.874754
Mg9	-3.224251	-0.705165	-2.006257
Mg10	-0.515321	0.380002	-0.810018
Mg11	-1.204324	-2.742827	-0.688536
Mg12	1.512498	-3.884670	0.449884
Mg13	2.319698	3.837298	-0.445481
Mg14	2.942956	1.010887	-1.452791

@mg14-isomer26 bp86/6-31G(d) Etot=-2801.247926 Eb=-12.20

Mg1	-1.411228	1.585684	-0.667277
Mg2	3.628730	0.126125	0.272047
Mg3	-2.710033	-1.329619	0.628833
Mg4	1.060620	2.446967	0.978739
Mg5	-3.792948	0.103727	-1.936649
Mg6	-1.572793	1.256428	2.441683
Mg7	3.565035	3.064781	-0.639412
Mg8	-0.443715	-3.343506	0.344191
Mg9	1.429938	0.966497	-1.840667
Mg10	2.120998	-2.052362	-1.283183
Mg11	-0.852147	-1.199839	-1.937160
Mg12	2.727956	-2.451379	1.653948
Mg13	-4.160483	1.348128	0.866153
Mg14	0.410070	-0.521633	1.118753

@mg14-isomer27 bp86/6-31G(d) Etot=-2801.247769 Eb=-12.19

Mg1	1.845603	1.617734	-3.153954
Mg2	-4.086543	-2.169343	0.699324
Mg3	2.846064	0.912428	2.574939
Mg4	0.587040	-0.768358	1.303506
Mg5	2.652985	1.584348	-0.299925
Mg6	1.563539	-1.105110	-1.815983
Mg7	-2.680695	2.989118	0.238901
Mg8	0.112563	2.235945	1.561291
Mg9	-1.380712	-2.016255	-0.824102

Mg10	-0.523247	1.060280	-1.221902
Mg11	-3.668700	0.162300	-1.230193
Mg12	-2.427874	0.203618	1.541729
Mg13	3.643741	-1.275457	0.558325
Mg14	1.516236	-3.431248	0.068043

@mg14-isomer28 bp86/6-31G(d) Etot=-2801.247394 Eb=-12.18

Mg1	-0.558776	1.864193	-1.555112
Mg2	-1.018235	-1.036004	-0.812329
Mg3	-3.512226	-2.483686	0.119873
Mg4	1.855402	-2.113692	-0.253324
Mg5	-3.518884	0.721185	-0.190689
Mg6	2.487607	1.323062	-0.905965
Mg7	0.930035	3.413105	0.696852
Mg8	-2.275247	3.707485	0.203631
Mg9	4.465449	-0.716621	0.310459
Mg10	-0.958555	1.087802	1.458527
Mg11	2.002296	0.516220	1.850884
Mg12	-0.106724	-1.783489	1.994296
Mg13	0.984279	-0.444063	-2.926968
Mg14	-0.776420	-4.055495	0.009865

@mg14-isomer29 bp86/6-31G(d) Etot=-2801.247150 Eb=-12.16

Mg1	0.687074	1.801952	1.361934
Mg2	-0.509758	-0.565518	-1.678290
Mg3	2.293812	-0.881289	1.282707
Mg4	-2.940742	-1.690336	0.454698
Mg5	3.865592	1.679248	1.264165
Mg6	-5.455200	0.061925	0.380339
Mg7	-2.407091	1.244451	1.004455
Mg8	4.836710	-0.413085	-0.590030
Mg9	-3.440057	0.665167	-1.815524
Mg10	2.099729	1.122544	-1.288757
Mg11	-0.727899	2.355670	-1.369602
Mg12	2.294866	-1.907058	-1.715585
Mg13	-0.628589	-0.751700	2.456382
Mg14	0.031551	-2.721972	0.253109

@mg14-isomer30 bp86/6-31G(d) Etot=-2801.247096 Eb=-12.16

Mg1	0.000338	-1.850218	-1.781024
Mg2	-0.002303	0.164853	0.819713
Mg3	0.001306	1.219541	-2.233418
Mg4	1.494318	2.901450	0.139634
Mg5	-0.000972	-4.709110	-0.302529
Mg6	4.378305	2.165723	-0.014010
Mg7	-2.607060	-0.184410	-1.054404
Mg8	1.738787	-2.494423	0.804124
Mg9	2.921931	0.195938	1.876721
Mg10	-1.744528	-2.495981	0.799510
Mg11	-2.925256	0.194724	1.875645
Mg12	-4.372338	2.173929	-0.013001
Mg13	2.605611	-0.189037	-1.053522
Mg14	-1.488138	2.907020	0.136560

@mg14-isomer31 bp86/6-31G(d) Etot=-2801.246231 Eb=-12.12

Mg1	1.262401	-2.995285	-0.263851
Mg2	-1.614540	0.464392	1.230470
Mg3	2.317099	1.545153	-1.290213
Mg4	-3.723228	2.427320	-0.144706
Mg5	2.827937	-1.325564	-2.256100
Mg6	-3.080760	-0.112660	-1.657723
Mg7	-1.933788	-2.523379	0.219464
Mg8	4.155628	2.059521	1.164650
Mg9	-4.372018	-0.735927	1.006776

Mg10	3.153374	-0.808973	0.735899
Mg11	0.516201	-1.463945	2.253153
Mg12	1.187525	1.484815	1.560788
Mg13	0.005334	-0.468652	-1.558910
Mg14	-0.701164	2.453184	-0.999697

@mg14-isomer32 bp86/6-31G(d) Etot=-2801.245807 Eb=-12.10

Mg1	1.262195	2.012918	-0.454440
Mg2	-0.012206	-2.362792	1.845050
Mg3	-3.642381	0.128280	-1.340477
Mg4	2.445508	-2.569162	-0.069154
Mg5	-0.703212	0.789644	-2.235523
Mg6	3.790946	0.133849	-0.466320
Mg7	3.566322	2.620792	1.346624
Mg8	-2.268960	2.804472	-0.335421
Mg9	2.063764	-0.040525	1.976935
Mg10	-0.837986	0.414224	1.082770
Mg11	-3.984748	0.954396	1.463768
Mg12	-2.997032	-1.983232	0.848859
Mg13	1.891103	-0.863958	-2.589148
Mg14	-0.573314	-2.038905	-1.073523

@mg14-isomer33 bp86/6-31G(d) Etot=-2801.245608 Eb=-12.10

Mg1	-1.837187	-2.656374	-0.620603
Mg2	-1.441936	0.107568	-1.456524
Mg3	-3.542106	1.912344	0.319129
Mg4	3.159930	-1.553734	1.191942
Mg5	1.069115	-1.729187	-1.151382
Mg6	3.778535	-0.186777	-1.531468
Mg7	1.210376	1.212426	-2.377915
Mg8	-3.144166	-0.825188	1.513669
Mg9	5.218927	0.760012	0.877329
Mg10	-4.530271	-0.598757	-1.121886
Mg11	1.708654	1.002293	0.760540
Mg12	-0.585829	2.727638	-0.348226
Mg13	-0.022749	-1.494598	1.690913
Mg14	-1.041292	1.322334	2.254482

@mg14-isomer34 bp86/6-31G(d) Etot=-2801.245413 Eb=-12.09

Mg1	-1.511951	-2.305570	-1.557774
Mg2	1.030595	1.451694	-0.000591
Mg3	-1.510566	-2.302756	1.559412
Mg4	1.102290	-0.708678	-2.209982
Mg5	-3.740851	-1.013133	0.001329
Mg6	-1.523358	0.696272	-1.616063
Mg7	3.730740	1.454446	-1.588004
Mg8	1.092652	-3.072466	0.000458
Mg9	3.729289	1.453015	1.589189
Mg10	-1.522056	0.698582	1.616283
Mg11	3.305609	-1.063837	-0.001255
Mg12	1.104204	-0.706993	2.208860
Mg13	-3.968169	2.034413	-0.000082
Mg14	-1.318428	3.385011	-0.001779

@mg14-isomer35 bp86/6-31G(d) Etot=-2801.244633 Eb=-12.05

Mg1	1.544274	0.886548	2.025326
Mg2	-1.832480	0.775043	-1.055099
Mg3	2.607521	-1.775201	0.135519
Mg4	0.353794	2.027849	-2.764336
Mg5	4.606713	0.295653	1.147351
Mg6	-1.585057	1.250207	1.918929
Mg7	-2.394358	-3.856219	0.217064
Mg8	0.491755	-3.919766	-0.612160
Mg9	-3.000025	3.374679	0.177630

Mg10	-0.398329	-1.335127	0.881373
Mg11	-3.554621	-1.053402	0.554486
Mg12	0.518389	-1.024044	-2.034955
Mg13	0.174582	3.091258	0.214082
Mg14	2.467843	1.262520	-0.805210

@mg14-isomer36 bp86/6-31G(d) Etot=-2801.243911 Eb=-12.02

Mg1	-0.686811	-0.821528	-3.273016
Mg2	0.770208	-0.012232	1.463152
Mg3	3.476010	-0.338020	-0.123175
Mg4	-4.372550	1.264234	0.837777
Mg5	0.803096	1.321532	-1.204326
Mg6	-1.300805	2.330487	0.954054
Mg7	-2.325648	0.676305	-1.268988
Mg8	1.004471	-1.899606	-1.025057
Mg9	-2.217644	-0.709889	1.645525
Mg10	-0.273053	-3.010635	1.530041
Mg11	-2.081934	-2.442683	-0.878227
Mg12	2.784270	-3.274896	0.994080
Mg13	0.940475	4.266597	0.290473
Mg14	3.479914	2.650333	0.057686

@mg14-isomer37 bp86/6-31G(d) Etot=-2801.243800 Eb=-12.01

Mg1	-2.508236	-0.690719	-3.265032
Mg2	1.401796	-0.382504	1.187118
Mg3	2.050925	-3.243891	0.026790
Mg4	3.775044	1.689391	1.191120
Mg5	0.107772	-1.248078	-1.630118
Mg6	-0.733400	1.607928	-1.876466
Mg7	-2.348315	2.931373	0.399590
Mg8	-2.973631	-0.095166	-0.402762
Mg9	0.713560	2.622654	0.679962
Mg10	-1.410410	0.615443	2.136973
Mg11	-3.740334	-1.525890	2.175594
Mg12	-0.968694	-2.281473	1.000869
Mg13	2.439032	1.099729	-1.470458
Mg14	4.194890	-1.098798	-0.153180

@mg14-isomer38 bp86/6-31G(d) Etot=-2801.243698 Eb=-12.01

Mg1	-1.192288	-2.687323	-2.083178
Mg2	-0.041430	-0.202069	-0.872490
Mg3	1.279583	2.405564	-1.673007
Mg4	-4.366502	1.789399	0.630821
Mg5	3.055981	-0.396769	-1.597701
Mg6	-2.059875	0.434209	1.899652
Mg7	1.626356	-2.714926	-0.105878
Mg8	3.718207	2.125068	0.083248
Mg9	-1.654068	-2.578501	0.831444
Mg10	3.522223	-0.724522	1.350255
Mg11	0.638873	-0.950406	2.365945
Mg12	0.671094	1.898491	1.237935
Mg13	-3.286851	-0.599997	-0.988618
Mg14	-1.911304	2.201782	-1.078428

@mg14-isomer39 bp86/6-31G(d) Etot=-2801.242392 Eb=-11.95

Mg1	1.120698	-1.315364	1.583884
Mg2	0.974646	1.755645	-1.835850
Mg3	-4.184419	1.339364	0.057702
Mg4	1.369392	2.030350	1.064245
Mg5	0.012047	0.856425	3.551949
Mg6	3.088050	-0.539910	-0.614923
Mg7	2.137630	-3.549668	-0.211326
Mg8	-2.944227	-1.905463	-0.333212
Mg9	3.834117	2.406476	-0.686343

Mg10	-0.841551	-4.130293	-0.059891
Mg11	0.129254	-1.337154	-1.298463
Mg12	-2.007699	0.795181	-1.938678
Mg13	-1.384671	0.331022	0.966305
Mg14	-1.303267	3.263390	-0.245399

@mg14-isomer40 bp86/6-31G(d) Etot=-2801.241813 Eb=-11.93

Mg1	0.556117	-0.202524	1.746818
Mg2	-0.860767	1.048854	-1.083060
Mg3	4.445136	1.304286	-0.861324
Mg4	-3.856795	1.564316	-0.012988
Mg5	1.676160	2.147287	0.254425
Mg6	-5.686572	-0.820818	0.177024
Mg7	-2.446545	-0.837371	1.128340
Mg8	3.624068	-0.046107	1.763457
Mg9	-3.169367	-0.901036	-1.790653
Mg10	1.842194	-2.789219	1.412177
Mg11	0.118004	-1.788672	-1.081456
Mg12	3.261669	-1.472169	-0.909147
Mg13	-1.206230	2.185737	1.750577
Mg14	1.702930	0.607436	-2.494189

@mg14-isomer41 bp86/6-31G(d) Etot=-2801.237177 Eb=-11.72

Mg1	-2.981505	-1.435868	-0.032916
Mg2	0.526249	2.643149	0.568120
Mg3	4.280866	0.118693	-1.165430
Mg4	-3.757673	1.364294	1.424637
Mg5	1.168474	0.612043	-1.748708
Mg6	-4.816448	0.873244	-1.430788
Mg7	-0.138550	-2.579563	0.584822
Mg8	2.291748	-2.189127	-1.355083
Mg9	-0.857603	0.201392	1.833306
Mg10	-0.810011	-1.822854	-2.180305
Mg11	1.119913	-1.783709	3.268657
Mg12	2.191258	-0.070683	1.112170
Mg13	-1.747438	1.216528	-0.965107
Mg14	3.530720	2.852461	0.086625

@mg14-isomer42 bp86/6-31G(d) Etot=-2801.234891 Eb=-11.62

Mg1	-0.390714	1.506228	-2.294507
Mg2	-0.250361	-0.016832	2.609864
Mg3	-0.318256	-4.146695	-0.377636
Mg4	4.326280	0.002193	0.050641
Mg5	-0.386050	-1.483020	-2.311780
Mg6	1.280783	1.507203	0.345720
Mg7	-0.318398	4.150140	-0.338452
Mg8	-3.113800	0.009310	-2.021746
Mg9	2.918481	-0.013438	2.748748
Mg10	-2.001210	-1.521153	0.423374
Mg11	-2.007378	1.518770	0.441932
Mg12	-3.446443	-0.016959	2.727579
Mg13	2.415560	0.017520	-2.331014
Mg14	1.291507	-1.513267	0.327276

@mg14-isomer43 bp86/6-31G(d) Etot=-2801.230817 Eb=-11.43

Mg1	-0.095627	2.093321	2.140604
Mg2	-2.438653	2.811024	-0.038115
Mg3	0.212225	1.078856	-0.690211
Mg4	3.002378	1.557740	-2.038357
Mg5	-0.615881	-2.146078	-0.690700
Mg6	-4.939601	0.723724	-0.116140
Mg7	2.528001	-1.195657	-0.765953
Mg8	0.831394	-0.928309	1.927895
Mg9	5.440908	0.419809	-0.464520

Mg10	1.788741	-3.666757	0.778589
Mg11	2.807082	1.425758	1.060946
Mg12	-2.097543	-0.084276	1.173029
Mg13	-3.884359	-2.221259	-0.407327
Mg14	-2.539065	0.132105	-1.869740

@mg14-isomer44 bp86/6-31G(d) Etot=-2801.228306 Eb=-11.32

Mg1	-2.269506	1.491833	1.167752
Mg2	-0.786531	1.609945	-1.487682
Mg3	-2.723215	-0.950490	-1.226355
Mg4	2.403909	-2.552628	-0.628080
Mg5	1.032686	2.331567	0.968286
Mg6	3.240252	-0.396934	1.539145
Mg7	4.218722	2.230247	0.455698
Mg8	-5.037857	0.087659	0.667447
Mg9	5.066581	-0.559566	-0.783936
Mg10	-3.908332	1.921478	-1.424141
Mg11	2.116384	0.478006	-1.239417
Mg12	-0.814767	-3.201864	-0.537056
Mg13	0.060382	-0.614233	0.851796
Mg14	-2.598710	-1.875021	1.676542

@mg15-isomer01 bp86/6-31G(d) Etot=-3001.368988 Eb=-13.53

Mg1	0.001496	1.916409	0.464728
Mg2	3.272404	1.771370	0.433003
Mg3	1.676895	-2.840460	-0.691831
Mg4	1.677456	2.018385	-2.112981
Mg5	-0.000227	-0.554307	-1.891594
Mg6	-3.272057	1.772854	0.433365
Mg7	-3.272236	-0.511028	-1.750163
Mg8	-3.272910	-1.259273	1.320149
Mg9	-1.679414	-2.839372	-0.691529
Mg10	0.000428	-1.361763	1.422375
Mg11	-1.673440	0.820491	2.802998
Mg12	-1.676789	2.018872	-2.111499
Mg13	3.271830	-0.511586	-1.749498
Mg14	1.674383	0.819352	2.803261
Mg15	3.272182	-1.259942	1.319217

@mg15-isomer02 bp86/6-31G(d) Etot=-3001.365066 Eb=-13.37

Mg1	4.006003	-0.001632	-0.513672
Mg2	2.982147	2.627484	0.676502
Mg3	-3.071190	-1.600948	1.406854
Mg4	-2.229374	-2.656034	-1.327721
Mg5	-3.719790	-0.002754	-1.185002
Mg6	-3.073472	1.603047	1.403208
Mg7	2.980224	-2.625665	0.684808
Mg8	0.019305	1.729396	0.586282
Mg9	1.863467	-1.652799	-1.964221
Mg10	-0.740708	-0.001988	-2.010664
Mg11	2.211857	0.002968	2.092184
Mg12	-2.231166	2.652417	-1.333378
Mg13	-0.880328	0.004919	2.863528
Mg14	1.864068	1.645940	-1.967923
Mg15	0.018955	-1.724351	0.589215

@mg15-isomer03 bp86/6-31G(d) Etot=-3001.364408 Eb=-13.34

Mg1	-0.000316	1.700329	-0.063323
Mg2	-2.587918	1.611071	1.792615
Mg3	-0.000120	-1.706046	-0.055179
Mg4	-4.039258	0.000710	-0.413702
Mg5	0.001102	0.004535	2.489726
Mg6	-2.744041	2.674319	-1.075554
Mg7	4.037193	0.000396	-0.415391

Mg8	-1.521985	-0.006913	-2.220176
Mg9	2.589193	1.610234	1.792456
Mg10	-2.747249	-2.679265	-1.063493
Mg11	1.520562	-0.004543	-2.219429
Mg12	2.745719	-2.679068	-1.066881
Mg13	2.589162	-1.602345	1.795894
Mg14	2.744109	2.676199	-1.074655
Mg15	-2.586152	-1.599614	1.797092

@mg15-isomer04 bp86/6-31G(d) Etot=-3001.363328 Eb=-13.30

Mg1	-3.232039	2.577092	0.402159
Mg2	-1.082979	-1.632015	-1.611768
Mg3	2.019827	2.494668	-0.957182
Mg4	-0.382656	2.515819	1.543315
Mg5	0.586074	-0.000042	0.421530
Mg6	-2.398060	-0.000685	1.704569
Mg7	-1.085768	1.630737	-1.608950
Mg8	-3.227004	-2.578757	0.401326
Mg9	-3.661425	-0.001833	-1.213647
Mg10	2.025530	-2.493174	-0.958085
Mg11	1.485342	0.000216	-2.619886
Mg12	3.800093	0.002968	-0.696190
Mg13	2.766617	-1.571822	1.823864
Mg14	2.767034	1.574015	1.822690
Mg15	-0.380588	-2.517186	1.546256

@mg15-isomer05 bp86/6-31G(d) Etot=-3001.358222 Eb=-13.08

Mg1	-1.385473	-0.000063	2.600059
Mg2	1.875157	0.000085	-2.470975
Mg3	-0.539258	0.000086	-0.521388
Mg4	3.358464	1.798005	-0.572453
Mg5	0.538310	2.618604	-1.376123
Mg6	-2.845406	1.591522	-1.752218
Mg7	-2.845378	-1.591396	-1.752276
Mg8	0.538090	-2.618438	-1.376329
Mg9	3.358338	-1.798101	-0.572602
Mg10	-3.814364	0.000015	0.792911
Mg11	-2.046288	-2.523721	0.979921
Mg12	1.108452	-1.652127	1.580120
Mg13	3.637018	-0.000160	1.881095
Mg14	1.108547	1.651997	1.580245
Mg15	-2.046208	2.523692	0.980012

@mg15-isomer06 bp86/6-31G(d) Etot=-3001.356777 Eb=-13.02

Mg1	0.014158	0.073565	-0.321273
Mg2	4.029666	1.664870	-0.021819
Mg3	1.650655	-2.874379	0.142112
Mg4	1.572900	1.882284	1.668810
Mg5	-0.001912	-0.997911	2.424254
Mg6	-4.005864	1.715900	-0.012428
Mg7	-3.118493	-0.732733	1.601566
Mg8	-2.897704	-0.711651	-1.578567
Mg9	-1.694021	-2.867679	0.158865
Mg10	-0.034093	-2.000733	-2.346488
Mg11	-1.622380	2.222807	-1.689721
Mg12	-1.530348	1.891730	1.657808
Mg13	3.113759	-0.771669	1.588121
Mg14	1.646700	2.239355	-1.673734
Mg15	2.876976	-0.733756	-1.597507

@mg15-isomer07 bp86/6-31G(d) Etot=-3001.356654 Eb=-13.02

Mg1	2.792306	-2.499600	-1.236208
Mg2	2.398189	-1.439147	1.563390
Mg3	-0.833648	1.410770	-1.582659

Mg4	-2.890601	-2.906444	0.432288
Mg5	1.944636	2.605652	-0.667120
Mg6	-0.118086	-1.616431	-0.817118
Mg7	1.711212	0.098630	-2.506488
Mg8	-2.988502	-0.966301	-1.857070
Mg9	0.274031	0.817355	1.319692
Mg10	-2.011024	2.832487	1.207808
Mg11	-2.994220	-0.036555	1.469033
Mg12	-0.568397	-1.962971	2.193713
Mg13	3.118639	1.608781	1.959275
Mg14	-3.845756	1.796761	-0.904433
Mg15	4.011220	0.257013	-0.574102

@mg15-isomer08 bp86/6-31G(d) Etot=-3001.352278 Eb=-12.84

Mg1	-3.803760	1.827728	-1.945378
Mg2	-1.569510	-0.190191	-2.132562
Mg3	1.072567	1.303631	-1.496779
Mg4	1.013957	-1.967487	-1.870320
Mg5	-3.555299	-0.189682	0.287338
Mg6	-1.901202	-2.753505	-0.614504
Mg7	-1.552478	2.263261	-0.062671
Mg8	3.667010	-0.526222	-1.450511
Mg9	2.719909	-2.725160	0.507227
Mg10	1.094547	2.158494	1.666474
Mg11	3.488614	2.490748	-0.217754
Mg12	-2.330805	-2.023611	2.260690
Mg13	0.126484	-0.737980	0.872855
Mg14	-1.802852	0.982258	2.616856
Mg15	3.332818	0.087717	1.579040

@mg15-isomer09 bp86/6-31G(d) Etot=-3001.352016 Eb=-12.82

Mg1	1.516498	-2.144980	-0.598571
Mg2	0.681081	3.366862	0.029265
Mg3	2.974953	-0.698820	1.794762
Mg4	-3.184031	1.258540	1.066295
Mg5	4.237540	-0.479594	-0.962245
Mg6	1.516264	0.776771	-1.629379
Mg7	-2.516849	-1.550515	1.760094
Mg8	-1.428797	1.384174	-1.406126
Mg9	-0.662002	-1.352735	-2.619370
Mg10	-1.322971	-3.398372	-0.443152
Mg11	3.375220	2.033599	0.587473
Mg12	-2.228797	4.073118	0.332383
Mg13	0.391421	-2.434946	2.133118
Mg14	-3.273022	-1.153737	-1.098642
Mg15	-0.076508	0.320636	1.054094

@mg15-isomer10 bp86/6-31G(d) Etot=-3001.351534 Eb=-12.80

Mg1	0.001065	1.148653	0.906823
Mg2	-1.516324	1.502624	-1.791744
Mg3	-1.807524	-3.030522	0.402516
Mg4	-3.077102	-1.278371	-1.669924
Mg5	-4.291830	1.351025	-0.667123
Mg6	0.000263	-1.169058	-1.484895
Mg7	3.077940	-1.280016	-1.669944
Mg8	-2.585285	2.633201	1.376491
Mg9	2.586113	2.634139	1.377503
Mg10	-2.834841	-0.423724	1.491627
Mg11	1.806840	-3.029889	0.402788
Mg12	2.833969	-0.423002	1.493652
Mg13	-0.001039	-1.487222	2.292927
Mg14	4.290495	1.349616	-0.667693
Mg15	1.517260	1.502546	-1.793005

@mg15-isomer11 bp86/6-31G(d) Etot=-3001.350995 Eb=-12.78

Mg1	0.130580	4.251728	0.386723
Mg2	2.357033	2.334154	-0.579530
Mg3	-1.940218	-0.940978	-2.412013
Mg4	0.942398	-1.953626	2.357496
Mg5	-0.394677	-2.488055	-0.215628
Mg6	-3.748230	0.492520	-0.377141
Mg7	-3.474646	-2.553913	-0.313683
Mg8	0.339814	0.641184	1.051633
Mg9	-2.204213	2.335428	1.445066
Mg10	-1.028168	1.905481	-1.315773
Mg11	1.007834	-0.289198	-1.945297
Mg12	3.419418	-0.091420	1.480776
Mg13	-2.136383	-0.759713	1.897928
Mg14	3.968248	-0.181476	-1.420771
Mg15	2.761209	-2.702113	-0.039785

@mg15-isomer12 bp86/6-31G(d) Etot=-3001.349753 Eb=-12.73

Mg1	-3.965233	-2.159670	0.164172
Mg2	-1.827369	-2.077320	-2.026187
Mg3	-1.038986	-2.212687	1.059319
Mg4	1.044597	-2.220952	-1.061926
Mg5	-2.882627	0.237206	1.892215
Mg6	-3.357912	0.460779	-1.121376
Mg7	3.967199	-2.155995	-0.158530
Mg8	1.829171	-2.069569	2.028953
Mg9	0.189867	0.517878	1.569340
Mg10	-0.003624	5.148858	-0.003279
Mg11	-0.189049	0.509188	-1.564546
Mg12	2.881042	0.237354	-1.892136
Mg13	-1.734008	2.657340	0.325651
Mg14	3.357050	0.468038	1.120665
Mg15	1.729881	2.659553	-0.332334

@mg15-isomer13 bp86/6-31G(d) Etot=-3001.348769 Eb=-12.69

Mg1	-2.638563	-1.159068	-1.809795
Mg2	-1.314857	2.892168	0.943291
Mg3	2.867554	0.560607	-1.482116
Mg4	1.900272	2.006172	1.177017
Mg5	-4.265141	-2.301315	0.599851
Mg6	-2.450292	2.005177	-1.755058
Mg7	-0.168868	0.280382	-0.634385
Mg8	-3.251384	0.585625	0.897645
Mg9	-1.291992	-2.131455	0.920164
Mg10	-0.577522	0.437640	2.593606
Mg11	1.657500	-1.479064	1.417414
Mg12	0.852763	2.838326	-1.660619
Mg13	3.670439	-2.287191	-0.775586
Mg14	0.809143	-2.282778	-1.757338
Mg15	4.200947	0.034775	1.325909

@mg15-isomer14 bp86/6-31G(d) Etot=-3001.348188 Eb=-12.66

Mg1	-3.005294	-0.954229	1.749202
Mg2	-3.412536	1.155012	-0.467701
Mg3	0.386813	-1.268025	1.948538
Mg4	-3.850386	-1.878340	-0.907084
Mg5	-0.711983	1.365093	1.079956
Mg6	-1.392304	-3.355122	0.340815
Mg7	-0.883110	-0.715303	-1.205196
Mg8	-1.923785	3.942422	-0.275781
Mg9	1.031008	4.001092	0.454209
Mg10	3.459169	-1.536363	1.740462
Mg11	1.145000	1.541404	-1.339033
Mg12	2.352850	1.249227	1.440961

Mg13	1.529658	-2.490146	-0.478072
Mg14	1.567776	-0.839924	-3.074812
Mg15	3.707122	-0.216798	-1.006462

@mg15-isomer15 bp86/6-31G(d) Etot=-3001.348056 Eb=-12.66

Mg1	-0.183919	0.268934	-1.756488
Mg2	1.268543	2.978745	-1.294483
Mg3	-0.511728	-1.518310	1.003065
Mg4	-0.981627	2.034538	0.745066
Mg5	-2.173960	2.689651	-1.927499
Mg6	3.109566	0.543033	-1.129219
Mg7	2.642699	-0.937326	1.573322
Mg8	1.466829	-2.202732	-1.292079
Mg9	-2.913514	0.189919	2.209799
Mg10	2.449265	2.193011	1.404753
Mg11	0.287311	0.588443	2.983821
Mg12	-3.496218	0.140413	-0.987641
Mg13	-1.799070	-2.406420	-1.726654
Mg14	4.386877	-2.225677	-0.517389
Mg15	-3.551055	-2.336221	0.711627

@mg15-isomer16 bp86/6-31G(d) Etot=-3001.347397 Eb=-12.63

Mg1	1.052377	2.036582	1.980735
Mg2	-1.720301	-2.625081	1.005539
Mg3	1.687989	4.292558	-0.029100
Mg4	-2.034129	-0.500470	-1.448331
Mg5	2.994077	-1.628761	-1.096831
Mg6	2.779298	1.411882	-0.600847
Mg7	1.458366	-3.316919	1.134002
Mg8	3.173197	-0.672306	1.747502
Mg9	-0.587789	2.366737	-0.734536
Mg10	-2.112787	0.888943	1.694515
Mg11	-4.284531	-0.867758	0.620911
Mg12	-3.673548	1.954727	-0.650804
Mg13	0.032444	-2.885338	-1.485048
Mg14	0.846633	0.006053	-2.619595
Mg15	0.388704	-0.460849	0.481887

@mg15-isomer17 bp86/6-31G(d) Etot=-3001.347092 Eb=-12.62

Mg1	-3.051373	-3.019702	-0.225392
Mg2	0.525424	-0.902006	2.703372
Mg3	-0.046659	0.990329	0.438379
Mg4	2.535111	-2.584086	-1.718730
Mg5	2.914216	-1.991469	1.207067
Mg6	-2.460336	-0.575310	1.723997
Mg7	-1.945559	-0.265528	-1.737449
Mg8	-2.883417	2.315474	0.036184
Mg9	3.680986	0.155223	-0.848226
Mg10	0.019545	-2.159543	-0.099215
Mg11	1.007055	0.069117	-2.227118
Mg12	2.699567	1.094554	1.864017
Mg13	-0.500962	4.379670	-0.080419
Mg14	-4.560878	-0.285298	-0.325106
Mg15	2.067279	2.778574	-0.711363

@mg15-isomer18 bp86/6-31G(d) Etot=-3001.347063 Eb=-12.62

Mg1	3.478538	-1.573267	0.560826
Mg2	3.745521	0.598243	-1.544750
Mg3	0.921952	1.712527	-1.386376
Mg4	-2.563965	-1.023387	1.873405
Mg5	0.576622	-1.310002	1.674726
Mg6	-3.618903	1.245873	0.172811
Mg7	2.516735	1.140501	1.411844
Mg8	-1.544637	3.357054	-0.565702

Mg9	-4.007004	-1.578525	-0.833270
Mg10	-0.585325	1.318909	1.429296
Mg11	1.266637	3.929856	0.758794
Mg12	1.499083	-3.905545	0.183929
Mg13	-1.260209	-2.778548	-0.398974
Mg14	-1.561548	0.104127	-1.741731
Mg15	1.136502	-1.237815	-1.594828

@mg15-isomer19 bp86/6-31G(d) Etot=-3001.346439 Eb=-12.59

Mg1	0.178411	0.750782	1.053847
Mg2	-2.179588	-1.344603	-2.121532
Mg3	-0.811278	-2.235801	0.805304
Mg4	1.965757	-1.409641	1.944600
Mg5	2.469715	1.441939	-1.716134
Mg6	3.256805	1.431098	1.177980
Mg7	3.764794	-1.110712	-0.487537
Mg8	-0.673289	1.458913	-1.730215
Mg9	-3.602107	0.930651	-0.605378
Mg10	-3.822179	-1.967382	0.304239
Mg11	-2.527778	0.187504	2.113249
Mg12	1.815464	-3.778253	-0.019539
Mg13	0.805239	-1.141832	-1.556667
Mg14	1.150611	3.764797	0.069429
Mg15	-1.790577	3.022540	0.768355

@mg15-isomer20 bp86/6-31G(d) Etot=-3001.345535 Eb=-12.55

Mg1	1.457548	-1.220462	1.890627
Mg2	1.732401	-3.081786	-0.725161
Mg3	-1.031678	-2.457190	0.467275
Mg4	-1.378976	-0.889996	3.163827
Mg5	4.096851	-1.378426	0.468767
Mg6	-3.649620	-0.525705	1.148467
Mg7	-0.505497	0.748000	0.843461
Mg8	2.823892	1.461896	0.662394
Mg9	2.729819	-0.360251	-1.913481
Mg10	-3.346278	-1.948381	-1.518887
Mg11	-0.378339	-1.046760	-2.086176
Mg12	0.527280	1.852857	-1.607029
Mg13	-2.712984	1.062185	-1.336302
Mg14	1.288189	4.138381	0.558343
Mg15	-1.652608	3.645639	-0.016126

@mg15-isomer21 bp86/6-31G(d) Etot=-3001.345333 Eb=-12.55

Mg1	-4.116991	0.575766	-0.620903
Mg2	0.288453	-1.649131	1.155886
Mg3	1.121281	-2.126435	-1.723780
Mg4	3.282964	-0.659336	0.097709
Mg5	-3.003923	3.444117	0.020818
Mg6	-3.188587	-1.916693	1.083063
Mg7	-1.922049	-1.242537	-1.566954
Mg8	-1.696696	0.809243	1.211470
Mg9	0.030119	3.486519	0.226381
Mg10	2.797167	-1.327873	2.964472
Mg11	2.899457	2.433190	-0.489626
Mg12	-1.142525	-4.016931	-0.372421
Mg13	2.992646	0.262379	-2.692225
Mg14	1.311555	1.166176	1.855073
Mg15	0.347129	0.761547	-1.148963

@mg15-isomer22 bp86/6-31G(d) Etot=-3001.344298 Eb=-12.50

Mg1	1.441807	-1.136612	1.983810
Mg2	-1.946865	3.125210	0.715671
Mg3	1.965871	-4.004900	0.614854
Mg4	-0.648882	0.946573	-0.906442

Mg5	2.387383	1.520924	-1.541641
Mg6	2.816235	-1.434150	-0.820489
Mg7	0.952359	1.834525	1.518123
Mg8	3.752013	0.742799	1.048024
Mg9	0.533738	-0.823434	-2.808228
Mg10	-1.447102	-0.077465	1.926273
Mg11	-3.918680	0.795701	0.196929
Mg12	-3.485444	-2.174299	0.804721
Mg13	0.888435	4.105784	-0.569593
Mg14	-2.850220	-1.160494	-1.977766
Mg15	-0.440649	-2.260162	-0.184247

@mg15-isomer23 bp86/6-31G(d) Etot=-3001.343148 Eb=-12.45

Mg1	-0.256108	1.089957	1.715824
Mg2	-1.509629	-1.559857	0.975716
Mg3	-0.525386	0.681339	-1.629098
Mg4	2.650543	0.467765	-1.764179
Mg5	-1.984169	2.965994	0.006410
Mg6	-3.769691	0.718524	-1.250088
Mg7	2.926943	0.850423	1.214969
Mg8	5.685511	0.121322	-0.403799
Mg9	-3.434966	0.790809	1.754480
Mg10	0.769555	-1.915410	-0.947221
Mg11	1.312154	2.883591	-0.381719
Mg12	1.275340	-1.521731	2.192448
Mg13	3.596546	-1.988615	0.255752
Mg14	-2.203532	-1.841704	-1.962762
Mg15	-4.533111	-1.742406	0.223266

@mg15-isomer24 bp86/6-31G(d) Etot=-3001.342225 Eb=-12.42

Mg1	0.734945	-0.518444	-1.040862
Mg2	-0.650542	2.291599	-1.099956
Mg3	0.081746	1.085326	1.639352
Mg4	-3.483886	0.943978	-0.907596
Mg5	-1.460068	0.014267	-3.015800
Mg6	2.508790	2.035331	-0.406514
Mg7	-0.133217	-1.952255	1.552142
Mg8	-2.685836	-0.255295	1.872319
Mg9	3.980335	-0.736667	-1.338251
Mg10	-2.426544	2.820172	1.306947
Mg11	2.929809	-0.473192	1.473530
Mg12	-2.137354	-1.886147	-0.716485
Mg13	5.426322	1.255606	0.425426
Mg14	2.456863	-3.213553	0.034408
Mg15	-5.141361	-1.410725	0.221341

@mg15-isomer25 bp86/6-31G(d) Etot=-3001.341684 Eb=-12.39

Mg1	2.762868	2.952988	-1.480500
Mg2	2.749054	-2.944172	-1.492960
Mg3	-1.790498	0.009356	-1.759119
Mg4	-0.223982	-2.607063	-1.887687
Mg5	-3.180910	-2.488905	-0.799248
Mg6	-3.179111	2.499876	-0.784287
Mg7	3.610053	-1.520168	1.042651
Mg8	-0.801030	1.667119	1.011391
Mg9	1.406271	-0.000489	2.509842
Mg10	-0.798160	-1.668218	1.005750
Mg11	3.617210	1.499554	1.037479
Mg12	-3.620879	-0.001367	0.918339
Mg13	-0.210146	2.621271	-1.868169
Mg14	-1.760672	-0.012720	3.310761
Mg15	1.419934	-0.007063	-0.764245

@mg15-isomer26 bp86/6-31G(d) Etot=-3001.341337 Eb=-12.38

Mg1	-4.386115	1.276091	0.022684
Mg2	0.055000	0.213520	1.361757
Mg3	-2.113975	2.457476	1.657942
Mg4	-2.866072	-1.140052	1.050418
Mg5	-3.631607	-0.993600	-1.943490
Mg6	-1.589084	1.210807	-1.251795
Mg7	3.399027	2.921414	-1.432919
Mg8	0.715496	2.860980	0.101339
Mg9	-0.430496	-2.699025	1.956189
Mg10	2.348427	-1.049872	3.016058
Mg11	1.514946	0.412983	-1.712522
Mg12	3.301114	0.893497	0.888750
Mg13	-0.671722	-1.875147	-1.133575
Mg14	1.983913	-2.491398	-2.759554
Mg15	2.371147	-1.997674	0.178718

@mg15-isomer27 bp86/6-31G(d) Etot=-3001.341173 Eb=-12.37

Mg1	-4.017805	0.748425	-1.311457
Mg2	1.117743	2.792794	-0.965026
Mg3	-2.842010	0.275939	1.410931
Mg4	-2.155269	3.048807	-0.082247
Mg5	-2.697220	-2.101521	-0.735987
Mg6	2.143730	-0.510701	2.945128
Mg7	2.948321	-1.885675	0.274157
Mg8	-0.721975	0.316056	-1.228251
Mg9	2.331652	0.107263	-2.013585
Mg10	3.164719	1.243476	0.672698
Mg11	-5.382898	-1.251464	0.533692
Mg12	0.592537	-2.395324	-1.581831
Mg13	0.201428	1.473703	1.622728
Mg14	5.420403	-0.278232	-0.770290
Mg15	-0.103355	-1.583545	1.229341

@mg15-isomer28 bp86/6-31G(d) Etot=-3001.340723 Eb=-12.35

Mg1	0.760412	-0.955451	2.322842
Mg2	2.831571	0.932480	1.127814
Mg3	-2.096795	-0.427829	1.270183
Mg4	2.789534	-2.038948	0.290828
Mg5	3.708111	0.660025	-1.740723
Mg6	0.711239	-0.094148	-1.320618
Mg7	-0.199257	1.900395	1.488350
Mg8	-0.361041	-2.660726	-0.061986
Mg9	-1.681152	1.899345	-1.138569
Mg10	-3.487538	2.203566	1.388009
Mg11	1.508486	2.811063	-0.966207
Mg12	-4.495094	0.283629	-0.626480
Mg13	-2.039836	-0.987753	-2.115321
Mg14	-3.558799	-2.791106	-0.147703
Mg15	5.610159	-0.734542	0.229581

@mg15-isomer29 bp86/6-31G(d) Etot=-3001.340546 Eb=-12.34

Mg1	1.790821	0.385801	-2.496957
Mg2	2.805846	-0.595609	2.327136
Mg3	-2.277315	2.995486	0.191258
Mg4	-2.561889	0.065502	1.641442
Mg5	-0.932170	0.350227	-1.035338
Mg6	-5.241692	-1.311130	0.904941
Mg7	0.163885	-1.663573	1.163442
Mg8	-2.779816	-2.125773	-0.651895
Mg9	3.128430	1.389687	0.036716
Mg10	0.788930	2.934600	-0.920694
Mg11	5.586037	-0.431955	0.430290
Mg12	0.410929	1.306333	1.707988
Mg13	2.967961	-1.739490	-0.522269

Mg14	0.328632	-2.297614	-1.816121
Mg15	-4.178590	0.737510	-0.959938

@mg15-isomer30 bp86/6-31G(d) Etot=-3001.340405 Eb=-12.34

Mg1	0.052747	-0.875858	1.022555
Mg2	3.085871	0.261975	1.629415
Mg3	0.589911	2.135588	0.343644
Mg4	-2.617373	-1.939286	-0.643017
Mg5	0.253634	-2.537129	-1.483848
Mg6	-1.699099	1.254062	2.163195
Mg7	-0.883229	0.298586	-1.802844
Mg8	2.277840	-0.009294	-1.313145
Mg9	-2.571076	-1.681192	2.413734
Mg10	2.994245	-2.572853	0.225406
Mg11	-3.906361	0.443399	-2.203560
Mg12	-4.288332	0.275726	0.736823
Mg13	5.400420	-0.160640	-0.270350
Mg14	3.774755	2.517794	-0.318962
Mg15	-2.463953	2.589121	-0.499046

@mg15-isomer31 bp86/6-31G(d) Etot=-3001.340233 Eb=-12.33

Mg1	2.237527	0.846899	0.724731
Mg2	4.033995	-0.696289	-1.521358
Mg3	3.099167	-2.035868	1.179181
Mg4	1.079477	-1.738004	-1.210861
Mg5	0.551778	3.103655	-0.333370
Mg6	0.019227	-1.340928	1.597688
Mg7	5.442687	0.004223	0.991545
Mg8	-0.946416	0.503239	-1.053166
Mg9	-1.992689	-2.276342	-0.722494
Mg10	-0.432270	1.623614	2.163080
Mg11	1.689680	1.139225	-2.424415
Mg12	-3.010340	-0.086842	1.497292
Mg13	-2.675287	2.753932	0.258583
Mg14	-4.160094	0.418512	-1.211286
Mg15	-4.936440	-2.219027	0.064848

@mg15-isomer32 bp86/6-31G(d) Etot=-3001.338341 Eb=-12.25

Mg1	2.862727	2.284273	-2.177739
Mg2	-0.185688	-2.382459	1.546193
Mg3	-1.141199	0.254242	0.440361
Mg4	3.679475	1.187708	0.710733
Mg5	1.749745	-0.378906	-1.101255
Mg6	-0.603182	1.252965	-2.517686
Mg7	-1.699939	2.749320	2.016767
Mg8	-4.073356	1.155242	0.762805
Mg9	-3.308824	-0.086296	-1.953434
Mg10	0.830514	2.516436	0.060242
Mg11	3.007106	-1.651437	1.509696
Mg12	-3.172193	-1.956743	0.683249
Mg13	1.111142	0.497613	2.482660
Mg14	-0.930494	-2.055907	-1.541487
Mg15	1.874166	-3.386052	-0.921106

@mg15-isomer33 bp86/6-31G(d) Etot=-3001.338115 Eb=-12.24

Mg1	-2.170577	1.973659	-0.998095
Mg2	-1.777856	-0.717886	1.517693
Mg3	-0.440184	-2.495655	-0.478525
Mg4	1.229765	-0.954444	1.664798
Mg5	-3.147824	1.915848	1.942573
Mg6	5.705926	-0.059464	-0.739782
Mg7	2.896940	1.342135	-0.023634
Mg8	0.285970	0.264214	-1.563623
Mg9	-3.573101	-2.884163	-0.028077

Mg10	4.343456	-1.065444	1.690970
Mg11	2.863709	-1.597081	-0.940620
Mg12	0.843346	3.261387	-1.178569
Mg13	-0.097051	1.798097	1.324092
Mg14	-4.485165	0.062820	-0.036454
Mg15	-2.477354	-0.844023	-2.152746

@mg15-isomer34 bp86/6-31G(d) Etot=-3001.336996 Eb=-12.20

Mg1	-2.563989	1.613909	-0.673530
Mg2	0.155408	1.600338	-1.972169
Mg3	0.111718	1.316936	1.098510
Mg4	0.874570	-1.173643	-0.844721
Mg5	-3.423213	-1.390937	0.149134
Mg6	-2.719563	0.778227	2.232422
Mg7	-0.681465	-1.508519	1.804035
Mg8	-5.434185	0.892653	0.279669
Mg9	2.412643	-0.880123	1.758531
Mg10	3.215936	1.151186	-0.677303
Mg11	-1.720539	-0.843997	-2.398650
Mg12	-1.330716	-3.367444	-0.648100
Mg13	5.348400	-0.217176	1.089123
Mg14	3.983277	-1.807801	-1.009179
Mg15	1.771717	3.836392	-0.187772

@mg15-isomer35 bp86/6-31G(d) Etot=-3001.334961 Eb=-12.11

Mg1	-1.329837	-1.855289	0.170200
Mg2	-1.344236	-0.489595	2.826960
Mg3	-0.226078	1.441797	0.607841
Mg4	-1.990018	3.500640	-0.735986
Mg5	0.830417	-0.344801	-1.615231
Mg6	2.846775	1.661676	-0.299769
Mg7	-2.007997	0.637984	-1.953658
Mg8	1.493112	-1.000945	1.418706
Mg9	-3.950295	-1.808301	1.666247
Mg10	-3.356267	1.057696	0.729544
Mg11	1.197522	-3.385308	-0.759270
Mg12	1.023606	4.169137	-0.443635
Mg13	-1.390707	-2.314575	-2.685821
Mg14	4.537239	0.149081	1.808139
Mg15	3.666765	-1.419197	-0.734268

@mg15-isomer36 bp86/6-31G(d) Etot=-3001.333253 Eb=-12.04

Mg1	-1.392119	-0.943795	2.523916
Mg2	-0.031055	2.210388	-1.181731
Mg3	-1.822578	1.777237	1.199248
Mg4	0.334481	-0.804307	-1.312822
Mg5	1.139218	0.616187	1.282774
Mg6	-4.685953	2.489592	-0.114009
Mg7	0.785957	-2.655952	1.176852
Mg8	-2.193394	-2.422115	0.058130
Mg9	3.046296	1.392466	-1.258452
Mg10	4.335862	1.334270	1.464761
Mg11	-4.172731	-0.291558	1.146987
Mg12	3.370319	-1.367801	0.209854
Mg13	5.881088	0.146315	-0.800548
Mg14	-1.942897	-2.001823	-2.930416
Mg15	-2.652491	0.520896	-1.464542

@mg15-isomer37 bp86/6-31G(d) Etot=-3001.328999 Eb=-11.86

Mg1	0.944796	-1.609582	-1.016275
Mg2	-1.390131	0.242299	-1.942054
Mg3	-4.107095	-0.304575	-0.122546
Mg4	3.465879	0.507702	-1.449132
Mg5	-0.806100	-0.386626	1.215008

Mg6	-3.194841	0.714159	2.711350
Mg7	2.492039	-0.245580	1.286067
Mg8	4.004729	-2.427682	-0.628844
Mg9	-4.024736	1.639749	-2.374465
Mg10	-2.052351	-2.581559	-1.023846
Mg11	3.724626	2.612933	0.901735
Mg12	0.720337	1.813139	-0.173191
Mg13	5.653543	-0.017352	0.545513
Mg14	-3.071490	-2.265501	1.903506
Mg15	-2.359205	2.308477	0.167173

@mg15-isomer38 bp86/6-31G(d) Etot=-3001.327049 Eb=-11.78

Mg1	-0.161813	1.291971	-0.428185
Mg2	-0.053652	-1.561728	-1.695128
Mg3	-1.011591	-1.564091	1.217367
Mg4	-2.271910	0.330190	-2.394714
Mg5	-3.027577	-2.328234	-0.993349
Mg6	2.853712	2.045265	0.753310
Mg7	-4.135650	-1.703272	1.735937
Mg8	-2.585758	0.974604	1.706589
Mg9	5.146970	0.341675	-0.133776
Mg10	2.645620	0.662791	-1.929199
Mg11	7.784627	-1.430200	0.205224
Mg12	-4.820399	0.216795	-0.443156
Mg13	2.185524	-0.879395	0.581902
Mg14	-2.862350	2.726282	-0.718204
Mg15	0.314245	0.877347	2.535381

@mg15-isomer39 bp86/6-31G(d) Etot=-3001.307793 Eb=-10.97

Mg1	0.069417	0.381156	-1.440141
Mg2	1.608349	-1.119123	0.902085
Mg3	4.518115	-0.936513	0.000208
Mg4	-1.353808	-0.447818	1.338539
Mg5	-2.165065	2.434566	-0.295220
Mg6	-3.068461	-0.305038	-1.430995
Mg7	3.094248	1.644504	-0.755025
Mg8	-4.327039	0.643659	1.181661
Mg9	0.661964	2.019660	1.256716
Mg10	-0.754067	-2.504529	-0.779045
Mg11	-6.032007	-1.201438	-0.579671
Mg12	-3.578995	-2.583388	0.731348
Mg13	3.626024	1.018011	2.132675
Mg14	0.611453	3.513160	-1.372749
Mg15	7.089871	-2.556869	-0.890384

@mg16-isomer01 bp86/6-31G(d) Etot=-3201.464716 Eb=-13.71

Mg1	3.441196	-1.431645	1.054762
Mg2	-3.542789	-0.000049	-0.000056
Mg3	0.362527	-0.205351	-1.834573
Mg4	0.362673	-1.486568	1.095671
Mg5	0.362701	1.692187	0.739790
Mg6	1.924621	0.338638	3.023469
Mg7	1.924109	2.449223	-1.804846
Mg8	1.924345	-2.787705	-1.218709
Mg9	-2.813666	2.758254	1.205885
Mg10	-2.813642	-0.334889	-2.991741
Mg11	-2.813791	-2.423496	1.785702
Mg12	-1.733466	0.281623	2.517718
Mg13	-1.733653	2.039581	-1.502899
Mg14	-1.733427	-2.321324	-1.014769
Mg15	3.441110	1.629369	0.711938
Mg16	3.441155	-0.197849	-1.767343

@mg16-isomer02 bp86/6-31G(d) Etot=-3201.464233 Eb=-13.69

Mg1	1.030505	-2.793023	0.725996
Mg2	0.658632	0.062197	-0.453691
Mg3	-3.444560	1.302232	0.995013
Mg4	1.408753	-0.363187	2.600676
Mg5	-2.110249	3.799148	-0.387292
Mg6	0.761821	2.928475	-1.210597
Mg7	-0.463675	2.005696	1.593761
Mg8	-1.524336	-0.991203	1.575546
Mg9	2.400986	-1.874243	-1.941558
Mg10	-1.988124	1.034484	-1.674584
Mg11	-0.862004	-2.050266	-1.874094
Mg12	-3.569733	-1.353933	-0.675946
Mg13	3.303956	1.095456	-1.629999
Mg14	2.705921	1.978747	1.221345
Mg15	-1.957056	-3.829211	0.392214
Mg16	3.649163	-0.951369	0.743209

@mg16-isomer03 bp86/6-31G(d) Etot=-3201.459142 Eb=-13.49

Mg1	-0.179953	0.762448	-1.665726
Mg2	-2.262343	-1.224059	-2.658362
Mg3	-0.690280	-2.017534	0.003152
Mg4	1.092582	-1.965672	-2.630969
Mg5	-3.308833	1.469118	-1.613087
Mg6	-0.183883	0.769229	1.660312
Mg7	4.777137	2.053936	-0.001200
Mg8	1.779901	2.362597	-0.003804
Mg9	-1.423264	3.128555	-0.006331
Mg10	-2.264909	-1.211875	2.663644
Mg11	3.028971	0.025962	-1.577930
Mg12	1.088009	-1.953250	2.638795
Mg13	2.487175	-2.588164	0.007191
Mg14	3.025909	0.032346	1.578594
Mg15	-3.654016	-1.119120	0.001460
Mg16	-3.312204	1.475484	1.604263

@mg16-isomer04 bp86/6-31G(d) Etot=-3201.458995 Eb=-13.49

Mg1	-3.902971	-0.585419	0.556227
Mg2	-2.510146	1.204298	2.639872
Mg3	2.929354	1.666560	1.579003
Mg4	-2.832748	2.150511	-0.188068
Mg5	-2.844098	-0.052295	-2.267830
Mg6	2.934002	-2.103367	-1.948361
Mg7	1.489649	-0.612859	2.919442
Mg8	-0.046750	0.800427	0.601055
Mg9	3.674682	-1.150817	0.860972
Mg10	2.658924	0.781911	-1.447180
Mg11	0.902167	-2.345722	0.369728
Mg12	1.788348	3.441152	-0.509017
Mg13	-1.531080	-1.585631	1.995295
Mg14	-2.189386	-2.660207	-0.812475
Mg15	0.056148	-0.969874	-2.187939
Mg16	-0.576095	2.021331	-2.160725

@mg16-isomer05 bp86/6-31G(d) Etot=-3201.458660 Eb=-13.47

Mg1	0.581581	0.066537	0.000123
Mg2	3.820799	-0.902595	-0.000065
Mg3	-1.099721	-1.734637	1.651626
Mg4	2.165679	-1.187013	2.578547
Mg5	1.571362	-2.794319	0.000047
Mg6	-1.099630	-1.734691	-1.651471
Mg7	-0.848593	1.377044	2.437798
Mg8	2.846048	1.547724	-1.570025
Mg9	-3.523005	-2.386615	-0.000008
Mg10	-2.428863	2.568900	-0.000100

Mg11	-0.848312	1.376902	-2.437753
Mg12	-3.410876	0.224154	-1.572116
Mg13	0.672817	2.993698	0.000052
Mg14	2.165530	-1.187017	-2.578537
Mg15	-3.410989	0.224193	1.571931
Mg16	2.846173	1.547734	1.569951

@mg16-isomer06 bp86/6-31G(d) Etot=-3201.458249 Eb=-13.46

Mg1	-3.687653	0.720909	-0.905992
Mg2	-1.471383	2.719463	-1.187771
Mg3	-0.848721	-0.455158	2.910613
Mg4	1.727076	1.435987	-2.508357
Mg5	-2.484958	1.789013	1.669850
Mg6	1.981206	-1.592244	1.583402
Mg7	1.574218	-1.500583	-1.722502
Mg8	3.955157	-2.678538	-0.399704
Mg9	-3.344754	-2.213651	-1.424831
Mg10	-0.885520	-2.194189	0.233621
Mg11	2.258317	1.252207	2.532444
Mg12	0.171339	0.668754	0.269126
Mg13	-3.432732	-1.130497	1.583732
Mg14	2.177773	3.031894	0.018128
Mg15	-1.252756	-0.218928	-2.396317
Mg16	3.563391	0.365560	-0.255441

@mg16-isomer07 bp86/6-31G(d) Etot=-3201.458040 Eb=-13.45

Mg1	1.426002	-3.306331	0.748576
Mg2	-1.571821	-3.547700	0.010598
Mg3	2.402779	0.750961	-2.197516
Mg4	0.665072	-1.733861	-1.779176
Mg5	3.476549	1.445644	0.569273
Mg6	-0.463027	0.962975	-1.260637
Mg7	-2.433330	1.367600	1.942791
Mg8	-3.511095	1.307195	-0.908318
Mg9	-2.443302	-1.348765	-1.946063
Mg10	-1.538828	3.557189	-0.012915
Mg11	-0.476654	-0.956382	1.257269
Mg12	-3.523651	-1.279447	0.906975
Mg13	2.387049	-0.770168	2.194745
Mg14	3.463848	-1.476159	-0.565401
Mg15	0.680027	1.731316	1.781879
Mg16	1.460383	3.295932	-0.742080

@mg16-isomer08 bp86/6-31G(d) Etot=-3201.457941 Eb=-13.44

Mg1	0.015798	1.577327	-2.479584
Mg2	0.009302	0.157244	0.063107
Mg3	1.534976	-1.569456	2.029340
Mg4	1.692094	1.708035	2.003447
Mg5	-3.816264	-0.121484	0.598866
Mg6	3.789964	-0.125678	0.648544
Mg7	2.582252	2.253017	-0.861756
Mg8	3.021150	-2.967532	-0.287910
Mg9	2.208268	-0.604543	-1.983279
Mg10	-1.722733	1.706359	1.981034
Mg11	-0.002904	3.687385	0.270605
Mg12	-2.163708	-0.628503	-1.984725
Mg13	-2.576355	2.243424	-0.897173
Mg14	-3.004641	-2.982375	-0.284742
Mg15	-1.577243	-1.537568	2.031084
Mg16	0.010045	-2.795651	-0.846858

@mg16-isomer09 bp86/6-31G(d) Etot=-3201.453783 Eb=-13.28

Mg1	0.041740	-0.355267	0.338303
Mg2	-2.695459	0.527955	-1.328589

Mg3	0.805046	2.849844	0.627693
Mg4	3.194032	1.654386	-0.857799
Mg5	-1.609329	3.591936	-1.239451
Mg6	4.315773	-0.946233	0.262118
Mg7	2.336286	-1.126784	-1.951418
Mg8	-0.498523	0.931791	2.878062
Mg9	2.453131	0.646251	1.991863
Mg10	-0.670399	-1.671226	-2.233738
Mg11	0.361388	1.367221	-2.111423
Mg12	-2.838763	-0.910850	1.598061
Mg13	-2.733234	2.134771	1.223321
Mg14	1.914525	-2.706239	0.850782
Mg15	-3.303084	-2.522871	-0.935637
Mg16	-1.073131	-3.464686	0.887852

@mg16-isomer10 bp86/6-31G(d) Etot=-3201.450791 Eb=-13.16

Mg1	-1.629312	0.205579	2.531979
Mg2	0.928446	0.616665	1.062244
Mg3	2.016522	3.410634	0.168708
Mg4	3.071508	-1.638169	0.701832
Mg5	-0.083602	-2.198365	1.271746
Mg6	-1.444798	-3.226070	-1.305787
Mg7	-1.672724	-0.256329	-1.040759
Mg8	3.909231	1.251998	1.598232
Mg9	-3.924766	1.135622	0.776149
Mg10	-3.188876	-1.945428	1.018911
Mg11	-2.981580	2.323712	-1.911510
Mg12	3.247722	1.016649	-1.322797
Mg13	-1.248959	2.702494	0.618429
Mg14	0.328051	1.908176	-1.898760
Mg15	1.149622	-1.239003	-1.652654
Mg16	1.523514	-4.068166	-0.615963

@mg16-isomer11 bp86/6-31G(d) Etot=-3201.446702 Eb=-13.00

Mg1	-2.739130	-1.306860	0.726026
Mg2	2.937229	-1.930659	-0.736967
Mg3	3.569580	1.064463	-1.377291
Mg4	-4.428458	0.890893	-0.902383
Mg5	-2.950656	1.733331	1.533485
Mg6	-0.929876	-3.117224	-1.008398
Mg7	-2.356419	-0.801455	-2.230151
Mg8	1.238936	3.034858	-1.489828
Mg9	0.488915	-0.118353	-1.439067
Mg10	0.544620	-1.626011	1.317786
Mg11	0.143070	1.668560	1.191715
Mg12	-1.650362	2.136785	-1.310890
Mg13	-1.461120	-0.264138	3.179700
Mg14	1.536460	-4.532742	0.106270
Mg15	3.034365	3.087626	0.877299
Mg16	3.022847	0.080925	1.562695

@mg16-isomer12 bp86/6-31G(d) Etot=-3201.445957 Eb=-12.97

Mg1	0.975837	-1.395167	-1.481029
Mg2	0.320378	-2.382645	1.571375
Mg3	-4.185367	-0.477890	-0.796197
Mg4	3.224950	-2.033969	0.505446
Mg5	-1.052314	-0.047297	0.436112
Mg6	0.491094	1.798489	-1.545412
Mg7	-2.024019	-2.689990	-0.978146
Mg8	-1.763978	-0.179820	-2.641699
Mg9	-2.734236	2.216828	-1.017275
Mg10	-0.451586	2.564124	1.560491
Mg11	2.420089	3.074237	0.494555
Mg12	-3.480953	1.220697	1.718273

Mg13	-3.009672	-1.909836	1.776152
Mg14	6.059906	-0.725494	-0.119558
Mg15	1.894409	0.381548	1.673753
Mg16	3.315462	0.586184	-1.156841

@mg16-isomer13 bp86/6-31G(d) Etot=-3201.443499 Eb=-12.88

Mg1	-4.518794	0.223587	1.895475
Mg2	-1.247536	3.150231	-0.480125
Mg3	2.945146	-0.481834	2.874887
Mg4	-1.668632	1.076390	1.751321
Mg5	2.642473	-2.888486	0.532804
Mg6	-2.522692	-1.789825	-2.527258
Mg7	2.144562	1.674736	-1.863502
Mg8	0.250469	-1.357911	1.712488
Mg9	-2.726872	-1.888385	0.499434
Mg10	-3.419469	0.827585	-0.906380
Mg11	3.683898	-0.103682	-0.000969
Mg12	-0.336817	0.059590	-0.975267
Mg13	2.082549	-1.464216	-2.207011
Mg14	1.474934	4.417672	-0.623247
Mg15	-0.144530	-3.067418	-0.814679
Mg16	1.361310	1.611964	1.132029

@mg16-isomer14 bp86/6-31G(d) Etot=-3201.443363 Eb=-12.87

Mg1	4.448308	0.053653	0.362653
Mg2	0.611377	1.960819	-0.194384
Mg3	0.615336	-1.364339	-0.862874
Mg4	2.440160	1.402712	2.269607
Mg5	3.470094	2.876928	-0.276116
Mg6	-2.272651	-2.202290	-1.519048
Mg7	-3.880634	0.521151	-1.598266
Mg8	-0.346815	0.022369	1.961466
Mg9	-3.276453	-0.846884	1.218584
Mg10	2.243261	-1.703670	1.782799
Mg11	-1.087312	-2.918947	1.218373
Mg12	-0.938614	0.622633	-2.430324
Mg13	-5.623530	1.285376	0.861066
Mg14	-2.396113	2.022710	0.511195
Mg15	2.561845	0.576774	-2.215580
Mg16	3.431744	-2.308996	-1.089150

@mg16-isomer15 bp86/6-31G(d) Etot=-3201.441165 Eb=-12.79

Mg1	-0.389530	-0.045177	-1.275145
Mg2	-0.226101	1.575657	1.548164
Mg3	1.955625	1.903059	-0.625515
Mg4	-2.982289	-0.433593	1.688141
Mg5	-2.372794	-2.277871	-0.674500
Mg6	1.384065	-2.554733	-1.227322
Mg7	3.804547	-0.749951	-0.609115
Mg8	-0.061280	-1.548855	1.475345
Mg9	-3.089519	2.661333	1.164067
Mg10	4.859570	1.862378	0.541273
Mg11	-1.299982	2.923493	-1.251208
Mg12	2.504200	0.340428	2.017683
Mg13	2.081235	-0.095919	-2.952224
Mg14	-3.497848	0.688140	-1.246587
Mg15	2.722395	-2.707295	1.525925
Mg16	-5.392295	-1.541094	-0.098982

@mg16-isomer16 bp86/6-31G(d) Etot=-3201.434989 Eb=-12.54

Mg1	-3.013916	-1.238740	-0.742176
Mg2	-0.783897	1.477466	1.499024
Mg3	1.539731	-5.060679	-0.626008
Mg4	0.051637	-0.174204	-1.089607

Mg5	3.593951	2.967311	-0.208658
Mg6	-5.001414	1.081685	-1.675082
Mg7	2.370593	-2.109000	-1.072268
Mg8	0.736015	2.839105	-0.780161
Mg9	-0.718846	-3.103171	0.028803
Mg10	2.054469	1.914780	2.308344
Mg11	3.568793	0.048037	0.534876
Mg12	-3.892897	0.949191	1.260752
Mg13	-2.116791	1.970209	-1.229307
Mg14	2.653607	0.901611	-2.318101
Mg15	1.064141	-0.999540	1.869338
Mg16	-2.105176	-1.464061	2.240229

@mg16-isomer17 bp86/6-31G(d) Etot=-3201.432908 Eb=-12.46

Mg1	2.362914	-1.578014	-1.581754
Mg2	4.525020	-0.005652	-0.060744
Mg3	2.367138	1.575345	-1.578915
Mg4	-2.840987	-1.593808	-0.182365
Mg5	-1.140775	0.003627	2.027902
Mg6	-5.679529	-0.008530	-0.415549
Mg7	-0.874203	2.803193	-2.203043
Mg8	0.322276	2.415366	0.705798
Mg9	-2.845179	1.600422	-0.181275
Mg10	1.872485	-0.000385	1.668622
Mg11	0.313492	-2.414346	0.707895
Mg12	-4.196542	0.004782	2.158826
Mg13	3.454077	-2.640294	1.159745
Mg14	-0.240242	0.002003	-1.176572
Mg15	-0.871719	-2.796103	-2.205844
Mg16	3.471773	2.632394	1.157273

@mg16-isomer18 bp86/6-31G(d) Etot=-3201.431513 Eb=-12.41

Mg1	-3.518220	0.110286	-1.464408
Mg2	-0.026613	0.328028	-1.260718
Mg3	4.790033	-0.321005	0.469984
Mg4	0.151138	-2.520416	0.306284
Mg5	1.985412	0.413179	-3.572617
Mg6	3.177465	-2.733066	1.280950
Mg7	-2.338936	2.687211	-0.064053
Mg8	-2.857176	-2.682970	0.023337
Mg9	2.919649	1.672458	-1.011497
Mg10	3.548896	2.087208	1.839770
Mg11	-5.088356	1.584349	0.674206
Mg12	0.575508	2.475187	0.916487
Mg13	2.577357	-1.522160	-1.358525
Mg14	1.506139	-0.228252	1.636813
Mg15	-1.860141	-0.018886	1.248957
Mg16	-5.542156	-1.331152	0.335031

@mg16-isomer19 bp86/6-31G(d) Etot=-3201.431453 Eb=-12.41

Mg1	1.277321	0.353452	1.294530
Mg2	3.435599	-2.176182	0.717092
Mg3	-1.123409	1.059459	3.008970
Mg4	0.735092	-2.011469	-0.925644
Mg5	-1.128603	-1.562202	1.402107
Mg6	-4.110988	-2.292373	0.976090
Mg7	-2.160941	-1.217467	-1.473433
Mg8	3.067245	0.043378	-1.555169
Mg9	0.076756	0.927511	-1.927382
Mg10	5.797882	-1.148804	-0.831929
Mg11	-2.881146	1.755547	-1.824980
Mg12	-3.412635	0.692690	1.025687
Mg13	-5.138683	-0.551807	-1.229761
Mg14	2.141821	2.768691	-0.214565

Mg15	-0.919987	2.584715	0.435373
Mg16	4.344675	0.774861	1.123016

@mg16-isomer20 bp86/6-31G(d) Etot=-3201.424242 Eb=-12.12

Mg1	0.919618	-0.219292	1.186709
Mg2	-1.449091	1.690560	1.550229
Mg3	3.259469	-2.119941	0.577860
Mg4	0.774831	-3.074011	2.102328
Mg5	-1.923512	-1.482500	1.133205
Mg6	-5.085866	-1.819038	0.466301
Mg7	-1.936154	3.241088	-0.941946
Mg8	3.816967	0.942713	0.979299
Mg9	1.213200	2.401501	-0.340206
Mg10	-0.115239	4.750736	1.032531
Mg11	2.238960	-0.167798	-1.810778
Mg12	-3.662720	0.652344	-0.442772
Mg13	0.242273	-2.521462	-0.871560
Mg14	-0.750595	0.251568	-1.706322
Mg15	5.312992	-0.428197	-1.199237
Mg16	-2.855133	-2.098271	-1.715641

@mg16-isomer21 bp86/6-31G(d) Etot=-3201.420679 Eb=-11.98

Mg1	-3.436694	-0.222219	-1.386624
Mg2	2.863776	-0.941598	-1.794470
Mg3	-6.425709	-0.018069	-0.375473
Mg4	4.007463	-0.926882	1.128152
Mg5	-1.401901	2.071706	-0.444928
Mg6	1.028925	0.347357	0.867488
Mg7	-4.690526	-2.006997	1.051519
Mg8	3.009795	1.763859	2.525728
Mg9	-0.250104	-0.755577	-1.686669
Mg10	0.999493	-2.722353	0.418896
Mg11	-1.635730	-1.002707	1.049703
Mg12	1.331379	1.765898	-2.310904
Mg13	1.172821	3.491090	0.317766
Mg14	3.769465	-3.675660	-0.148776
Mg15	3.723911	1.691023	-0.436210
Mg16	-4.066365	1.141129	1.224802

@mg16-isomer22 bp86/6-31G(d) Etot=-3201.419627 Eb=-11.94

Mg1	1.643708	-0.220472	1.549710
Mg2	0.118033	2.365470	-0.002143
Mg3	1.638399	-0.224624	-1.547997
Mg4	3.497955	1.823435	-0.003331
Mg5	1.855012	2.687778	-2.507238
Mg6	-1.063616	-0.829658	0.005559
Mg7	-3.650365	0.242288	-1.538402
Mg8	4.330907	-1.131277	-0.002126
Mg9	-0.906947	1.199547	2.617577
Mg10	-3.647625	0.295472	1.509079
Mg11	-6.266691	-0.566740	0.000914
Mg12	4.048686	-4.208225	-0.000344
Mg13	1.861864	2.695133	2.501777
Mg14	-0.914438	1.190480	-2.619635
Mg15	1.310883	-2.863799	0.004753
Mg16	-3.855766	-2.454809	0.031846

@mg17-isomer01 bp86/6-31G(d) Etot=-3401.582481 Eb=-14.68

Mg1	-1.345089	-3.451999	-0.601941
Mg2	2.008285	0.881402	-2.141075
Mg3	-0.795697	-2.036344	2.143372
Mg4	-2.005359	-0.881103	-2.142759
Mg5	2.039259	-0.796665	2.142058
Mg6	0.879714	-2.000008	-2.143542

Mg7	3.392981	1.489162	0.606143
Mg8	0.791995	2.037359	2.144407
Mg9	-3.396170	-1.490338	0.602172
Mg10	1.347526	3.453926	-0.600658
Mg11	-0.875751	2.000003	-2.143310
Mg12	3.454786	-1.347666	-0.602663
Mg13	-2.042474	0.796128	2.141113
Mg14	-3.453297	1.347132	-0.605421
Mg15	-1.490011	3.394188	0.599654
Mg16	1.489227	-3.394802	0.602131
Mg17	0.000074	-0.000376	0.000321

@mg17-isomer02 bp86/6-31G(d) Etot=-3401.572397 Eb=-14.31

Mg1	-0.044754	-0.017622	-0.016256
Mg2	-0.187086	2.253470	2.022737
Mg3	-2.928908	-1.397114	-1.356588
Mg4	2.464343	-0.524287	1.937198
Mg5	-0.274606	-0.684811	-2.785667
Mg6	2.079128	1.235113	-2.012378
Mg7	-2.366692	1.586581	-1.826411
Mg8	-2.211138	-2.806751	1.200134
Mg9	2.584420	2.423075	0.788421
Mg10	2.222379	-1.925439	-1.239709
Mg11	4.308717	0.101031	-0.290104
Mg12	-0.566409	-3.423625	-1.286850
Mg13	0.896813	-3.140149	1.326369
Mg14	-2.578790	3.380490	0.526610
Mg15	-2.967211	0.399870	1.226880
Mg16	-0.535712	-0.792477	2.745235
Mg17	0.105507	3.332645	-0.959619

@mg17-isomer03 bp86/6-31G(d) Etot=-3401.570567 Eb=-14.24

Mg1	-0.338321	-1.568412	2.337863
Mg2	2.220430	-2.647778	0.821798
Mg3	0.230909	0.022563	-0.107385
Mg4	-2.694191	-2.968597	1.191853
Mg5	-2.631899	1.620206	-1.539346
Mg6	-0.671305	-0.295444	-2.855692
Mg7	-0.176959	1.772185	2.251572
Mg8	-0.061758	3.345608	-0.867141
Mg9	2.491481	2.461530	0.647575
Mg10	2.040964	1.414139	-2.152052
Mg11	-2.419247	3.283918	0.977440
Mg12	2.389782	-0.047130	2.390625
Mg13	2.001617	-1.747883	-2.029336
Mg14	3.900377	-0.201512	-0.216538
Mg15	-3.050583	-1.430911	-1.376047
Mg16	-0.444052	-3.203912	-0.776494
Mg17	-2.787245	0.191430	1.301305

@mg17-isomer04 bp86/6-31G(d) Etot=-3401.566267 Eb=-14.08

Mg1	-0.145961	0.072734	-0.717228
Mg2	2.525445	-1.769569	0.373559
Mg3	-1.557191	-2.247677	-2.081945
Mg4	1.225426	0.485815	2.060696
Mg5	0.548413	2.826059	-1.952097
Mg6	2.352756	3.006763	0.467947
Mg7	-1.721619	-0.108887	1.954415
Mg8	-2.461432	2.596663	-1.520892
Mg9	0.294890	-2.483209	2.279226
Mg10	4.148478	0.708615	1.184626
Mg11	-0.662620	2.825107	1.083626
Mg12	-3.341042	-0.264505	-0.690602
Mg13	0.399812	-3.933502	-0.374155

Mg14	1.436305	-1.768719	-2.422992
Mg15	-3.668409	2.173079	1.191304
Mg16	2.901390	0.774808	-1.603707
Mg17	-2.274643	-2.893574	0.768219

@mg17-isomer05 bp86/6-31G(d) Etot=-3401.561595 Eb=-13.91

Mg1	0.923258	-0.400499	-2.507065
Mg2	0.629412	-2.225751	1.484602
Mg3	2.212639	-2.929534	-1.047374
Mg4	3.613457	-1.907572	1.458607
Mg5	0.912522	3.705400	0.996827
Mg6	-2.223658	0.430470	-2.134625
Mg7	-0.157389	0.559528	-0.019126
Mg8	3.627549	-0.133492	-0.965377
Mg9	-3.353933	0.285943	0.828616
Mg10	2.057736	2.414493	-1.443560
Mg11	2.316501	0.920519	1.709243
Mg12	-1.902165	2.925360	1.328960
Mg13	-3.778157	-2.024136	-1.078040
Mg14	-0.856384	3.316902	-1.576736
Mg15	-0.826020	-2.585081	-1.264820
Mg16	-2.327131	-2.557963	1.513317
Mg17	-0.868240	0.205412	2.716552

@mg17-isomer06 bp86/6-31G(d) Etot=-3401.560659 Eb=-13.87

Mg1	-1.522362	0.639789	1.916140
Mg2	-3.798658	-0.030517	-0.000050
Mg3	-1.522231	0.639949	-1.916048
Mg4	1.522368	0.639772	-1.916130
Mg5	3.798662	-0.030543	0.000064
Mg6	1.522236	0.639947	1.916046
Mg7	-2.743192	-2.414017	-1.537942
Mg8	0.000061	-2.092288	-2.827080
Mg9	2.743211	-2.414264	-1.537701
Mg10	2.743166	-2.414042	1.537941
Mg11	-0.000072	-2.092263	2.827086
Mg12	-2.743222	-2.414246	1.537705
Mg13	-0.000011	-1.322207	-0.000001
Mg14	2.491040	2.797679	-0.000148
Mg15	0.000088	3.534787	1.531017
Mg16	-2.491019	2.797693	0.000141
Mg17	-0.000064	3.534769	-1.531040

@mg17-isomer07 bp86/6-31G(d) Etot=-3401.559621 Eb=-13.83

Mg1	-0.296557	-0.250450	1.859728
Mg2	-0.260089	1.180588	-0.892584
Mg3	-0.486662	-1.994068	-0.999409
Mg4	1.677390	-0.383020	-2.584452
Mg5	-3.337147	-0.006760	1.844274
Mg6	-1.586205	2.548250	1.490205
Mg7	2.643157	-3.040629	-1.484353
Mg8	1.846137	1.941026	1.407939
Mg9	-1.967028	-0.180542	-3.007523
Mg10	3.340107	-0.379033	-0.064586
Mg11	1.428910	-2.715051	1.222484
Mg12	-1.945717	-2.763301	1.546612
Mg13	2.626816	2.352248	-1.518293
Mg14	-3.361294	1.470756	-0.834231
Mg15	0.508251	4.305051	-0.119676
Mg16	2.732418	-0.486065	2.926143
Mg17	-3.562487	-1.599000	-0.792279

@mg17-isomer08 bp86/6-31G(d) Etot=-3401.558788 Eb=-13.80

Mg1	-0.773030	2.952805	1.790880
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Mg2	-0.916233	2.424925	-1.319168
Mg3	2.248644	2.045817	1.465259
Mg4	2.390647	2.346119	-1.709738
Mg5	0.713841	-0.163035	-2.209710
Mg6	-0.532192	-2.789890	-0.916238
Mg7	2.345562	-2.780426	-2.203674
Mg8	-2.284571	-0.373609	-1.818023
Mg9	-3.180899	1.389109	0.813177
Mg10	-0.231890	0.032284	0.776070
Mg11	3.110346	-0.398472	-0.314805
Mg12	-4.975674	-0.440100	-0.775967
Mg13	2.086522	-0.818588	2.510095
Mg14	1.101657	4.432095	-0.024791
Mg15	-0.376081	-2.753254	2.176333
Mg16	-2.986415	-1.791507	1.031447
Mg17	2.259767	-3.314273	0.728852

@mg17-isomer09 bp86/6-31G(d) Etot=-3401.557482 Eb=-13.75

Mg1	-2.794921	0.807203	2.483449
Mg2	-2.082156	-2.001555	1.270075
Mg3	0.248532	0.155955	3.036931
Mg4	3.275960	-0.414769	2.581772
Mg5	-0.577591	0.453968	0.218864
Mg6	1.703789	-2.677271	-1.870632
Mg7	-2.030756	1.308669	-2.365298
Mg8	-2.724761	2.878081	0.236895
Mg9	3.404593	-0.447275	-0.499954
Mg10	-0.650379	-4.178586	-0.426314
Mg11	3.106329	2.399850	-1.615872
Mg12	-3.788092	0.008726	-0.266123
Mg13	-1.783831	-1.684964	-1.867805
Mg14	1.207201	-2.050729	1.016627
Mg15	2.303712	2.038328	1.230678
Mg16	0.207177	3.164415	-0.853470
Mg17	0.975195	0.239953	-2.309823

@mg17-isomer10 bp86/6-31G(d) Etot=-3401.554738 Eb=-13.65

Mg1	1.954207	1.098367	2.116054
Mg2	-1.952924	1.096138	-2.116885
Mg3	-2.437209	-1.971084	1.517656
Mg4	2.437727	-1.972955	-1.515477
Mg5	0.000002	-0.271957	0.000534
Mg6	-1.954477	1.098351	2.115955
Mg7	1.953157	1.096167	-2.116781
Mg8	2.436984	-1.971104	1.517751
Mg9	-2.437430	-1.973035	-1.515586
Mg10	3.860996	0.213067	-0.000251
Mg11	-3.860998	0.213028	-0.000631
Mg12	0.000214	-1.035708	-3.010203
Mg13	-0.000205	-1.031107	3.012003
Mg14	-0.000021	2.848928	-0.000999
Mg15	0.000029	-3.578398	0.000585
Mg16	2.996130	3.070672	-0.001737
Mg17	-2.996182	3.070628	-0.001988

@mg17-isomer11 bp86/6-31G(d) Etot=-3401.553766 Eb=-13.62

Mg1	0.800675	4.463441	0.202108
Mg2	-1.907164	3.148550	0.225201
Mg3	-2.872387	0.987746	-1.605965
Mg4	-3.822606	0.758854	1.346646
Mg5	-3.577780	-1.806154	-0.453783
Mg6	0.223216	0.722799	-1.321274
Mg7	-1.740894	-1.433465	-2.853238
Mg8	-0.867835	0.693894	1.557642

Mg9	-0.539301	-2.122890	-0.095339
Mg10	-2.438477	-1.810523	2.385145
Mg11	1.405894	-2.109805	-2.583075
Mg12	2.695964	2.701492	-1.415905
Mg13	3.225306	-0.254440	-1.107649
Mg14	1.003827	-1.469320	2.469876
Mg15	2.090525	1.434746	1.251127
Mg16	2.476567	-2.985714	0.097650
Mg17	3.844469	-0.919212	1.900834

@mg17-isomer12 bp86/6-31G(d) Etot=-3401.552315 Eb=-13.56

Mg1	-2.306819	0.227149	-3.252603
Mg2	-2.770382	-1.709500	-1.007442
Mg3	2.202998	-3.025067	-0.300974
Mg4	2.119346	-1.391383	2.440013
Mg5	0.248957	-0.906086	-1.648567
Mg6	-0.729506	2.191447	-1.425025
Mg7	-0.487184	-2.447319	1.002439
Mg8	-1.874499	2.907744	1.382825
Mg9	-2.672703	-0.017382	1.919014
Mg10	2.895939	1.604849	1.921336
Mg11	3.969075	-0.613408	0.167456
Mg12	-3.539708	1.294875	-0.673462
Mg13	3.094737	-1.121763	-2.661842
Mg14	-3.529478	-2.892014	1.615445
Mg15	0.921283	3.854685	0.605216
Mg16	0.177996	0.541214	1.076002
Mg17	2.279948	1.501960	-1.159833

@mg17-isomer13 bp86/6-31G(d) Etot=-3401.549641 Eb=-13.47

Mg1	0.830299	1.976420	-1.757431
Mg2	2.011357	1.988445	1.230974
Mg3	1.711049	-0.747825	-2.849760
Mg4	-0.073566	4.141611	0.235999
Mg5	3.552092	0.805227	-1.098905
Mg6	-2.303329	2.329383	-0.914796
Mg7	-0.889899	1.369744	1.743707
Mg8	2.832180	-2.080842	-0.197130
Mg9	-1.683338	-0.037029	-2.857614
Mg10	4.017032	-0.186605	1.830469
Mg11	-0.089799	-0.606768	-0.372325
Mg12	1.221504	-1.054363	2.277370
Mg13	-3.695124	0.771799	2.239766
Mg14	-3.495186	-0.374529	-0.519545
Mg15	0.273542	-3.570938	0.540698
Mg16	-2.075092	-1.820284	1.766341
Mg17	-2.143722	-2.903445	-1.297817

@mg17-isomer14 bp86/6-31G(d) Etot=-3401.548790 Eb=-13.43

Mg1	1.457121	0.360014	2.266863
Mg2	-2.825656	-2.463407	0.994553
Mg3	2.744254	2.651380	0.561996
Mg4	0.151206	-1.931621	0.417061
Mg5	0.387554	1.082764	-0.615579
Mg6	-1.487476	0.440077	1.635833
Mg7	4.051905	-0.111888	0.896969
Mg8	-2.146432	-2.245254	-1.972822
Mg9	-1.833346	0.734219	-2.798708
Mg10	-2.217084	2.769258	-0.423643
Mg11	3.064895	0.596994	-1.905589
Mg12	0.255050	4.472569	0.332364
Mg13	-3.662448	0.061041	-0.570990
Mg14	0.743677	-1.276632	-2.572848
Mg15	-4.309215	-0.214066	2.502543

Mg16	2.985137	-2.402259	-0.900651
Mg17	2.640860	-2.523188	2.152646

@mg17-isomer15 bp86/6-31G(d) Etot=-3401.545950 Eb=-13.33

Mg1	1.536324	1.028219	1.634560
Mg2	0.142585	2.007711	-1.514484
Mg3	-1.112170	0.047761	0.457116
Mg4	1.706234	3.821471	0.486227
Mg5	0.462955	-2.043071	1.876060
Mg6	3.262359	-1.345539	0.824183
Mg7	-2.864904	-1.902305	1.876263
Mg8	3.166725	1.338297	-0.922332
Mg9	6.009436	0.000952	-0.192055
Mg10	-1.206363	2.889382	1.244749
Mg11	-3.813197	1.074255	1.509048
Mg12	-4.027489	-0.956037	-0.864359
Mg13	1.622745	-3.824929	-0.337904
Mg14	1.216916	-0.964053	-1.418409
Mg15	-1.379961	-2.783555	-0.753724
Mg16	-1.667577	-0.359448	-2.626210
Mg17	-3.054619	1.970890	-1.278730

@mg17-isomer16 bp86/6-31G(d) Etot=-3401.541588 Eb=-13.17

Mg1	-0.180849	-0.941287	-2.482609
Mg2	2.717706	-1.425706	-1.374505
Mg3	3.613103	1.067839	0.261068
Mg4	-0.701243	1.152110	-0.413543
Mg5	3.098899	-1.753910	1.573317
Mg6	1.503829	3.300959	0.334306
Mg7	-2.371354	-2.762633	-1.315828
Mg8	-4.273472	-0.981047	0.404065
Mg9	-3.119493	0.206019	-2.148486
Mg10	-1.396026	4.263622	0.602464
Mg11	5.781243	-1.192740	0.070556
Mg12	-3.558573	1.953715	0.349043
Mg13	1.110405	0.664350	2.017817
Mg14	0.168441	-1.879899	0.468359
Mg15	-1.838584	-0.081310	2.134573
Mg16	-2.392146	-3.114831	1.715496
Mg17	1.838115	1.524748	-2.196092

@mg17-isomer17 bp86/6-31G(d) Etot=-3401.540947 Eb=-13.14

Mg1	-1.935261	2.662904	-1.008200
Mg2	-0.661514	-1.998518	-2.290635
Mg3	-3.028389	-3.168560	-0.770538
Mg4	-3.933977	-1.187834	1.550757
Mg5	3.123122	1.215523	0.164177
Mg6	1.174747	0.027334	2.288860
Mg7	1.289884	2.719151	-1.878606
Mg8	5.214590	-0.980938	-0.495822
Mg9	2.089090	-1.825691	0.009812
Mg10	2.244963	-0.153580	-2.546628
Mg11	-4.498485	1.633480	0.506841
Mg12	-1.016491	-1.955211	1.167968
Mg13	-3.067013	-0.225494	-1.407828
Mg14	4.120670	-1.013808	2.293702
Mg15	0.758258	2.892530	1.143046
Mg16	-1.825953	1.001252	1.858025
Mg17	-0.048239	0.357461	-0.584932

@mg17-isomer18 bp86/6-31G(d) Etot=-3401.540629 Eb=-13.13

Mg1	-2.564977	-1.275420	2.041585
Mg2	-4.081521	1.035909	0.643950
Mg3	-1.495056	1.781690	2.064016

Mg4	0.941260	-2.164539	1.964741
Mg5	-3.483368	-1.514466	-0.880363
Mg6	1.548783	1.032306	1.862183
Mg7	-0.534813	-0.256364	0.087875
Mg8	-1.278767	-3.569676	0.250357
Mg9	-2.535293	3.597701	-0.207883
Mg10	-2.402588	1.165072	-2.009828
Mg11	3.445795	-0.927211	0.556555
Mg12	0.305919	2.597940	-0.751568
Mg13	6.179388	0.728840	0.100162
Mg14	1.543154	-2.874566	-0.947439
Mg15	-0.808250	-1.481126	-2.511233
Mg16	1.843229	0.023086	-1.910376
Mg17	3.377104	2.100824	-0.352736

@mg17-isomer19 bp86/6-31G(d) Etot=-3401.539847 Eb=-13.10

Mg1	-2.087151	0.102017	-1.360425
Mg2	-3.255278	-1.833218	1.254111
Mg3	-0.051436	2.071658	1.117800
Mg4	-4.944598	0.451531	0.117682
Mg5	-0.295609	-0.904280	1.710591
Mg6	-0.982784	-2.611872	-0.813707
Mg7	-4.201139	-2.136097	-1.512546
Mg8	1.994376	-2.605816	0.225542
Mg9	1.019837	-0.197690	-1.220183
Mg10	3.954585	-1.115219	-1.744528
Mg11	5.106348	1.210202	0.062264
Mg12	-2.913087	2.716303	-0.190514
Mg13	-0.337347	2.408310	-1.977650
Mg14	4.737992	-1.616797	1.060987
Mg15	2.494403	2.441342	-0.723686
Mg16	-2.694315	1.024411	2.260625
Mg17	2.455203	0.595213	1.733638

@mg17-isomer20 bp86/6-31G(d) Etot=-3401.539602 Eb=-13.09

Mg1	1.485574	1.215900	-1.600271
Mg2	1.946354	-1.428114	1.500460
Mg3	3.881837	0.418840	0.068308
Mg4	-0.672781	0.066190	0.358147
Mg5	1.562132	1.783407	1.450586
Mg6	-1.486641	1.582591	-2.344140
Mg7	0.370384	-3.617659	-0.123718
Mg8	-1.606386	2.344620	2.183649
Mg9	7.012427	0.684541	0.255560
Mg10	-0.539275	-1.441411	-2.207564
Mg11	-3.388858	2.474768	-0.191690
Mg12	-3.514509	-0.370926	-1.365737
Mg13	2.418333	-1.779310	-1.520150
Mg14	-3.403089	-0.212946	1.648549
Mg15	-0.361976	3.564657	-0.317440
Mg16	-2.763094	-3.000432	-0.026809
Mg17	-0.940432	-2.284716	2.232258

@mg17-isomer21 bp86/6-31G(d) Etot=-3401.539266 Eb=-13.08

Mg1	-4.885036	0.693391	0.659154
Mg2	-2.757317	3.047916	0.183882
Mg3	3.311372	1.744053	1.477159
Mg4	0.978537	-0.149710	2.403482
Mg5	3.536387	-1.389411	1.242008
Mg6	-1.481270	-4.553237	0.132513
Mg7	-1.066368	-2.275579	-1.965247
Mg8	0.416241	2.657944	0.991494
Mg9	-0.028890	0.037366	-0.406212
Mg10	-2.857482	0.435455	-1.641619

Mg11	2.229072	1.856299	-1.542363
Mg12	-1.945628	0.718820	1.948498
Mg13	-2.861244	-1.819240	0.498867
Mg14	2.304431	-1.317026	-1.792724
Mg15	-0.699010	2.746404	-1.938674
Mg16	4.840373	0.362483	-0.838564
Mg17	0.965831	-2.795927	0.588346

@mg17-isomer22 bp86/6-31G(d) Etot=-3401.537401 Eb=-13.01

Mg1	-1.570035	-1.899636	2.080496
Mg2	-0.071415	0.911834	2.245930
Mg3	1.607312	-1.668371	1.592008
Mg4	2.901987	1.076354	1.177076
Mg5	1.239490	3.704607	1.632128
Mg6	4.591953	-1.437080	0.428451
Mg7	-3.084324	0.661814	1.298546
Mg8	-0.514893	-3.561525	-0.310845
Mg9	-0.160730	-0.500052	-0.536472
Mg10	-3.258067	-1.950404	-0.374325
Mg11	-1.011460	2.573612	-0.129542
Mg12	2.428270	-3.084719	-1.145555
Mg13	2.241424	2.861029	-1.156259
Mg14	2.864057	-0.076195	-1.796128
Mg15	-2.751568	0.713527	-1.820577
Mg16	-5.715346	0.361016	-0.370791
Mg17	0.263346	1.314191	-2.814142

@mg17-isomer23 bp86/6-31G(d) Etot=-3401.537228 Eb=-13.01

Mg1	0.011564	0.067144	-2.193513
Mg2	3.023812	-0.258666	-1.463597
Mg3	1.890750	2.587540	-1.583768
Mg4	2.558634	-0.814295	1.549591
Mg5	1.112434	2.152614	1.584886
Mg6	5.697266	-0.778836	0.447947
Mg7	-0.445639	-0.361081	0.935281
Mg8	-4.063260	2.653986	0.039433
Mg9	-2.126076	-2.082758	-1.232246
Mg10	-3.082463	0.699727	-2.072090
Mg11	3.929107	1.826709	0.591879
Mg12	-0.982612	2.508627	-0.624195
Mg13	-2.271161	-2.721831	1.765418
Mg14	-1.957464	1.980873	2.205690
Mg15	1.231153	-2.530472	-0.668991
Mg16	-3.742622	-0.204078	0.841404
Mg17	-0.783421	-4.725204	-0.123129

@mg17-isomer24 bp86/6-31G(d) Etot=-3401.534829 Eb=-12.92

Mg1	2.283001	1.032485	1.478578
Mg2	-0.390623	-0.626573	-0.971935
Mg3	-2.645405	-1.410890	1.314483
Mg4	0.442020	2.325237	-0.978699
Mg5	-0.740288	1.019518	1.720341
Mg6	5.548172	0.695898	0.168936
Mg7	0.700559	-1.786772	1.767023
Mg8	3.633887	-1.693930	0.873375
Mg9	-2.416540	3.058042	0.013903
Mg10	-4.427581	0.480245	-0.393491
Mg11	-2.186264	1.288203	-2.403178
Mg12	3.534847	2.823555	-0.544321
Mg13	1.719782	-2.963012	-1.102244
Mg14	-0.992389	-3.770868	-0.036295
Mg15	-3.628968	1.302013	2.339413
Mg16	2.617420	-0.007370	-1.502049
Mg17	-3.051629	-1.765781	-1.743839

@mg17-isomer25 bp86/6-31G(d) Etot=-3401.532875 Eb=-12.85

Mg1	2.284279	2.044007	1.752849
Mg2	0.439539	-0.059256	2.895363
Mg3	-2.278932	-0.035567	-1.989004
Mg4	-2.841907	-0.675823	3.131663
Mg5	5.671730	-1.285170	-0.136019
Mg6	-1.811943	1.391758	1.111195
Mg7	3.796732	0.864351	-1.261422
Mg8	1.938977	3.253549	-0.966367
Mg9	3.029281	-1.002892	1.682766
Mg10	-1.260950	-1.793461	0.841951
Mg11	-1.021983	2.656965	-1.575415
Mg12	-0.109626	-2.229249	-2.023608
Mg13	0.805585	0.310491	-0.419718
Mg14	-4.130100	2.089333	-0.946685
Mg15	-3.102258	-2.841688	-1.380602
Mg16	-4.255798	-0.568586	0.442443
Mg17	2.847375	-2.118762	-1.159390

@mg17-isomer26 bp86/6-31G(d) Etot=-3401.532148 Eb=-12.82

Mg1	0.981566	-1.502319	-0.669773
Mg2	-1.743400	-3.136267	-0.335164
Mg3	3.534305	-0.667387	-2.045056
Mg4	0.388112	1.676999	1.614202
Mg5	-4.215032	-1.834783	-1.711798
Mg6	-0.683384	-1.164722	1.823360
Mg7	5.347260	-0.346393	0.446686
Mg8	3.763375	-2.816270	0.180422
Mg9	2.900868	1.650081	0.011857
Mg10	-1.811139	2.845377	-0.488534
Mg11	-3.869389	-1.528586	1.223497
Mg12	0.943177	3.978275	-0.429826
Mg13	2.399488	-0.508886	2.042831
Mg14	0.844368	1.272655	-2.046803
Mg15	-1.630701	-0.146287	-1.117842
Mg16	-2.650874	1.227982	1.958267
Mg17	-4.498598	1.000533	-0.456329

@mg17-isomer27 bp86/6-31G(d) Etot=-3401.531506 Eb=-12.80

Mg1	-0.119318	1.081147	0.043726
Mg2	-2.377984	3.226800	0.936504
Mg3	2.776763	1.903351	0.250068
Mg4	-1.977126	0.534779	2.412187
Mg5	4.003391	-0.779503	1.277391
Mg6	-0.718075	-0.475277	-2.370803
Mg7	-0.949855	-1.843567	0.896650
Mg8	-4.196259	-1.686407	1.202300
Mg9	-3.201958	0.459642	-0.685404
Mg10	0.303790	-3.286030	-1.524511
Mg11	-1.607910	2.751789	-2.036524
Mg12	1.916347	-3.021232	1.123295
Mg13	1.201039	-0.173354	2.378386
Mg14	2.128852	-0.820648	-1.145966
Mg15	0.492904	4.136847	-0.122817
Mg16	5.231365	0.527260	-1.202264
Mg17	-2.905967	-2.535597	-1.432216

@mg17-isomer28 bp86/6-31G(d) Etot=-3401.529931 Eb=-12.74

Mg1	-2.057334	-0.955716	1.583746
Mg2	-3.048853	1.912094	-1.474679
Mg3	-0.109668	1.394734	-2.272237
Mg4	0.381458	-0.473425	-0.003976
Mg5	-0.760665	-3.330127	-0.003340

Mg6	-3.049026	1.913175	1.477583
Mg7	2.326389	-2.940413	-0.004861
Mg8	-0.825359	3.505339	0.000452
Mg9	2.891306	-0.150167	-1.685085
Mg10	5.181421	-1.578618	0.003085
Mg11	-0.109079	1.389008	2.269884
Mg12	5.076405	1.418776	0.006275
Mg13	-2.059733	-0.955629	-1.585981
Mg14	-3.839951	-3.120813	0.004099
Mg15	2.884402	-0.153872	1.686055
Mg16	1.926314	2.302489	-0.002734
Mg17	-4.808027	-0.176835	0.001712

@mg17-isomer29 bp86/6-31G(d) Etot=-3401.528626 Eb=-12.69

Mg1	-0.392039	3.011658	0.571043
Mg2	-1.872908	0.349155	0.957110
Mg3	2.151156	2.916138	-1.142625
Mg4	0.799354	-1.125410	1.582229
Mg5	4.859970	1.186697	-0.290248
Mg6	-0.584915	1.428459	-1.919960
Mg7	-0.625995	-1.543939	-1.117682
Mg8	2.198529	-3.139421	-0.188565
Mg9	-3.266318	-2.411672	0.291187
Mg10	-0.087842	1.329219	3.185488
Mg11	-3.573333	-0.340222	-2.027912
Mg12	-0.590552	-4.069076	0.703432
Mg13	-3.322595	2.533526	-0.687827
Mg14	-5.073872	0.119987	0.429630
Mg15	2.455503	1.615926	1.572182
Mg16	2.017504	-0.096530	-1.057745
Mg17	4.908353	-1.764494	-0.859738

@mg17-isomer30 bp86/6-31G(d) Etot=-3401.525161 Eb=-12.56

Mg1	-2.169444	-0.799877	-0.875937
Mg2	-4.914812	-1.074882	0.515520
Mg3	0.725594	-0.439747	-1.459617
Mg4	0.906267	2.479734	-0.639098
Mg5	2.541904	0.521406	1.050862
Mg6	-0.276042	-0.772616	1.431017
Mg7	2.448049	-2.556380	0.222077
Mg8	-0.405988	-3.285815	-0.317849
Mg9	-3.396305	-3.677479	0.047154
Mg10	-4.101991	1.621990	-0.790779
Mg11	-2.793711	0.910761	1.765321
Mg12	-1.842240	3.439683	0.117060
Mg13	5.339128	-1.377520	0.767733
Mg14	-0.005101	2.104632	2.206345
Mg15	-1.363195	1.679284	-2.461307
Mg16	3.945959	-0.395737	-1.700200
Mg17	5.361928	1.622562	0.121698

@mg17-isomer31 bp86/6-31G(d) Etot=-3401.520313 Eb=-12.38

Mg1	0.667805	-2.337457	-0.564345
Mg2	-1.922056	-2.252261	1.062118
Mg3	0.633802	-0.751836	2.220577
Mg4	0.610601	-0.108187	-2.683066
Mg5	-2.111795	-1.746265	-1.956483
Mg6	0.917986	2.971673	-1.677365
Mg7	-3.163702	2.785123	0.765561
Mg8	-1.323146	4.693359	-0.672407
Mg9	-2.265932	0.502669	2.611205
Mg10	-0.981694	0.724224	-0.200933
Mg11	3.290880	-1.897950	1.022435
Mg12	-4.581044	-2.902856	-0.396432

Mg13	5.277170	0.319884	0.046489
Mg14	-4.091884	-0.024862	0.042977
Mg15	3.553101	0.697170	2.636864
Mg16	3.325409	-1.407091	-2.088385
Mg17	2.164498	0.734663	-0.168810

@mg17-isomer32 bp86/6-31G(d) Etot=-3401.519025 Eb=-12.34

Mg1	-0.279693	1.487616	-1.847208
Mg2	0.703798	-1.362850	-1.630441
Mg3	1.744379	-1.723870	1.148827
Mg4	4.780197	-0.216952	1.720413
Mg5	5.462897	1.687517	-0.539799
Mg6	-2.282870	-0.774773	-2.234021
Mg7	-2.623130	1.243035	0.077253
Mg8	-1.357541	-2.009423	0.497481
Mg9	2.228546	1.238341	0.088247
Mg10	6.900716	-0.915858	-0.307800
Mg11	-0.276972	0.391320	1.974196
Mg12	-5.173154	0.588325	-1.860118
Mg13	-0.131744	3.064599	0.653978
Mg14	-4.632973	-1.802434	-0.126924
Mg15	-3.167065	-0.497011	2.470695
Mg16	-5.811920	0.646230	1.065295
Mg17	3.916530	-1.043812	-1.150074

@mg17-isomer33 bp86/6-31G(d) Etot=-3401.505416 Eb=-11.83

Mg1	0.748049	0.609784	-1.388731
Mg2	2.157150	-1.586397	-3.069867
Mg3	-1.444365	2.794862	-1.985038
Mg4	2.514634	-2.183735	-0.204995
Mg5	3.859336	0.545370	-1.620580
Mg6	-3.541607	2.437198	0.294483
Mg7	-0.588075	1.975341	0.954610
Mg8	5.133047	2.350693	0.531004
Mg9	2.350089	1.039792	1.212795
Mg10	-2.901186	0.039657	2.228092
Mg11	0.005094	-1.030489	1.405442
Mg12	-2.343993	-0.296045	-0.777498
Mg13	-5.317208	0.036139	0.328233
Mg14	5.040747	-0.690811	0.934792
Mg15	2.693443	-1.902139	2.728130
Mg16	-7.985839	-1.620539	-0.173013
Mg17	-0.379314	-2.518681	-1.397859

@mg17-isomer34 bp86/6-31G(d) Etot=-3401.497030 Eb=-11.52

Mg1	-1.419566	2.830875	-0.260131
Mg2	-0.009284	0.976528	-2.269043
Mg3	-2.835037	-1.414868	1.238700
Mg4	-4.025039	1.472247	0.775691
Mg5	-2.731427	-0.002014	-1.551706
Mg6	-0.093507	-1.345661	2.397169
Mg7	-1.549350	1.416314	2.503562
Mg8	0.919376	1.047069	0.844779
Mg9	-5.398955	-1.011305	-0.286465
Mg10	-0.169741	-1.576883	-0.646037
Mg11	-8.149633	-2.228257	-1.293734
Mg12	2.875337	-1.408525	1.292164
Mg13	4.058914	1.568797	0.784697
Mg14	2.854023	-0.089338	-1.479546
Mg15	5.573260	-0.841743	-0.002775
Mg16	2.018299	3.153002	-1.157106
Mg17	8.082331	-2.546237	-0.890218

@mg17-isomer35 bp86/6-31G(d) Etot=-3401.491364 Eb=-11.31

Mg1	3.011726	1.119350	0.006721
Mg2	3.070829	-1.850686	1.596556
Mg3	4.516752	0.512662	2.666182
Mg4	1.314927	-3.712996	-0.014886
Mg5	0.223832	2.270545	0.006269
Mg6	-1.825765	0.800665	1.697809
Mg7	1.201266	0.673750	2.628876
Mg8	1.201293	0.691743	-2.627294
Mg9	3.072199	-1.838456	-1.610143
Mg10	-2.715533	3.313867	0.011546
Mg11	-1.823667	0.813668	-1.697126
Mg12	-4.513286	0.978972	-0.001091
Mg13	-7.131900	-0.673764	0.000298
Mg14	-10.104541	-2.140792	-0.002850
Mg15	4.514705	0.537750	-2.656229
Mg16	5.551607	-0.678603	-0.000739
Mg17	0.435555	-0.817676	-0.003900

@mg18-isomer01 bp86/6-31G(d) Etot=-3601.685070 Eb=-15.01

Mg1	-2.206106	2.669656	1.467582
Mg2	2.827436	1.661637	0.000107
Mg3	3.379945	0.000126	-2.419497
Mg4	-2.206139	-2.669634	-1.467672
Mg5	0.347571	-3.568204	-0.000219
Mg6	0.782617	-1.649730	-2.370990
Mg7	-2.206136	-2.669821	1.467343
Mg8	-3.402129	0.000053	-0.000045
Mg9	-0.246741	-0.000110	0.000025
Mg10	-1.883419	0.000192	-2.699147
Mg11	-1.883463	-0.000156	2.699180
Mg12	0.347665	3.568249	0.000206
Mg13	0.782598	1.649951	-2.370740
Mg14	3.379853	-0.000140	2.419544
Mg15	2.827386	-1.661635	-0.000054
Mg16	-2.206023	2.669946	-1.467405
Mg17	0.782518	1.649681	2.370936
Mg18	0.782567	-1.650060	2.370844

@mg18-isomer02 bp86/6-31G(d) Etot=-3601.683618 Eb=-14.96

Mg1	-0.084801	0.000145	0.000004
Mg2	0.891372	-1.621122	-2.377562
Mg3	2.764008	-2.328890	-0.000009
Mg4	0.891363	-1.621158	2.377554
Mg5	-2.264492	-2.595418	1.520395
Mg6	-2.264489	-2.595395	-1.520417
Mg7	0.105078	-3.607444	-0.000019
Mg8	2.763979	2.328795	0.000014
Mg9	-1.817961	0.000006	-2.762381
Mg10	3.379513	0.000018	-1.662830
Mg11	3.379497	0.000000	1.662827
Mg12	-1.817957	-0.000020	2.762377
Mg13	-3.284103	-0.000001	0.000004
Mg14	0.105087	3.607369	0.000014
Mg15	0.891440	1.621133	2.377684
Mg16	-2.264486	2.595402	1.520419
Mg17	-2.264488	2.595423	-1.520410
Mg18	0.891440	1.621155	-2.377663

@mg18-isomer03 bp86/6-31G(d) Etot=-3601.682770 Eb=-14.93

Mg1	-0.061733	-0.147694	0.252560
Mg2	1.748575	-0.089355	2.801583
Mg3	-2.308774	1.537384	1.837266
Mg4	0.901163	-2.888163	1.768461
Mg5	3.410050	1.654959	1.047919

Mg6	1.337752	2.395794	-1.216322
Mg7	-1.493609	1.053348	-2.246627
Mg8	-3.890949	2.077687	-0.747670
Mg9	0.691666	2.617998	1.884641
Mg10	-1.531180	-1.981381	-2.349358
Mg11	-1.688760	-3.490771	0.299221
Mg12	-1.290661	3.537299	-0.265962
Mg13	-1.655885	-1.351590	2.539004
Mg14	2.942263	-1.225915	0.097320
Mg15	3.853203	0.907216	-1.893577
Mg16	-3.160067	-0.801215	-0.096926
Mg17	1.257330	-0.468474	-2.484766
Mg18	0.939616	-3.337127	-1.226765

@mg18-isomer04 bp86/6-31G(d) Etot=-3601.682467 Eb=-14.92

Mg1	-0.171562	-0.000448	0.127225
Mg2	-2.771196	2.707199	-0.658160
Mg3	2.284535	-2.149802	-0.381360
Mg4	1.256236	1.531888	2.558183
Mg5	1.307274	-0.000640	-2.559451
Mg6	-1.898003	1.548497	2.235357
Mg7	-0.257704	-2.572401	-2.156998
Mg8	-3.520099	0.005663	0.246402
Mg9	-0.219365	-3.626637	0.750398
Mg10	-0.206480	3.627399	0.752843
Mg11	4.084328	-0.006623	-1.566391
Mg12	-0.248394	2.576113	-2.155639
Mg13	3.530928	-0.006938	1.462875
Mg14	-2.024428	0.004258	-2.406441
Mg15	1.248445	-1.535722	2.557992
Mg16	-2.780840	-2.697451	-0.660585
Mg17	-1.905554	-1.546260	2.234267
Mg18	2.291879	2.141904	-0.380517

@mg18-isomer05 bp86/6-31G(d) Etot=-3601.680814 Eb=-14.86

Mg1	-0.068913	0.086627	0.064009
Mg2	-2.997972	-0.753533	0.922476
Mg3	3.972272	0.169157	-1.670069
Mg4	3.395517	1.237597	1.070502
Mg5	0.383243	-3.457881	-1.182928
Mg6	-2.301999	-3.572952	0.088963
Mg7	1.731475	2.281234	-1.260227
Mg8	0.037172	-2.680376	1.809789
Mg9	0.677399	2.619224	1.735855
Mg10	2.631119	-1.808908	0.221288
Mg11	-2.483103	2.271144	1.566532
Mg12	1.315581	-0.887193	-2.492510
Mg13	-2.027119	-1.375937	-2.031689
Mg14	-1.014566	0.131672	2.985685
Mg15	-3.298894	1.418395	-1.211019
Mg16	-1.098741	3.530317	-0.714760
Mg17	1.986709	-0.537485	2.889522
Mg18	-0.839180	1.328898	-2.791418

@mg18-isomer06 bp86/6-31G(d) Etot=-3601.679725 Eb=-14.82

Mg1	-3.035310	0.854072	-1.940953
Mg2	3.459386	-0.832042	0.474111
Mg3	1.495355	-2.869841	1.298624
Mg4	3.045379	0.815281	-1.943527
Mg5	1.503540	3.115222	-1.000878
Mg6	-0.028360	-4.203756	-0.968792
Mg7	-1.681660	-1.803879	-1.865976
Mg8	-1.468193	3.139739	-1.001547
Mg9	-3.467429	-0.788091	0.476160

Mg10	0.016880	2.544286	1.742718
Mg11	0.003337	0.783934	-2.696708
Mg12	0.001561	-0.044583	0.143356
Mg13	-1.622511	-0.055838	2.730733
Mg14	-1.536016	-2.855851	1.299564
Mg15	1.657707	-1.825449	-1.867825
Mg16	1.626778	-0.071295	2.730513
Mg17	3.111712	2.029443	1.193693
Mg18	-3.082157	2.068649	1.196736

@mg18-isomer07 bp86/6-31G(d) Etot=-3601.679706 Eb=-14.82

Mg1	0.000001	-0.089703	0.000002
Mg2	1.975168	-2.136328	-1.605725
Mg3	-0.000002	-0.502832	3.327620
Mg4	0.000002	2.615215	-1.662846
Mg5	2.468951	0.852447	-2.452349
Mg6	1.975147	-2.135913	1.606270
Mg7	0.000001	2.615628	1.662190
Mg8	0.000000	-0.503705	-3.327490
Mg9	-0.000003	-3.756929	0.000470
Mg10	-2.468962	0.853074	2.452137
Mg11	-1.975170	-2.136326	-1.605726
Mg12	-1.975153	-2.135910	1.606269
Mg13	-2.568451	2.612704	-0.000333
Mg14	2.568457	2.612699	-0.000332
Mg15	3.688449	-0.234823	0.000030
Mg16	2.468962	0.853071	2.452138
Mg17	-3.688449	-0.234819	0.000029
Mg18	-2.468946	0.852450	-2.452352

@mg18-isomer08 bp86/6-31G(d) Etot=-3601.676804 Eb=-14.72

Mg1	3.525720	-0.000911	1.586668
Mg2	0.080073	-3.690993	0.450918
Mg3	-1.857849	1.575576	1.514995
Mg4	0.945363	2.222672	-2.204369
Mg5	-3.365739	0.001789	-0.772981
Mg6	-1.856322	-1.570565	1.513145
Mg7	0.084541	3.688238	0.453631
Mg8	-4.398985	0.000060	2.138998
Mg9	2.881939	-0.001371	-1.605341
Mg10	0.236077	0.001380	-0.090451
Mg11	2.885720	-2.572478	0.105852
Mg12	2.888238	2.569225	0.105766
Mg13	-2.028001	-2.608063	-1.518267
Mg14	1.107181	-1.538929	2.469331
Mg15	-1.153820	0.000763	-2.896777
Mg16	1.106189	1.534701	2.470740
Mg17	0.941614	-2.222154	-2.203557
Mg18	-2.021939	2.611060	-1.518301

@mg18-isomer09 bp86/6-31G(d) Etot=-3601.673078 Eb=-14.59

Mg1	2.083502	-0.036539	-2.784785
Mg2	-2.224068	2.167505	-1.471204
Mg3	0.906119	2.646300	-1.749528
Mg4	-1.902891	-0.614015	-2.643516
Mg5	-2.316533	-3.080110	-0.933799
Mg6	-3.263053	-0.282068	0.169565
Mg7	0.001821	0.011082	-0.326923
Mg8	0.794870	2.390460	1.589076
Mg9	0.185504	-2.857899	1.001249
Mg10	1.835789	-0.462219	2.182962
Mg11	3.132028	1.246484	-0.213912
Mg12	-2.445602	2.410901	1.619713
Mg13	-0.851409	4.394625	0.023972

Mg14	2.891779	-1.871910	-0.458483
Mg15	-2.780844	-2.703585	2.005662
Mg16	0.472657	-2.595801	-2.150615
Mg17	4.697544	-0.561296	1.628250
Mg18	-1.217214	-0.201915	2.512317

@mg18-isomer10 bp86/6-31G(d) Etot=-3601.659401 Eb=-14.11

Mg1	0.159366	-1.509601	-2.348509
Mg2	0.932698	1.603253	-2.674388
Mg3	0.934047	1.603491	2.674269
Mg4	-0.681364	3.778145	-1.447936
Mg5	2.984997	-0.156597	1.520791
Mg6	2.985672	-0.152284	-1.519019
Mg7	-2.173386	1.089226	2.220761
Mg8	0.156677	-1.507884	2.350537
Mg9	4.525663	-2.247311	-0.002930
Mg10	2.120937	2.611444	0.000131
Mg11	1.624113	-2.851702	0.002371
Mg12	-3.503713	-0.594899	-0.000803
Mg13	-0.677732	3.779297	1.447191
Mg14	-1.451628	-2.974180	0.000770
Mg15	-2.842552	-1.962963	2.534710
Mg16	-0.079564	0.371074	-0.000401
Mg17	-2.840458	-1.965569	-2.534444
Mg18	-2.173772	1.087061	-2.223099

@mg18-isomer11 bp86/6-31G(d) Etot=-3601.658836 Eb=-14.09

Mg1	-4.086348	-1.684687	-0.654226
Mg2	-1.434700	-2.927564	-0.284230
Mg3	0.999826	3.729566	-0.439980
Mg4	0.829938	1.297091	-2.440184
Mg5	-2.903283	-1.567001	2.108028
Mg6	2.692384	1.234138	-0.054666
Mg7	2.087799	-0.476018	2.427844
Mg8	-0.171444	-2.538088	2.563498
Mg9	3.034647	-0.937726	-2.218542
Mg10	0.201227	-2.026785	-2.655267
Mg11	-2.021454	-0.069612	-2.154775
Mg12	1.272516	2.463498	2.396919
Mg13	-1.645575	2.918317	-1.522718
Mg14	-3.107701	1.087021	0.554655
Mg15	-1.342150	3.474203	1.422708
Mg16	4.230807	-1.483039	0.485683
Mg17	1.543675	-2.643402	0.022796
Mg18	-0.180165	0.150089	0.442456

@mg18-isomer12 bp86/6-31G(d) Etot=-3601.647065 Eb=-13.68

Mg1	-0.696011	-0.077579	0.748433
Mg2	1.923768	2.029528	0.092327
Mg3	-2.562902	2.086405	1.787632
Mg4	3.968126	-0.240578	-0.389058
Mg5	2.307212	-2.718003	0.063852
Mg6	-0.520619	3.956007	0.393723
Mg7	0.362499	1.936071	2.647919
Mg8	-3.847711	-0.097337	0.152648
Mg9	-2.816668	2.610247	-1.169434
Mg10	-1.756617	-0.101548	-2.159869
Mg11	-0.569637	-2.887163	-1.043986
Mg12	1.214731	-0.360083	-1.725871
Mg13	-3.569069	-2.571768	-1.677418
Mg14	0.007856	2.479107	-2.196395
Mg15	0.098193	-2.743475	2.130493
Mg16	2.219308	-0.426047	2.113164
Mg17	7.043657	-0.049054	-0.979754

Mg18	-2.806118	-2.824728	1.211594
@mg18-isomer13 bp86/6-31G(d) Etot=-3601.646592 Eb=-13.67			
Mg1	-1.364573	-0.719837	-2.634905
Mg2	-3.722288	-1.893586	-1.138725
Mg3	-3.492458	1.272652	-1.631154
Mg4	-0.784044	-2.948763	-0.584266
Mg5	-4.501294	0.256716	1.004186
Mg6	-0.347549	2.020941	-1.472175
Mg7	1.442823	-0.548547	-1.083783
Mg8	2.281513	-3.179947	0.296326
Mg9	-1.438101	-0.089222	0.422484
Mg10	-2.876000	-2.336982	1.752906
Mg11	4.807444	-1.864955	-0.716832
Mg12	2.571345	2.357945	-0.501953
Mg13	-2.381159	2.659194	1.001068
Mg14	5.282670	1.052838	-0.591696
Mg15	0.289798	4.297520	0.538793
Mg16	0.404681	-1.680315	2.088589
Mg17	0.674010	1.603222	1.795147
Mg18	3.153184	-0.258874	1.455989
@mg18-isomer14 bp86/6-31G(d) Etot=-3601.641979 Eb=-13.51			
Mg1	-0.779311	-3.182791	-0.200398
Mg2	1.350695	-1.681800	1.554335
Mg3	0.571785	-0.586900	-1.246452
Mg4	-3.572179	-2.886958	0.720849
Mg5	0.979330	1.434276	1.114194
Mg6	1.841982	2.094220	-1.810477
Mg7	4.337840	-1.579329	0.614554
Mg8	3.539455	-0.544097	-2.176955
Mg9	3.278912	0.324110	2.786129
Mg10	-1.933046	2.747055	1.511015
Mg11	2.253385	-3.080119	-0.995984
Mg12	-5.681220	-0.864864	0.116180
Mg13	-4.337285	1.703999	-0.090130
Mg14	-1.675147	-0.369079	1.219973
Mg15	-1.482670	1.836432	-1.362219
Mg16	0.083473	4.243682	-0.311276
Mg17	4.051674	1.432293	0.084696
Mg18	-2.827675	-1.040128	-1.528033
@mg18-isomer15 bp86/6-31G(d) Etot=-3601.639848 Eb=-13.43			
Mg1	-1.870680	-0.912271	1.416347
Mg2	-3.309169	2.135642	-1.151759
Mg3	-0.541388	1.668555	-2.366038
Mg4	0.416279	-0.574906	-0.670957
Mg5	-4.876878	-0.012190	0.375093
Mg6	-1.115783	-3.368635	-0.381644
Mg7	1.545535	-1.512574	2.009862
Mg8	4.920447	1.224910	-0.520619
Mg9	4.350172	-1.536839	0.551067
Mg10	1.995492	2.157353	-0.678995
Mg11	1.984359	-3.114042	-0.570164
Mg12	-2.741056	2.050404	1.773885
Mg13	-4.072909	-2.885419	0.218315
Mg14	0.265934	1.338888	1.840494
Mg15	-2.522914	-0.831235	-1.638867
Mg16	3.268944	1.113378	1.980688
Mg17	3.059393	-0.617771	-2.153417
Mg18	-0.755780	3.676751	-0.033293
@mg18-isomer16 bp86/6-31G(d) Etot=-3601.639772 Eb=-13.43			
Mg1	-1.209532	4.047203	0.561234

Mg2	-0.157853	-3.027128	-1.121783
Mg3	0.866694	-0.035855	-0.860705
Mg4	-0.692674	-1.322214	1.489340
Mg5	2.819441	-2.073001	-1.953142
Mg6	3.625873	0.988111	-1.899813
Mg7	-2.818852	-3.356016	0.370513
Mg8	1.238013	2.962111	-1.078744
Mg9	3.442658	1.895136	0.888664
Mg10	4.550274	-0.860731	0.339153
Mg11	-5.119474	-1.396343	0.397724
Mg12	2.399541	-0.425123	2.595796
Mg13	0.409777	1.698063	1.662584
Mg14	-1.694553	2.038609	-1.580640
Mg15	-2.390168	-0.871260	-1.199734
Mg16	2.143970	-2.765035	0.847600
Mg17	-4.788568	1.337325	-0.756546
Mg18	-2.624565	1.166148	1.298499

@mg18-isomer17 bp86/6-31G(d) Etot=-3601.638001 Eb=-13.37

Mg1	-1.075336	-2.626418	-1.484147
Mg2	1.571824	1.704222	2.579487
Mg3	0.254972	0.018883	-2.419978
Mg4	3.722688	0.338446	0.946479
Mg5	-0.432117	-3.034343	1.523201
Mg6	-2.629628	-4.603949	0.110838
Mg7	-2.892399	-0.225258	-2.023785
Mg8	-3.333981	-1.752334	0.694181
Mg9	1.794643	-1.271014	2.630552
Mg10	1.508277	2.154153	-0.482658
Mg11	3.361611	0.253882	-2.087345
Mg12	-0.585581	0.010857	0.735397
Mg13	1.810640	-1.846752	-0.415053
Mg14	-0.923027	3.048926	1.428382
Mg15	-1.474717	2.436306	-1.525965
Mg16	-3.598341	1.260685	0.666296
Mg17	6.323241	-0.014520	-0.869332
Mg18	-3.402769	4.148226	-0.006547

@mg18-isomer18 bp86/6-31G(d) Etot=-3601.634101 Eb=-13.23

Mg1	2.195888	3.124835	1.276219
Mg2	1.794971	-1.640339	-2.463684
Mg3	0.788219	4.166386	-1.237216
Mg4	-0.642831	-2.184331	1.539280
Mg5	1.899027	1.228748	-1.360852
Mg6	-5.578209	-0.513200	1.029435
Mg7	4.563898	-1.079507	-1.248100
Mg8	0.537919	0.579495	1.444544
Mg9	-0.413233	-3.484204	-1.317192
Mg10	-2.508667	0.626725	1.156018
Mg11	2.257183	-2.723706	0.235662
Mg12	3.510446	0.260885	1.176130
Mg13	1.973547	-1.699810	2.995534
Mg14	-1.657714	2.424782	-1.577387
Mg15	-0.713059	-0.450345	-1.253637
Mg16	-3.897171	0.230226	-1.575550
Mg17	-3.176741	-2.311865	-0.029818
Mg18	-0.933475	3.445225	1.210615

@mg18-isomer19 bp86/6-31G(d) Etot=-3601.631658 Eb=-13.15

Mg1	0.532443	-1.913976	1.314941
Mg2	0.956283	2.580909	-1.444731
Mg3	-1.952209	-3.769311	1.898730
Mg4	-4.966307	0.604348	-0.190453
Mg5	-2.444211	-0.852564	0.916910

Mg6	-1.153354	4.142353	0.263737
Mg7	-3.088833	-0.994493	-2.217999
Mg8	3.447060	-1.341195	0.755179
Mg9	5.643691	0.414578	-0.484868
Mg10	-0.106593	-0.382146	-1.578652
Mg11	2.082348	0.198809	3.000401
Mg12	1.806763	-2.707642	-1.436149
Mg13	-2.231769	1.785434	-1.298814
Mg14	-1.344730	-3.334453	-1.056704
Mg15	-3.020003	2.153067	1.711006
Mg16	3.040519	1.953960	0.653030
Mg17	2.858727	0.235063	-1.965913
Mg18	-0.059826	1.227260	1.160351

@mg18-isomer20 bp86/6-31G(d) Etot=-3601.631164 Eb=-13.13

Mg1	-2.223437	1.699881	0.404753
Mg2	-3.954007	0.170885	2.418607
Mg3	-2.872593	0.323117	-2.232067
Mg4	4.147380	1.401431	0.805469
Mg5	0.016380	1.109925	-1.827775
Mg6	2.483489	2.923902	-1.367976
Mg7	-0.623946	-3.981207	-0.006616
Mg8	-0.590781	3.986341	-0.821255
Mg9	-0.956911	-0.063904	2.596026
Mg10	2.500859	-0.108306	2.900286
Mg11	-2.536866	-1.551514	0.301635
Mg12	0.793584	-1.122793	0.443954
Mg13	-5.443390	0.047763	-0.222463
Mg14	-0.764224	-1.860864	-2.217189
Mg15	2.862278	-0.107967	-1.688344
Mg16	3.978671	-1.680194	0.775787
Mg17	2.185594	-3.079011	-1.351068
Mg18	0.997920	1.892515	1.088236

@mg18-isomer21 bp86/6-31G(d) Etot=-3601.630070 Eb=-13.09

Mg1	-0.351041	0.253949	-0.842587
Mg2	2.050799	1.369924	-2.064232
Mg3	-3.267379	1.307683	-0.500367
Mg4	1.387000	-1.654072	-2.236890
Mg5	-1.780232	0.257356	2.032350
Mg6	3.301854	-1.074048	2.033977
Mg7	3.876308	-0.734443	-0.846300
Mg8	1.145083	1.116942	1.767848
Mg9	2.639893	-3.423509	0.180473
Mg10	1.617278	3.658133	-0.118647
Mg11	3.956940	1.809846	0.844531
Mg12	-5.925274	-0.329829	-0.900056
Mg13	-4.471379	-1.031969	1.617053
Mg14	-2.431267	-1.950656	-0.449888
Mg15	-0.711176	3.041145	-1.904324
Mg16	-1.235555	3.082113	1.070874
Mg17	-0.188700	-3.897562	-1.020483
Mg18	0.386848	-1.801004	1.336668

@mg18-isomer22 bp86/6-31G(d) Etot=-3601.629585 Eb=-13.07

Mg1	0.597071	2.022666	1.864620
Mg2	2.640716	2.297667	-0.465781
Mg3	2.647637	-0.261890	1.455946
Mg4	-2.387835	0.644637	1.190729
Mg5	-1.523348	2.775307	-0.803335
Mg6	0.249260	0.265320	-0.656389
Mg7	0.665638	4.580694	0.295654
Mg8	-1.867975	-2.592108	-0.371277
Mg9	-0.216239	-1.321982	2.110786

Mg10	2.997179	-0.586312	-1.689636
Mg11	-0.118819	-2.045544	-2.620696
Mg12	-4.805192	-1.120568	-0.109546
Mg13	4.638013	-2.331689	0.310193
Mg14	-2.477003	-0.004275	-1.979868
Mg15	1.492560	-2.784078	-0.063840
Mg16	5.328559	0.715894	-0.042556
Mg17	-3.243440	-2.151714	2.248598
Mg18	-4.616781	1.897974	-0.673600

@mg18-isomer23 bp86/6-31G(d) Etot=-3601.629296 Eb=-13.06

Mg1	-1.491970	1.010796	1.685080
Mg2	-0.346419	0.878583	-1.400807
Mg3	0.291189	-1.091945	3.177700
Mg4	2.623724	1.424787	-0.501461
Mg5	-2.781294	-1.710533	2.229256
Mg6	2.665537	-1.176826	1.292896
Mg7	3.335849	-3.708641	-0.473355
Mg8	1.831080	-1.320070	-1.715130
Mg9	-0.432350	-1.946137	0.304271
Mg10	-2.691863	2.656137	-0.552278
Mg11	0.321959	3.344398	0.509110
Mg12	-4.432131	0.392839	0.615145
Mg13	-1.297095	-1.790032	-2.679432
Mg14	-3.418509	0.313631	-2.331023
Mg15	1.750904	1.505743	2.454755
Mg16	-3.478244	-2.294489	-0.675888
Mg17	4.958612	-1.027584	-0.831791
Mg18	2.591023	4.539343	-1.107049

@mg19-isomer01 bp86/6-31G(d) Etot=-3801.797339 Eb=-15.62

Mg1	-0.100383	3.710950	0.051661
Mg2	2.728553	-0.000427	2.336681
Mg3	0.428991	-1.977902	2.482297
Mg4	-2.369543	-2.625379	-1.552683
Mg5	0.495253	2.148154	-2.453582
Mg6	-2.432722	2.618135	1.494618
Mg7	4.612153	0.002499	-0.013547
Mg8	-1.915576	-0.003575	2.802412
Mg9	2.378891	2.024049	0.041095
Mg10	-0.096825	-3.710379	0.047153
Mg11	2.617495	0.002407	-2.289090
Mg12	0.427770	1.974556	2.484558
Mg13	-3.117663	-0.000907	-0.072362
Mg14	-0.029685	-0.000647	-0.028241
Mg15	0.498039	-2.145216	-2.456758
Mg16	-2.372704	2.627755	-1.550033
Mg17	-1.701367	0.001523	-2.854233
Mg18	2.380521	-2.021806	0.038661
Mg19	-2.431198	-2.623791	1.491391

@mg19-isomer02 bp86/6-31G(d) Etot=-3801.794159 Eb=-15.52

Mg1	-1.604211	-1.024764	2.450441
Mg2	-0.000951	-3.516771	1.569856
Mg3	-0.002940	-3.518575	-1.566451
Mg4	1.562035	2.851205	-0.001946
Mg5	3.308308	0.130754	-0.000864
Mg6	3.021239	1.799039	-2.455459
Mg7	-3.020300	1.804605	2.453399
Mg8	-1.606078	-1.027066	-2.449085
Mg9	0.000472	-0.211166	0.000028
Mg10	-3.022615	1.803806	-2.451601
Mg11	1.602461	-1.029917	-2.451811
Mg12	3.025111	1.801882	2.451453

Mg13	-0.001197	1.817036	-2.438456
Mg14	0.002417	1.819285	2.437067
Mg15	2.377993	-2.729186	-0.000592
Mg16	-2.380534	-2.726907	0.002866
Mg17	-3.308912	0.133375	0.000626
Mg18	-1.557580	2.850553	0.000195
Mg19	1.605283	-1.027188	2.450334

@mg19-isomer03 bp86/6-31G(d) Etot=-3801.793940 Eb=-15.51

Mg1	-3.948639	-0.518704	2.031056
Mg2	-0.006901	0.109364	-0.158053
Mg3	3.961811	-0.703157	1.993306
Mg4	-2.864232	-1.519016	-0.653411
Mg5	-0.601227	3.285448	1.553983
Mg6	-1.326517	-2.371462	-3.079910
Mg7	-1.823925	0.667575	-2.578441
Mg8	-1.145196	0.518264	2.703784
Mg9	1.764795	1.404063	2.098594
Mg10	1.536750	-1.434595	-2.587695
Mg11	3.053174	0.529375	-0.645528
Mg12	1.119904	-1.740272	2.145270
Mg13	1.109883	1.648242	-2.702266
Mg14	-0.986891	3.427210	-1.448717
Mg15	1.778095	3.340718	-0.254853
Mg16	-1.762742	-2.571810	1.992178
Mg17	-0.036671	-3.113799	-0.444217
Mg18	-2.771686	1.594326	0.218653
Mg19	2.950216	-2.551770	-0.183732

@mg19-isomer04 bp86/6-31G(d) Etot=-3801.791717 Eb=-15.44

Mg1	0.494067	-3.264925	1.471945
Mg2	-0.647746	2.407694	-2.632342
Mg3	-3.226126	1.358347	-1.763580
Mg4	-0.206108	-0.015796	0.007160
Mg5	-2.224358	-2.333933	2.003415
Mg6	0.037155	-0.570336	3.013808
Mg7	-1.413454	-3.558064	-0.811393
Mg8	3.706324	1.337110	-0.190655
Mg9	4.024990	-1.282918	-1.630538
Mg10	1.723854	0.589326	-2.340155
Mg11	-1.886889	3.348677	0.005764
Mg12	2.288693	1.538876	2.494298
Mg13	-2.657623	0.743332	1.569305
Mg14	1.256841	-2.419651	-1.417625
Mg15	-0.488620	2.626145	2.538521
Mg16	1.121890	2.867362	-0.155649
Mg17	2.563906	-1.153051	1.144178
Mg18	-3.289221	-1.310787	-0.579201
Mg19	-1.177576	-0.907408	-2.727256

@mg19-isomer05 bp86/6-31G(d) Etot=-3801.791042 Eb=-15.42

Mg1	-0.123748	-0.071515	-0.000192
Mg2	1.995411	-2.367391	0.004523
Mg3	2.316876	0.015780	2.072049
Mg4	0.566801	2.696020	1.558862
Mg5	0.567920	2.690894	-1.567575
Mg6	2.318609	0.008402	-2.070676
Mg7	-0.314246	0.443743	3.520884
Mg8	-1.647091	4.054809	-0.007173
Mg9	-0.311703	0.431341	-3.522070
Mg10	0.509756	-2.491748	-2.574670
Mg11	0.507794	-2.482572	2.583018
Mg12	4.458573	-0.611679	0.002648
Mg13	-2.391529	1.485653	-1.568713

Mg14	-2.334318	-1.690103	-2.627773
Mg15	-1.118295	-3.118472	0.004780
Mg16	-2.336352	-1.680648	2.632039
Mg17	-2.392578	1.490924	1.562284
Mg18	-3.314591	-0.933324	0.000382
Mg19	3.042710	2.129886	-0.002626

@mg19-isomer06 bp86/6-31G(d) Etot=-3801.789742 Eb=-15.37

Mg1	2.048384	-0.120085	-2.253023
Mg2	-2.529493	-2.112574	-1.708801
Mg3	2.105478	-2.535907	-0.223536
Mg4	0.561583	2.568213	-1.375008
Mg5	3.823251	-0.064448	0.226060
Mg6	-1.119089	0.334172	-2.809945
Mg7	-2.367749	-1.613406	1.387979
Mg8	2.488528	-0.507500	2.781108
Mg9	3.511172	2.494107	-1.212946
Mg10	-3.127375	0.632888	-0.492929
Mg11	-3.244134	1.237331	2.449354
Mg12	0.296453	-2.540955	2.337024
Mg13	1.842174	2.144799	1.404471
Mg14	-0.673867	-3.843731	-0.155172
Mg15	-2.331652	3.166959	-1.780024
Mg16	0.027259	-0.213486	0.036241
Mg17	-0.353209	0.639094	3.011016
Mg18	-1.193647	2.904752	1.073328
Mg19	0.235933	-2.570222	-2.695198

@mg19-isomer07 bp86/6-31G(d) Etot=-3801.780937 Eb=-15.08

Mg1	1.498251	3.224790	-2.531591
Mg2	-1.275928	-2.544194	-2.340395
Mg3	2.701846	-1.484496	-0.469385
Mg4	-1.319789	2.524294	-2.342205
Mg5	0.749174	0.004811	-2.562005
Mg6	0.169887	3.284305	0.313389
Mg7	1.551087	-3.207288	-2.527460
Mg8	-1.300334	1.579547	2.638198
Mg9	1.701933	1.625304	2.430056
Mg10	-2.827275	2.562187	0.199219
Mg11	2.680648	1.528935	-0.469136
Mg12	-1.275502	-1.598978	2.637851
Mg13	-0.130313	0.000693	0.269169
Mg14	-2.785713	-2.607012	0.199657
Mg15	-2.624081	-0.020940	-1.532237
Mg16	4.158307	0.032500	1.754486
Mg17	1.726027	-1.594637	2.430570
Mg18	-3.620829	-0.028205	1.585387
Mg19	0.222603	-3.281619	0.316432

@mg19-isomer08 bp86/6-31G(d) Etot=-3801.780243 Eb=-15.06

Mg1	0.152330	-0.084412	-0.156194
Mg2	-1.340925	0.157253	-2.826635
Mg3	2.488600	-2.183133	-0.470474
Mg4	-1.731043	-1.626926	2.056883
Mg5	-1.555479	2.993961	-1.641072
Mg6	-4.515571	-1.515219	1.144697
Mg7	0.041869	-2.711823	-2.470295
Mg8	2.026032	-0.507998	-2.903401
Mg9	0.823430	3.137666	0.392348
Mg10	-0.720862	1.242105	2.532865
Mg11	2.306192	1.479940	2.459026
Mg12	-2.082104	3.564508	1.256986
Mg13	3.060971	1.077863	-0.494073
Mg14	4.040172	-0.853768	1.742221

Mg15	-2.449445	-2.145877	-1.037822
Mg16	-2.767433	0.783218	0.060571
Mg17	1.237987	-1.621359	2.464404
Mg18	1.130750	2.362093	-2.541011
Mg19	-0.145471	-3.548092	0.430973

@mg19-isomer09 bp86/6-31G(d) Etot=-3801.755395 Eb=-14.24

Mg1	2.678683	-2.617336	-1.073957
Mg2	0.177836	0.002917	-0.216791
Mg3	-0.039065	-2.200146	-2.435903
Mg4	0.176532	-3.689233	0.343742
Mg5	-1.292469	-1.528020	2.053149
Mg6	-2.465438	-2.556295	-0.643379
Mg7	1.827361	1.558999	1.839608
Mg8	2.180654	0.001166	-2.625714
Mg9	-2.079575	0.012705	-2.280481
Mg10	-1.283546	1.527411	2.061624
Mg11	-3.495957	0.009962	0.680504
Mg12	0.197087	3.689036	0.360121
Mg13	-0.027038	2.215575	-2.427507
Mg14	3.829576	-0.009445	-0.034826
Mg15	-2.449656	2.575598	-0.631196
Mg16	1.817671	-1.575299	1.832872
Mg17	2.693381	2.609449	-1.062296
Mg18	4.184585	-0.018213	3.023825
Mg19	-6.630622	-0.008831	1.236605

@mg19-isomer10 bp86/6-31G(d) Etot=-3801.740949 Eb=-13.76

Mg1	-4.910424	-0.822719	0.010620
Mg2	2.239894	1.453334	2.108791
Mg3	-2.553728	0.253410	-1.744936
Mg4	1.329743	3.319854	-0.438186
Mg5	-0.116311	-1.617168	-1.589318
Mg6	-0.176233	-3.982638	0.334861
Mg7	-3.052705	1.298066	1.453026
Mg8	2.734890	-2.303564	-0.906122
Mg9	4.169411	2.109440	-0.203718
Mg10	-0.583671	0.385355	3.153355
Mg11	-1.858741	3.219097	-0.844257
Mg12	4.316477	-0.629621	1.141040
Mg13	2.002706	0.628560	-1.886421
Mg14	-1.970840	-1.623813	1.390378
Mg15	-4.776498	2.140133	-0.863394
Mg16	1.389967	-1.495276	1.659621
Mg17	-0.218891	0.829478	0.177042
Mg18	-2.917614	-2.811101	-1.167261
Mg19	4.952568	-0.350826	-1.785119

@mg19-isomer11 bp86/6-31G(d) Etot=-3801.734358 Eb=-13.54

Mg1	-0.696794	0.105308	-0.606339
Mg2	0.054572	-1.467588	1.996584
Mg3	1.487285	0.555598	-2.584473
Mg4	-2.944296	-1.173977	1.458613
Mg5	-5.176058	0.215718	-0.490777
Mg6	1.896674	-1.694562	-0.571098
Mg7	1.741247	1.111115	1.401303
Mg8	-2.932314	2.236306	-0.578570
Mg9	-1.257114	-2.718589	-0.742740
Mg10	-2.892285	-0.270198	-2.520258
Mg11	0.143938	2.892249	-0.461543
Mg12	-1.305465	1.442506	2.062640
Mg13	3.092024	-1.386124	2.374887
Mg14	3.163203	2.459169	-0.967073
Mg15	-4.250815	-2.550494	-1.055352

Mg16	-4.387376	1.424114	2.099087
Mg17	4.402014	-0.073088	-2.022977
Mg18	4.855734	0.860757	1.023561
Mg19	5.005824	-1.968218	0.184525

@mg19-isomer12 bp86/6-31G(d) Etot=-3801.732760 Eb=-13.49

Mg1	0.315605	2.159022	-1.624258
Mg2	-2.798491	1.454482	-1.965776
Mg3	1.232140	-2.770309	0.425229
Mg4	-0.915718	-0.622403	-0.838880
Mg5	3.337144	2.499704	-1.264142
Mg6	-1.419611	2.103849	0.785497
Mg7	-4.918069	-0.048257	-0.305410
Mg8	-1.155632	-3.958519	-0.935030
Mg9	-2.938480	-2.091853	0.909427
Mg10	4.796088	0.984779	0.902866
Mg11	-4.299716	2.841294	0.329952
Mg12	-3.389250	0.453427	2.335828
Mg13	5.116534	0.008284	-1.932379
Mg14	-3.379626	-1.761455	-2.166993
Mg15	1.762359	2.171330	1.419946
Mg16	4.459239	-1.984705	0.286521
Mg17	-0.508196	-0.505399	2.190404
Mg18	2.548535	-0.682505	2.352691
Mg19	2.155144	-0.250766	-0.905491

@mg19-isomer13 bp86/6-31G(d) Etot=-3801.729414 Eb=-13.38

Mg1	-0.772136	-1.795329	-1.697802
Mg2	1.880693	-0.237985	-1.202063
Mg3	2.327105	1.342185	1.533660
Mg4	4.759031	-1.656204	-1.198864
Mg5	4.558341	1.297425	-0.615026
Mg6	-4.299920	1.637528	-0.690021
Mg7	0.859566	2.562337	-0.849816
Mg8	-2.697483	-1.991716	0.715661
Mg9	3.396718	4.042247	-0.028457
Mg10	-3.655605	-1.046471	-2.122527
Mg11	-5.426543	-0.829950	0.565326
Mg12	-1.686585	1.233638	-2.248846
Mg13	-3.400658	0.791166	2.153243
Mg14	0.268614	-2.749546	1.025522
Mg15	1.153207	-0.795385	3.368864
Mg16	2.128011	-3.292765	-1.213113
Mg17	3.140781	-1.735349	1.336581
Mg18	-1.900618	2.968275	0.409872
Mg19	-0.632519	0.255898	0.757807

@mg19-isomer14 bp86/6-31G(d) Etot=-3801.718532 Eb=-13.02

Mg1	-2.522677	0.064928	-1.455136
Mg2	0.011764	1.180730	-0.290950
Mg3	-2.386462	1.729838	1.800450
Mg4	-2.580903	-2.867632	-0.492326
Mg5	-2.188830	3.133461	-1.010954
Mg6	0.105829	-1.497518	-1.666386
Mg7	-4.151147	-0.908263	1.724978
Mg8	2.391158	0.648226	-2.007233
Mg9	2.034556	-1.068834	1.190202
Mg10	4.781366	-0.229967	-0.168147
Mg11	0.636720	1.190286	2.657793
Mg12	-5.324783	-1.378422	-0.947298
Mg13	7.740643	-0.074896	0.792601
Mg14	-4.902573	1.575205	0.106988
Mg15	-1.086404	-1.144772	1.420223
Mg16	3.006704	-2.408173	-1.278233

Mg17	2.955342	2.069823	0.659331
Mg18	1.002821	3.687045	-1.427172
Mg19	0.476878	-3.701066	0.391268

@mg19-isomer15 bp86/6-31G(d) Etot=-3801.710890 Eb=-12.77

Mg1	-2.069079	-1.244760	-0.665902
Mg2	0.380549	1.355714	-0.504476
Mg3	0.896245	-1.897994	0.406182
Mg4	-0.448245	0.242123	2.266457
Mg5	-3.491683	-0.201909	2.434075
Mg6	-2.411077	2.236400	0.807996
Mg7	2.636146	0.411352	1.500770
Mg8	2.004511	-3.246286	-2.132404
Mg9	5.387203	0.405807	-0.001433
Mg10	2.807339	-0.248977	-1.721903
Mg11	-1.569522	-2.646162	1.986145
Mg12	4.856864	2.848620	1.933350
Mg13	3.298543	2.585614	-0.649818
Mg14	-4.830441	0.521411	-0.196481
Mg15	3.972920	-2.391990	0.291209
Mg16	-4.671077	3.271136	-1.497583
Mg17	-2.256987	1.365189	-2.162463
Mg18	-4.553915	-2.472916	0.630253
Mg19	0.061703	-0.892374	-2.723974

@mg20-isomer01 bp86/6-31G(d) Etot=-4001.911195 Eb=-16.23

Mg1	0.001896	0.000327	-3.051814
Mg2	2.033383	4.094754	-0.491722
Mg3	2.613445	-0.952119	-1.538777
Mg4	2.330608	1.886642	-2.477025
Mg5	0.470129	-2.959974	-2.477563
Mg6	-0.479328	2.735567	-1.537588
Mg7	2.330453	-1.564399	1.541603
Mg8	-0.234702	-3.049405	0.576596
Mg9	-4.563535	-0.287815	-0.496907
Mg10	-2.521934	-1.236646	1.537291
Mg11	0.000311	-0.000699	0.119248
Mg12	1.547820	0.779981	3.372689
Mg13	2.530855	-3.807668	-0.490501
Mg14	0.187565	2.800537	1.539063
Mg15	2.758623	1.321779	0.578836
Mg16	-1.452825	0.953588	3.370711
Mg17	-2.128822	-1.783649	-1.541480
Mg18	-0.103111	-1.733075	3.370632
Mg19	-2.796227	1.075686	-2.479390
Mg20	-2.524603	1.726587	0.576098

@mg20-isomer02 bp86/6-31G(d) Etot=-4001.907113 Eb=-16.10

Mg1	-2.096549	-1.681955	-2.633356
Mg2	2.224336	0.718125	1.947062
Mg3	-3.103184	-0.455825	-0.001915
Mg4	0.835314	-2.130833	2.158499
Mg5	-2.100823	-1.686095	2.628414
Mg6	-0.090560	2.699131	1.754890
Mg7	-2.746739	1.279208	2.694664
Mg8	-0.123008	0.040835	0.001103
Mg9	2.875020	-1.539462	0.002378
Mg10	1.392300	-4.266886	-0.000534
Mg11	4.499497	1.092363	0.002372
Mg12	2.348512	3.172269	0.001943
Mg13	0.837976	-2.126732	-2.157891
Mg14	-2.539037	2.498537	0.001096
Mg15	2.224543	0.716195	-1.943191
Mg16	-2.741879	1.282387	-2.696303

Mg17	-0.151235	0.333124	-3.694163
Mg18	-0.089649	2.697610	-1.751567
Mg19	-0.156812	0.329534	3.689518
Mg20	-1.298024	-2.971527	-0.003021

@mg20-isomer03 bp86/6-31G(d) Etot=-4001.906578 Eb=-16.08

Mg1	-0.085647	0.008128	0.002681
Mg2	-0.756950	-3.673811	0.019802
Mg3	3.325921	-0.447553	-0.031283
Mg4	1.415202	-2.249199	1.551625
Mg5	3.203307	-0.442934	-3.155733
Mg6	1.932369	1.800870	-1.578641
Mg7	0.157970	-0.034987	-3.339232
Mg8	-1.578106	-2.308143	-2.462396
Mg9	0.224419	-0.015674	3.342385
Mg10	3.266988	-0.424392	3.094030
Mg11	-2.659268	0.364175	1.573485
Mg12	-1.534242	-2.286798	2.504299
Mg13	1.386424	-2.258455	-1.561909
Mg14	-2.663630	2.992696	0.015414
Mg15	0.240073	3.747610	-0.010902
Mg16	-0.915453	2.621522	-2.479863
Mg17	-2.684572	0.353133	-1.532036
Mg18	1.958949	1.807171	1.530927
Mg19	-3.362578	-2.184730	0.035049
Mg20	-0.871177	2.631370	2.482298

@mg20-isomer04 bp86/6-31G(d) Etot=-4001.900667 Eb=-15.90

Mg1	-2.673391	-1.757529	-0.479205
Mg2	-1.829842	-0.918727	-3.246817
Mg3	-1.236970	-4.368556	0.302773
Mg4	-1.821875	-2.360548	2.415787
Mg5	-2.681942	1.284677	-1.272086
Mg6	0.127324	-2.629157	-1.720523
Mg7	-2.674472	0.451564	1.754952
Mg8	-1.256047	1.917908	-3.930817
Mg9	0.122412	-0.174421	3.136286
Mg10	-0.013898	-0.001332	-0.001165
Mg11	1.129535	-2.647175	1.324591
Mg12	-1.840768	3.266270	0.834177
Mg13	-1.254897	2.439635	3.630379
Mg14	0.110139	2.804037	-1.415221
Mg15	1.117774	0.179028	-2.956017
Mg16	1.112193	2.474011	1.630412
Mg17	2.808320	-1.532168	-0.996590
Mg18	2.806364	-0.086726	1.830875
Mg19	2.797359	1.641203	-0.837753
Mg20	5.152684	0.018004	-0.004037

@mg20-isomer05 bp86/6-31G(d) Etot=-4001.900006 Eb=-15.88

Mg1	2.511619	1.766785	-0.797812
Mg2	0.004793	-1.877366	-3.371871
Mg3	3.025952	-1.004343	0.462697
Mg4	2.594986	-0.614501	-2.628243
Mg5	2.726131	1.448440	2.246362
Mg6	0.190548	1.182939	-2.875703
Mg7	1.134491	-3.093857	1.503141
Mg8	-0.226556	1.324757	2.780271
Mg9	-1.471378	2.287593	-0.369597
Mg10	-2.970822	0.869667	1.903085
Mg11	0.153723	-0.198987	0.045683
Mg12	-1.133118	-2.903218	-0.582259
Mg13	1.592327	-1.024457	3.579130
Mg14	-2.210024	-0.399026	-1.966829

Mg15	1.814466	-3.233728	-1.410156
Mg16	-3.663749	-1.637945	0.460350
Mg17	0.915855	3.569467	1.095368
Mg18	-1.321502	-1.598706	2.504034
Mg19	0.711965	3.979456	-1.876038
Mg20	-4.379708	1.157029	-0.701614

@mg20-isomer06 bp86/6-31G(d) Etot=-4001.899622 Eb=-15.87

Mg1	0.046289	0.008943	0.000106
Mg2	-0.355720	1.871062	2.581073
Mg3	2.541932	1.820891	-0.522661
Mg4	-2.295584	-0.456744	2.381894
Mg5	-2.315448	-0.205851	-2.398533
Mg6	0.655812	-1.102855	2.913616
Mg7	-1.452690	-3.287112	2.573873
Mg8	-4.267724	-0.610178	-0.014169
Mg9	0.800808	-3.141958	0.460659
Mg10	2.945656	-1.032499	0.537419
Mg11	2.804289	-3.171886	-1.761997
Mg12	-2.543180	1.772921	0.338028
Mg13	-1.937764	-2.410053	-0.348847
Mg14	2.843529	-0.350679	-2.599472
Mg15	-2.303424	2.746467	-2.584705
Mg16	0.204934	-1.892530	-2.579092
Mg17	-0.111870	3.238943	-0.458674
Mg18	0.340736	1.243146	-2.911510
Mg19	2.612712	1.131526	2.614797
Mg20	1.786705	3.828446	1.778193

@mg20-isomer07 bp86/6-31G(d) Etot=-4001.893814 Eb=-15.68

Mg1	-0.014329	3.186668	1.994377
Mg2	-1.488203	3.559623	-0.625839
Mg3	-2.436442	1.449338	1.337054
Mg4	0.003414	0.436189	3.400606
Mg5	1.451373	3.571987	-0.627759
Mg6	-0.010714	2.118194	-2.910962
Mg7	-3.910501	-1.042728	0.011139
Mg8	2.421216	1.468616	1.335726
Mg9	-2.362187	0.836138	-1.717075
Mg10	-0.003690	0.076725	0.223331
Mg11	0.014207	-2.604917	2.504786
Mg12	-2.882829	-2.018851	-2.785771
Mg13	2.349407	0.855699	-1.715959
Mg14	2.537731	-1.226290	2.651588
Mg15	-2.518300	-1.245070	2.656209
Mg16	0.002163	-1.083842	-2.621423
Mg17	-1.456945	-2.679163	-0.158558
Mg18	3.924599	-1.006223	0.002267
Mg19	1.482157	-2.659804	-0.160950
Mg20	2.897874	-1.992288	-2.792788

@mg20-isomer08 bp86/6-31G(d) Etot=-4001.892691 Eb=-15.65

Mg1	-0.413194	-0.457167	-0.011410
Mg2	0.538363	-2.351449	2.582418
Mg3	-3.666072	-0.000574	0.055838
Mg4	-0.151597	0.673209	3.091217
Mg5	-2.816517	1.730509	2.385658
Mg6	0.091788	1.050182	-2.960577
Mg7	0.218069	-3.419989	-0.371227
Mg8	1.931574	-1.105868	-1.756575
Mg9	2.885216	-2.646886	0.770054
Mg10	-2.605383	-0.127141	-2.715084
Mg11	-2.621362	-2.663326	-0.926680
Mg12	0.680350	3.805541	-1.361563

Mg13	1.519705	1.655728	0.614220
Mg14	2.843408	1.911870	-2.210731
Mg15	-2.249745	-1.426699	2.192329
Mg16	-0.561836	-2.128774	-3.124125
Mg17	3.978986	0.117001	0.018584
Mg18	-0.505264	3.525250	1.727020
Mg19	2.636040	-0.286382	2.687180
Mg20	-1.732530	2.144966	-0.686545

@mg20-isomer09 bp86/6-31G(d) Etot=-4001.887140 Eb=-15.47

Mg1	-0.601044	3.594372	-1.606627
Mg2	-2.424186	-3.848980	-1.962422
Mg3	-3.093627	0.819454	1.694488
Mg4	1.038346	-1.623093	2.601387
Mg5	-0.375190	1.269090	3.134498
Mg6	-0.767206	-1.411693	-2.348705
Mg7	2.014040	-0.606572	-3.177505
Mg8	2.504919	0.932772	1.761912
Mg9	-2.439055	1.182513	-1.375208
Mg10	-1.926489	-1.645649	2.826794
Mg11	1.840383	1.833953	-1.345881
Mg12	4.008726	-0.082834	-0.764908
Mg13	-0.197050	0.106252	0.281059
Mg14	1.787595	-2.080059	-0.518514
Mg15	3.912517	-1.682781	1.804560
Mg16	0.835056	3.274610	1.097685
Mg17	-0.297606	1.307961	-3.642133
Mg18	-0.697188	-3.224335	0.577392
Mg19	-3.074167	-1.551680	-0.105550
Mg20	-2.048772	3.436699	1.067678

@mg20-isomer10 bp86/6-31G(d) Etot=-4001.886343 Eb=-15.45

Mg1	0.413031	0.221808	3.169317
Mg2	-2.318827	0.254802	-2.641123
Mg3	1.558182	-2.379144	1.455329
Mg4	-1.096962	2.588512	1.818312
Mg5	1.285799	-2.959998	-1.792871
Mg6	3.249340	-0.043507	2.224602
Mg7	-2.854913	-1.545071	0.033001
Mg8	0.601744	-0.337834	-3.185831
Mg9	-0.428035	2.376132	-1.550048
Mg10	2.868165	-0.734059	-0.809064
Mg11	-0.166027	-0.245290	0.011012
Mg12	-2.565038	0.158506	2.723146
Mg13	-2.446002	4.271548	-0.486079
Mg14	1.613750	2.146553	0.838906
Mg15	-3.177780	1.414132	0.008249
Mg16	-0.873427	-3.733161	0.126274
Mg17	-1.108134	-2.424778	2.883207
Mg18	2.434035	1.892525	-2.176991
Mg19	4.476480	1.657237	0.038850
Mg20	-1.465381	-2.578913	-2.688200

@mg20-isomer11 bp86/6-31G(d) Etot=-4001.878604 Eb=-15.21

Mg1	1.509309	-0.599696	2.817460
Mg2	1.193409	-3.283426	1.522018
Mg3	-2.024258	2.558956	-0.000438
Mg4	2.780764	-1.040591	0.000356
Mg5	-0.151042	-0.013907	0.001492
Mg6	2.804817	1.765373	-1.521023
Mg7	-4.870674	1.293514	0.001635
Mg8	-0.138554	2.016489	-2.481886
Mg9	5.557518	0.635800	0.002250
Mg10	-0.136382	2.023242	2.480116

Mg11	-2.920155	0.828502	2.334516
Mg12	1.511992	-0.602344	-2.818421
Mg13	0.864927	3.413896	-0.003002
Mg14	-3.108892	-1.164411	0.000628
Mg15	-2.925418	0.829116	-2.333699
Mg16	-1.311735	-1.784266	2.457550
Mg17	1.193657	-3.283650	-1.521480
Mg18	-1.310657	-1.780299	-2.456734
Mg19	-1.323465	-3.579541	-0.000456
Mg20	2.804839	1.767243	1.519118

@mg20-isomer12 bp86/6-31G(d) Etot=-4001.875771 Eb=-15.12

Mg1	-1.840281	0.849532	2.277376
Mg2	0.330580	0.039677	-0.042457
Mg3	3.172266	-1.494808	-1.695612
Mg4	1.168257	1.195414	2.927725
Mg5	-0.443951	3.428903	1.613275
Mg6	-2.021927	1.949374	-0.618757
Mg7	0.483165	3.700672	-1.275546
Mg8	2.403655	2.982647	0.849371
Mg9	-2.497878	-0.368083	-2.643025
Mg10	3.318481	0.121237	0.927463
Mg11	-3.510794	-0.670633	0.248307
Mg12	-1.306847	-2.146424	1.790884
Mg13	3.828352	-2.842687	0.914406
Mg14	2.600629	1.496266	-1.796675
Mg15	0.354644	-1.575872	-2.820491
Mg16	-0.189976	1.449246	-3.093243
Mg17	1.004578	-3.027405	-0.128991
Mg18	-6.600377	-0.536889	1.013406
Mg19	1.573271	-1.783902	2.639976
Mg20	-1.825847	-2.766267	-1.087394

@mg20-isomer13 bp86/6-31G(d) Etot=-4001.875247 Eb=-15.10

Mg1	-0.300822	0.089516	0.028801
Mg2	-1.420516	3.569741	-0.711713
Mg3	1.023800	2.734859	-2.072520
Mg4	-1.393925	2.573571	2.180401
Mg5	1.057596	-2.823444	-0.363008
Mg6	1.411043	-0.259071	-2.581395
Mg7	1.135686	0.869294	2.703612
Mg8	1.098233	3.460315	0.912408
Mg9	-2.136977	-0.405510	2.515791
Mg10	-3.588231	-1.162741	-1.832020
Mg11	-1.571561	1.110100	-2.651930
Mg12	-0.954436	-2.196547	-2.526832
Mg13	2.939937	-1.442240	1.689141
Mg14	3.654162	-1.783901	-1.315505
Mg15	2.648240	1.043922	-0.053579
Mg16	-1.903367	-2.725817	0.356552
Mg17	0.243277	-2.290734	2.535520
Mg18	-4.555371	-1.453450	0.981707
Mg19	5.781069	-0.082612	0.167696
Mg20	-3.167838	1.174750	0.036871

@mg20-isomer14 bp86/6-31G(d) Etot=-4001.872824 Eb=-15.03

Mg1	-1.814121	1.472419	-2.205491
Mg2	0.779319	-2.386062	2.470299
Mg3	-1.600237	3.575232	0.040611
Mg4	3.124765	-1.513055	0.964625
Mg5	-1.617450	-1.788908	-1.988792
Mg6	1.530606	0.637434	2.639104
Mg7	0.714763	3.034356	-1.763389
Mg8	3.554997	-1.284634	-2.072968

Mg9	-3.216036	0.976534	0.527885
Mg10	-0.280243	0.032552	0.203787
Mg11	-3.889697	-1.950509	0.303850
Mg12	-1.210741	2.052334	2.633397
Mg13	0.909353	0.020488	-2.613577
Mg14	5.811538	-0.066833	-0.249017
Mg15	-1.328724	-3.320333	0.619824
Mg16	-4.272128	-0.358289	-2.111230
Mg17	-2.006832	-1.031006	2.610296
Mg18	2.621418	1.227537	-0.318325
Mg19	1.100970	-2.671724	-0.990484
Mg20	1.088480	3.342467	1.299597

@mg20-isomer15 bp86/6-31G(d) Etot=-4001.872318 Eb=-15.01

Mg1	-5.479966	-0.699085	0.040702
Mg2	-2.728291	0.424415	-1.259167
Mg3	-2.766389	-2.431972	0.453133
Mg4	0.212770	0.622104	-3.022642
Mg5	-1.457735	3.070608	-2.447767
Mg6	-2.916253	0.199279	1.909920
Mg7	-1.428122	-2.101036	-2.174290
Mg8	-1.634520	2.630505	0.530899
Mg9	0.058753	-0.146145	0.003439
Mg10	-0.998164	-1.926772	2.784328
Mg11	0.253343	-3.225790	0.257762
Mg12	3.197891	-2.544333	-0.273842
Mg13	1.235408	2.919072	-1.212092
Mg14	-0.155822	1.160798	2.813311
Mg15	0.768548	3.960997	1.632648
Mg16	1.531594	-2.153354	-2.663289
Mg17	1.967665	-1.310539	2.153225
Mg18	2.925407	0.313811	-1.574487
Mg19	2.516212	1.557509	1.202685
Mg20	4.897670	-0.320072	0.845523

@mg20-isomer16 bp86/6-31G(d) Etot=-4001.871870 Eb=-15.00

Mg1	3.020626	-0.674244	-1.395075
Mg2	5.526679	-0.373744	0.967316
Mg3	2.512440	1.210827	0.980007
Mg4	-4.385430	-1.900836	-0.863693
Mg5	-4.215611	0.664476	0.604422
Mg6	-2.315499	-1.574476	1.496061
Mg7	0.954712	3.660649	-0.235049
Mg8	2.205272	1.977015	-2.361305
Mg9	0.413988	-0.610888	-3.008167
Mg10	-2.538339	0.305670	-1.914589
Mg11	-0.648811	2.538283	-2.586858
Mg12	-0.032663	0.016699	-0.102871
Mg13	0.106601	-3.296780	1.290212
Mg14	-1.880470	2.596796	0.216907
Mg15	2.703570	-1.946390	1.311819
Mg16	-1.445534	-2.544475	-1.300848
Mg17	0.441504	-0.595115	2.851550
Mg18	1.474248	-3.172876	-1.355144
Mg19	0.307100	2.651466	2.493832
Mg20	-2.204384	1.067942	2.911472

@mg20-isomer17 bp86/6-31G(d) Etot=-4001.869593 Eb=-14.92

Mg1	-1.358278	-2.818798	-0.027404
Mg2	-3.426559	-0.722751	0.830579
Mg3	3.768842	1.610731	2.021934
Mg4	-2.021517	-0.305073	-1.854530
Mg5	0.918421	-2.724806	2.165015
Mg6	-3.718774	1.965799	-0.436155

Mg7	2.827725	-1.540048	-2.248613
Mg8	1.566651	-3.675227	-0.583789
Mg9	0.380552	-0.216070	0.049083
Mg10	1.113843	0.471637	2.951678
Mg11	3.244039	1.184111	-0.891419
Mg12	-0.874618	2.507401	-1.003608
Mg13	-6.407351	0.161684	-0.454594
Mg14	0.018244	-2.407195	-2.780953
Mg15	-1.579293	1.641573	1.851253
Mg16	0.899491	0.730251	-2.855720
Mg17	1.788514	3.609649	-1.772039
Mg18	3.169451	-1.250744	0.866974
Mg19	-1.521484	-1.174433	2.998111
Mg20	1.212101	2.952308	1.174197

@mg20-isomer18 bp86/6-31G(d) Etot=-4001.868503 Eb=-14.89

Mg1	-0.698920	2.756364	-2.165400
Mg2	4.569717	-0.690895	1.545429
Mg3	-0.771081	-1.397765	2.550004
Mg4	-5.413348	0.607063	-0.077280
Mg5	2.123530	3.546656	-1.956819
Mg6	3.195301	1.399733	-0.131343
Mg7	-0.984017	1.806153	2.708388
Mg8	1.612901	0.532709	-2.642877
Mg9	2.119725	-2.340862	2.159309
Mg10	1.894019	0.776977	2.558558
Mg11	0.575901	3.178600	0.622481
Mg12	0.774395	-2.392531	-2.744849
Mg13	-1.661072	-0.148971	-2.383920
Mg14	-2.664898	-1.513684	0.169081
Mg15	-3.499942	0.272596	2.469840
Mg16	0.121896	-3.264570	0.114102
Mg17	-2.437756	1.876555	0.049553
Mg18	2.876333	-1.747757	-0.758388
Mg19	-1.966147	-3.251251	-2.150109
Mg20	0.233463	-0.005118	0.064241

@mg20-isomer19 bp86/6-31G(d) Etot=-4001.867180 Eb=-14.85

Mg1	-0.669577	-1.069406	2.709740
Mg2	-0.144018	2.024718	2.778951
Mg3	-3.349823	1.974791	-1.519234
Mg4	-0.144661	-2.024490	-2.778729
Mg5	2.450161	-0.358979	-2.416765
Mg6	1.955640	3.297671	1.182391
Mg7	0.538597	0.000130	-0.000202
Mg8	3.819891	-1.395547	0.177100
Mg9	1.663875	2.706012	-1.841431
Mg10	-0.672423	1.068235	-2.708988
Mg11	-3.348332	-1.976368	1.522164
Mg12	1.667026	-2.705662	1.839555
Mg13	-0.783071	3.007941	-0.155842
Mg14	1.956593	-3.295589	-1.183079
Mg15	-2.481740	-0.956749	-1.261044
Mg16	-2.481115	0.954519	1.263618
Mg17	3.816765	1.397468	-0.178939
Mg18	2.451466	0.359778	2.415527
Mg19	-0.781235	-3.008649	0.157264
Mg20	-5.464018	0.000177	-0.002060

@mg20-isomer20 bp86/6-31G(d) Etot=-4001.866647 Eb=-14.83

Mg1	1.813066	2.545163	-1.184636
Mg2	3.405848	0.620014	0.717932
Mg3	1.685668	2.928470	1.914334
Mg4	-0.393137	4.056033	-2.638924

Mg5	-0.893653	3.159819	0.263376
Mg6	2.706459	-0.211516	-2.177614
Mg7	-1.618242	1.321626	-2.201979
Mg8	-0.848998	1.751088	2.955943
Mg9	0.355600	0.096344	-0.032661
Mg10	1.788077	0.139399	3.234525
Mg11	4.539576	-1.920725	-0.373258
Mg12	-2.670923	0.627926	0.711570
Mg13	-0.166884	-1.342109	-2.846579
Mg14	1.974982	-3.136638	-1.548919
Mg15	-2.972671	-1.330869	-1.715009
Mg16	-0.830644	-1.363171	2.413119
Mg17	1.975757	-2.242517	1.389606
Mg18	-0.728686	-2.953213	-0.222881
Mg19	-3.393461	-2.354438	1.116344
Mg20	-5.727734	-0.390686	0.225711

@mg20-isomer21 bp86/6-31G(d) Etot=-4001.865117 Eb=-14.78

Mg1	-0.331820	0.065538	0.141119
Mg2	0.493959	2.459889	2.348987
Mg3	-1.431695	-1.934811	2.634749
Mg4	2.607972	-1.034316	-0.508850
Mg5	-2.000283	1.006123	3.153253
Mg6	3.062458	1.542284	1.203276
Mg7	0.878424	0.635133	-2.729803
Mg8	0.305240	-2.258668	-2.102103
Mg9	5.737739	-0.022003	0.157665
Mg10	-4.343183	1.754990	-1.306925
Mg11	-1.537906	2.525764	-2.282228
Mg12	0.860956	-3.016922	1.029909
Mg13	1.421572	-0.556123	2.696282
Mg14	0.977858	2.921151	-0.661001
Mg15	-2.102592	-2.768687	-0.206779
Mg16	3.545970	1.588697	-1.790262
Mg17	-0.191854	-4.968960	-0.957273
Mg18	-2.344408	-0.499021	-2.256660
Mg19	-3.455251	-0.194448	0.755475
Mg20	-2.153156	2.754389	0.681169

@mg20-isomer22 bp86/6-31G(d) Etot=-4001.861063 Eb=-14.66

Mg1	-2.344160	3.102684	-0.866437
Mg2	-3.274032	-1.247991	1.446266
Mg3	1.892444	-0.434955	-1.436897
Mg4	-1.851227	0.624362	-2.627363
Mg5	3.529967	2.184765	-1.924733
Mg6	-0.698337	-0.056188	0.123459
Mg7	-2.585185	1.725752	1.954248
Mg8	5.091075	0.408201	0.026196
Mg9	-0.614266	-2.180825	-2.303076
Mg10	-3.505843	-1.772813	-1.603295
Mg11	0.304542	1.027103	2.936767
Mg12	2.381752	-0.966958	1.820500
Mg13	-0.500073	-2.018178	2.481990
Mg14	-1.702214	-3.542780	0.183822
Mg15	2.367959	1.925181	0.864888
Mg16	-4.344361	0.856768	-0.455510
Mg17	0.496698	2.370895	-1.555794
Mg18	4.266084	-2.383156	-0.315610
Mg19	-0.184847	3.520270	1.271009
Mg20	1.274023	-3.142137	-0.020429

@mg20-isomer23 bp86/6-31G(d) Etot=-4001.857508 Eb=-14.54

Mg1	-0.241487	-0.326188	-0.215576
Mg2	0.700753	1.802617	-2.308586

Mg3	-2.317610	3.537255	1.636673
Mg4	3.007160	0.056602	-1.421557
Mg5	-1.772690	0.064114	-3.173435
Mg6	0.636309	-0.297972	2.836868
Mg7	-1.863480	-2.767628	-2.085756
Mg8	-2.044714	2.243819	-1.099207
Mg9	-4.708268	1.820440	0.592542
Mg10	0.417966	2.409000	0.995387
Mg11	5.772557	1.028163	-0.187812
Mg12	-1.982819	-2.420902	1.340175
Mg13	2.962184	2.924258	-0.613684
Mg14	2.393511	-1.931422	0.801906
Mg15	3.071175	0.940302	1.708888
Mg16	0.229242	-3.855142	-0.247552
Mg17	0.515292	-3.394286	2.730287
Mg18	-3.485823	-0.555422	-0.694188
Mg19	0.965891	-1.820259	-2.570105
Mg20	-2.255148	0.542649	1.974732

@mg20-isomer24 bp86/6-31G(d) Etot=-4001.857468 Eb=-14.54

Mg1	-0.545381	0.201660	-0.001787
Mg2	-2.221558	2.515371	1.796130
Mg3	2.313922	2.315806	0.007190
Mg4	0.314465	-1.139207	-2.930116
Mg5	2.731844	-0.105033	-1.631113
Mg6	-2.638255	-0.490471	-2.415800
Mg7	4.330819	-2.270895	-0.011797
Mg8	1.269386	-2.394851	-0.008517
Mg9	0.326599	-1.162081	2.930228
Mg10	-3.720716	-2.099877	0.001543
Mg11	-2.220881	2.516321	-1.789889
Mg12	-1.354034	-3.133563	-1.513281
Mg13	2.734393	-0.116118	1.626900
Mg14	-0.223918	3.777272	0.006044
Mg15	0.610948	1.979687	-2.504741
Mg16	0.605401	1.960213	2.512216
Mg17	-3.937769	0.780189	0.004182
Mg18	-1.350381	-3.139541	1.502861
Mg19	5.597158	0.497687	0.001905
Mg20	-2.622042	-0.492569	2.417843

@mg20-isomer25 bp86/6-31G(d) Etot=-4001.855002 Eb=-14.47

Mg1	0.341180	2.568260	1.797742
Mg2	0.970983	-2.703744	1.512613
Mg3	-1.089311	-3.036828	-0.928483
Mg4	0.782548	1.848736	-2.183883
Mg5	-2.152281	0.224650	-2.382179
Mg6	-3.865476	-1.785284	-0.793190
Mg7	5.223986	0.431414	0.699903
Mg8	0.775578	4.347527	-0.596423
Mg9	-2.074750	-1.997783	1.731805
Mg10	-4.413284	1.220653	-0.455818
Mg11	-1.813610	2.766757	-0.497474
Mg12	2.020435	-3.256648	-1.290290
Mg13	3.963928	-2.260650	0.966578
Mg14	-0.238449	-0.072745	0.164066
Mg15	3.054178	2.508552	0.297657
Mg16	-2.371897	1.154905	2.035111
Mg17	0.581047	-1.123274	-2.817679
Mg18	2.225920	0.055348	2.051442
Mg19	-4.817784	-0.637731	1.851413
Mg20	2.897058	-0.252116	-1.162910

@mg20-isomer26 bp86/6-31G(d) Etot=-4001.853966 Eb=-14.43

Mg1	2.445500	0.490840	-2.014929
Mg2	5.352272	0.517636	-0.589043
Mg3	-1.986378	-1.773607	-1.473470
Mg4	0.052930	0.022902	-0.070912
Mg5	0.670205	2.979123	-1.351894
Mg6	-4.186607	-1.148780	0.678721
Mg7	3.414394	2.771234	-0.218177
Mg8	0.541475	-0.282897	2.959435
Mg9	3.904382	-2.046029	-0.717773
Mg10	1.068706	-2.234980	-1.871087
Mg11	-1.938960	1.362479	-1.871934
Mg12	-1.729204	3.336956	0.441501
Mg13	2.997382	0.110729	1.341052
Mg14	-0.510407	-4.198242	-0.234126
Mg15	1.004707	2.559804	1.736379
Mg16	-2.179573	0.830108	2.153482
Mg17	-4.589861	-0.200678	-2.147087
Mg18	1.565000	-2.739800	1.355822
Mg19	-1.520888	-2.190703	1.787889
Mg20	-4.375075	1.833905	0.106151

@mg20-isomer27 bp86/6-31G(d) Etot=-4001.849707 Eb=-14.30

Mg1	0.183751	-0.821012	-0.002255
Mg2	4.333647	2.094056	-0.002338
Mg3	-0.876284	1.182119	1.838861
Mg4	-3.764951	0.529823	2.632894
Mg5	0.892530	-2.461994	-2.493252
Mg6	-3.428784	2.095123	-0.002103
Mg7	2.436515	0.071186	1.708258
Mg8	0.894953	-2.454152	2.496435
Mg9	1.740427	3.076013	-1.517134
Mg10	-4.592482	-0.744036	0.002169
Mg11	-0.868621	3.693211	-0.002574
Mg12	-2.138802	-1.913587	-1.571259
Mg13	-0.132428	-3.870737	0.004947
Mg14	-3.768896	0.521174	-2.632226
Mg15	2.438841	0.064532	-1.711554
Mg16	-2.136693	-1.908336	1.576973
Mg17	-0.880701	1.179840	-1.841465
Mg18	5.178255	-0.769870	0.001146
Mg19	1.741974	3.084279	1.512694
Mg20	2.747748	-2.647632	0.001784

@mg20-isomer28 bp86/6-31G(d) Etot=-4001.848398 Eb=-14.26

Mg1	2.345567	1.752040	0.357273
Mg2	4.303956	0.883202	-2.107406
Mg3	0.766437	-3.172297	0.683673
Mg4	-1.804751	1.022694	-2.128881
Mg5	-0.571606	-2.144861	-2.039921
Mg6	4.779916	-0.334822	0.548147
Mg7	-4.392638	0.977472	-0.484583
Mg8	-2.188613	-2.746842	0.615531
Mg9	0.036241	1.589999	2.732982
Mg10	0.466599	4.206770	1.383702
Mg11	2.043290	-0.698438	2.302577
Mg12	-4.999511	-1.621480	0.833455
Mg13	0.175391	3.360468	-1.444489
Mg14	-2.033037	2.611873	0.666350
Mg15	-2.652397	-0.017139	2.228226
Mg16	1.241663	0.718569	-2.435968
Mg17	2.602508	-1.688042	-1.272268
Mg18	-0.219595	-0.184548	0.256747
Mg19	-3.573959	-1.524085	-1.997730
Mg20	3.674541	-2.990533	1.302582

@mg20-isomer29 bp86/6-31G(d) Etot=-4001.848187 Eb=-14.25

Mg1	2.883953	-2.084260	0.639905
Mg2	-1.540957	-1.687747	-1.132706
Mg3	3.306810	1.986771	-1.767833
Mg4	4.980653	0.264100	0.251964
Mg5	-3.773294	-0.284803	-2.859082
Mg6	-4.487000	-1.159932	-0.063244
Mg7	0.712769	-1.734986	2.746261
Mg8	-4.522954	1.816282	-0.725064
Mg9	1.098512	-0.088424	-1.070438
Mg10	3.783437	-1.204361	-2.079701
Mg11	0.040954	-3.861406	0.767832
Mg12	-1.545200	1.434282	-1.617495
Mg13	3.785191	3.065409	0.931110
Mg14	2.242552	0.725835	1.936175
Mg15	-2.257066	-1.972583	1.889314
Mg16	-2.210814	3.267641	0.675252
Mg17	0.869600	2.993908	-0.072316
Mg18	-3.702500	0.928325	2.079853
Mg19	1.138938	-3.002194	-1.836113
Mg20	-0.803583	0.598144	1.306328

@mg20-isomer30 bp86/6-31G(d) Etot=-4001.843548 Eb=-14.11

Mg1	0.498404	-1.519064	2.560456
Mg2	2.211317	0.450055	1.043301
Mg3	4.629426	2.445005	1.175543
Mg4	-0.070118	-1.028354	-0.473580
Mg5	0.606241	-3.540109	-1.873021
Mg6	-2.547522	-2.705363	-1.180377
Mg7	-0.665033	1.248591	1.518675
Mg8	-2.462422	-1.508860	1.604563
Mg9	-1.669449	3.457815	-0.311169
Mg10	0.529404	1.663958	-1.710092
Mg11	-4.842300	-0.799204	-0.194507
Mg12	-2.379268	0.604200	-1.359107
Mg13	1.448479	3.457017	0.517959
Mg14	4.859717	-0.589765	0.005121
Mg15	2.486453	-0.956440	-1.990784
Mg16	-3.703285	1.475940	1.546670
Mg17	-4.779113	2.550084	-0.932227
Mg18	2.664684	-2.772550	0.533413
Mg19	3.583581	1.934665	-1.487550
Mg20	-0.399197	-3.867620	1.006714

@mg20-isomer31 bp86/6-31G(d) Etot=-4001.843275 Eb=-14.10

Mg1	3.559478	0.803755	-0.732847
Mg2	-2.055344	0.277618	-0.470031
Mg3	-2.009745	2.759443	1.483381
Mg4	-1.743921	-2.086630	-2.540893
Mg5	0.865613	1.869405	0.525740
Mg6	1.012302	-0.799395	-1.691128
Mg7	-0.455804	3.465794	-4.203326
Mg8	-1.304015	3.223102	-1.328057
Mg9	1.672191	2.178317	-2.512323
Mg10	-1.162024	0.633561	-3.478704
Mg11	2.891416	-2.318224	0.343282
Mg12	-2.553941	-2.619283	0.685898
Mg13	-2.677498	-0.362763	2.559571
Mg14	-2.225930	-4.806885	-1.351889
Mg15	0.177412	-1.348393	1.635211
Mg16	0.422078	-3.664058	-0.498763
Mg17	5.283746	-0.713937	1.208538
Mg18	0.156477	1.181959	3.525800

Mg19	2.749518	0.271548	2.493851
Mg20	-2.602007	2.055065	4.346688

@mg20-isomer32 bp86/6-31G(d) Etot=-4001.842833 Eb=-14.08

Mg1	-1.834550	1.187857	1.402033
Mg2	-2.330544	0.676957	-2.427756
Mg3	-2.606114	3.228298	-0.602238
Mg4	0.958116	-3.241199	-2.071683
Mg5	-0.545394	-0.919863	-0.627470
Mg6	-0.258150	3.791587	1.361838
Mg7	1.113270	-0.315650	-3.049577
Mg8	3.003722	-1.230901	-0.867440
Mg9	4.861665	0.911643	0.602758
Mg10	-4.239935	-0.542330	2.133338
Mg11	-4.650759	1.001277	-0.443345
Mg12	0.202772	2.139190	-1.100280
Mg13	4.018658	-1.529692	1.973967
Mg14	-3.489088	-1.799503	-0.516760
Mg15	1.253321	0.248667	1.590672
Mg16	-1.375031	-1.708981	2.139733
Mg17	-1.202023	-3.872797	-0.021056
Mg18	1.337814	-2.870839	1.284857
Mg19	2.625200	3.035741	0.961812
Mg20	3.157051	1.810537	-1.723404

@mg20-isomer33 bp86/6-31G(d) Etot=-4001.841127 Eb=-14.03

Mg1	-0.873698	-2.007116	-2.010640
Mg2	2.130242	-2.085457	-1.844484
Mg3	3.359548	0.706130	-2.292102
Mg4	-3.869842	-1.784490	-2.445757
Mg5	0.410692	-2.074790	1.003205
Mg6	0.640272	0.434770	-0.887912
Mg7	3.045328	-3.589380	0.591184
Mg8	-2.772576	-1.590823	0.351098
Mg9	-2.415823	0.760500	-1.803183
Mg10	4.653991	-1.168898	-0.292506
Mg11	2.232131	3.493325	-1.473041
Mg12	-0.762110	3.304501	-1.281850
Mg13	-4.637070	0.399931	2.125158
Mg14	-5.636230	-0.246249	-0.584318
Mg15	3.299963	1.436965	0.777411
Mg16	-1.839425	-0.780624	2.993050
Mg17	0.843558	0.681538	2.311697
Mg18	-1.863910	1.675009	1.121720
Mg19	3.187669	-1.195126	2.386680
Mg20	0.867292	3.630285	1.254589

@mg20-isomer34 bp86/6-31G(d) Etot=-4001.840705 Eb=-14.02

Mg1	-1.110844	-0.714683	2.088135
Mg2	2.707418	-0.680611	-2.590011
Mg3	1.039349	-0.670746	-0.156826
Mg4	-1.302144	1.674939	-0.049612
Mg5	1.362189	1.462370	1.951724
Mg6	-3.343524	1.197547	-2.314461
Mg7	2.149123	-1.712323	2.301184
Mg8	4.130794	-1.809743	-0.068309
Mg9	4.648255	1.078222	-1.013310
Mg10	-4.226553	2.980096	-0.078142
Mg11	1.740629	2.073629	-1.256055
Mg12	-3.630927	0.940065	2.155418
Mg13	-2.248061	-1.367939	-0.836097
Mg14	-3.925878	-2.077423	1.620841
Mg15	0.277183	-2.869497	-2.259940
Mg16	4.287175	0.455210	1.959556

Mg17	-5.255444	0.068676	-0.240581
Mg18	-0.485420	0.183245	-2.713038
Mg19	-0.338539	-3.439373	0.620182
Mg20	3.525217	3.228338	0.879339

@mg20-isomer35 bp86/6-31G(d) Etot=-4001.838549 Eb=-13.95

Mg1	-1.006777	1.320575	-1.393357
Mg2	-2.191176	-1.517751	-1.492896
Mg3	-0.893991	-0.841685	1.294217
Mg4	2.123142	-1.261238	1.289424
Mg5	2.956950	-3.544476	-0.657530
Mg6	5.110985	-1.967503	0.711771
Mg7	-4.038949	1.006998	-0.813146
Mg8	-5.120012	-1.943369	-0.592304
Mg9	3.895791	-0.716102	-1.650621
Mg10	2.066582	1.766867	-1.408118
Mg11	-2.927543	-3.412105	0.867463
Mg12	-2.157608	1.975291	1.490067
Mg13	0.836957	-1.109947	-1.570662
Mg14	0.995977	1.541512	1.542042
Mg15	4.135410	1.099874	0.778130
Mg16	-3.921905	-0.575231	1.777952
Mg17	3.023183	3.912347	0.616332
Mg18	-2.931812	3.850372	-0.852704
Mg19	0.027072	3.956390	-0.067404
Mg20	0.017725	-3.540819	0.131345

@mg20-isomer36 bp86/6-31G(d) Etot=-4001.837671 Eb=-13.92

Mg1	0.516098	-2.064055	-0.753361
Mg2	2.281835	0.497068	-0.134345
Mg3	1.931965	-1.560341	2.086847
Mg4	-1.256320	-1.831261	1.975269
Mg5	0.208090	0.996990	1.962769
Mg6	3.602905	-2.622680	-0.399029
Mg7	-2.894614	0.912188	2.508916
Mg8	-1.842385	-0.138538	-0.368100
Mg9	-1.664451	2.926191	0.193395
Mg10	-2.636811	-3.095834	-0.582932
Mg11	4.797004	-0.571647	1.653007
Mg12	-4.585430	-0.998180	-1.714763
Mg13	0.194984	1.231178	-2.101052
Mg14	-3.006175	1.524961	-2.475945
Mg15	-4.377467	-1.412415	1.328195
Mg16	2.495203	-0.866660	-2.826594
Mg17	-4.630973	1.475565	0.127127
Mg18	1.301621	3.340185	0.245198
Mg19	5.120516	-0.115868	-1.368698
Mg20	4.444405	2.373153	0.644096

@mg20-isomer37 bp86/6-31G(d) Etot=-4001.834153 Eb=-13.81

Mg1	0.189791	-2.450752	1.225734
Mg2	-2.003852	-1.994037	-0.830776
Mg3	-2.337815	1.273697	0.058477
Mg4	0.856453	-2.634488	-1.749249
Mg5	-0.695842	0.309348	-2.320562
Mg6	1.553566	-0.111974	-0.343118
Mg7	-3.669515	-0.032221	-2.548415
Mg8	4.767740	-0.425031	0.531577
Mg9	0.274002	2.695852	-0.480384
Mg10	-5.501289	1.542173	-0.682783
Mg11	-5.021714	-1.322065	0.030324
Mg12	3.693243	1.774897	-1.400304
Mg13	3.223337	-3.082809	0.350268
Mg14	2.600431	4.514149	-0.119002

Mg15	2.972796	1.889271	1.528046
Mg16	2.636941	-1.009472	2.568107
Mg17	-2.467639	-1.185404	2.090491
Mg18	3.756912	-1.320638	-2.143153
Mg19	-4.712657	0.867315	2.168021
Mg20	-0.114889	0.702188	2.066700

@mg20-isomer38 bp86/6-31G(d) Etot=-4001.833754 Eb=-13.80

Mg1	-4.404177	0.104485	-2.630736
Mg2	-4.996660	-1.238299	-0.000988
Mg3	-1.762108	1.269190	-1.572228
Mg4	3.154646	0.551307	-1.829366
Mg5	5.147243	1.879623	0.001584
Mg6	2.884593	-2.499779	1.526134
Mg7	2.444802	3.339473	0.001490
Mg8	-2.316026	-1.812176	1.522384
Mg9	-4.396412	1.711524	0.000589
Mg10	0.519316	-0.793196	-2.575514
Mg11	-2.315174	-1.809289	-1.523213
Mg12	-1.761633	1.266248	1.572576
Mg13	2.884829	-2.497396	-1.527453
Mg14	-0.463447	3.773350	0.002699
Mg15	0.222781	-2.562179	-0.001038
Mg16	5.086393	-1.165329	0.000496
Mg17	0.518093	-0.796101	2.573501
Mg18	0.806879	0.626545	-0.001228
Mg19	-4.405983	0.102381	2.630435
Mg20	3.152044	0.549617	1.829874

@mg20-isomer39 bp86/6-31G(d) Etot=-4001.830347 Eb=-13.69

Mg1	2.178483	-1.397969	1.790198
Mg2	0.521191	-0.338296	-0.931921
Mg3	-0.589175	2.371362	-0.133655
Mg4	-2.005306	0.796223	-2.578978
Mg5	2.227041	1.684389	-2.248009
Mg6	-2.380343	-0.057052	0.576010
Mg7	4.920962	0.034456	1.870284
Mg8	-1.965237	-2.135049	-1.569435
Mg9	-0.730048	-2.384092	1.319459
Mg10	4.995972	1.802300	-0.747986
Mg11	-5.508202	0.373882	1.051506
Mg12	-0.018552	0.620608	2.451333
Mg13	-4.227364	-2.399079	0.622031
Mg14	3.663084	-0.926022	-0.979615
Mg15	-4.713161	-0.479033	-1.753551
Mg16	2.321133	1.571552	0.880475
Mg17	-3.121679	2.121875	2.303572
Mg18	6.835036	-0.499689	-0.375288
Mg19	-3.820592	2.338861	-0.729206
Mg20	1.416757	-3.099228	-0.817223

@mg20-isomer40 bp86/6-31G(d) Etot=-4001.830270 Eb=-13.69

Mg1	-2.606886	-2.563205	0.785768
Mg2	-0.413354	-0.523088	-0.280639
Mg3	0.243136	-2.672694	2.011372
Mg4	4.182522	0.749760	0.410524
Mg5	-1.195064	2.522481	0.607480
Mg6	5.411152	-1.979974	0.154872
Mg7	1.809430	1.167007	-1.435836
Mg8	-3.461493	0.275066	-0.273254
Mg9	1.889041	3.019300	1.020865
Mg10	0.406105	3.892268	-1.571747
Mg11	-0.003004	2.555524	3.367328
Mg12	2.367782	-2.033155	-0.229630

Mg13	1.531278	0.155177	1.985726
Mg14	-2.299070	-1.699049	-2.393374
Mg15	-1.267932	1.512673	-2.377909
Mg16	-1.648657	-0.045715	2.490877
Mg17	4.266699	-0.757407	-2.329892
Mg18	-4.762419	-0.789298	2.266430
Mg19	-0.317332	-3.569595	-0.937986
Mg20	-4.131935	0.783923	-3.270974

@mg20-isomer41 bp86/6-31G(d) Etot=-4001.828515 Eb=-13.64

Mg1	0.041456	-1.715824	1.441339
Mg2	5.022353	1.513751	-0.128000
Mg3	3.044860	0.373433	-2.434203
Mg4	-2.732189	0.443151	-2.580190
Mg5	3.296370	2.962757	1.906913
Mg6	-1.656611	-2.008149	-1.067337
Mg7	-4.609080	0.750256	1.635853
Mg8	0.262970	2.898295	1.153634
Mg9	4.674724	-1.465276	-0.617012
Mg10	-2.485690	2.388309	-0.169126
Mg11	2.923238	-2.881523	1.316826
Mg12	2.354970	2.935842	-0.928470
Mg13	0.523812	-4.431390	0.126452
Mg14	-3.043865	-1.890721	1.787595
Mg15	1.543189	-1.978507	-1.335942
Mg16	-1.618061	0.733000	2.113421
Mg17	2.332088	0.209106	0.913515
Mg18	-0.031890	0.719997	-1.220332
Mg19	-5.281700	1.658882	-1.223421
Mg20	-4.560944	-1.215389	-0.691514

@mg20-isomer42 bp86/6-31G(d) Etot=-4001.827175 Eb=-13.59

Mg1	-1.297822	0.189985	0.212930
Mg2	1.678771	0.138488	0.942518
Mg3	-2.615602	-2.294240	-1.633005
Mg4	2.529682	-2.137878	2.710922
Mg5	-4.302019	0.344108	-0.924229
Mg6	4.859488	-1.119118	0.922903
Mg7	-2.249540	2.845127	-0.914467
Mg8	0.359619	-1.410993	-2.026153
Mg9	0.198997	2.905846	1.008309
Mg10	3.176498	-0.034098	-1.888950
Mg11	-0.267129	-2.523105	1.072009
Mg12	5.772342	1.373976	-0.365390
Mg13	-2.648352	-4.411526	0.570473
Mg14	-3.598461	1.439628	1.895313
Mg15	-2.326143	4.164195	2.126941
Mg16	-2.029052	0.436811	-2.930902
Mg17	0.589083	1.709789	-1.748612
Mg18	-3.500215	-1.615194	1.337951
Mg19	2.538618	-2.679086	-0.286245
Mg20	3.131233	2.677283	-0.082316

@mg20-isomer43 bp86/6-31G(d) Etot=-4001.817073 Eb=-13.28

Mg1	1.307872	0.551760	0.333445
Mg2	-0.459434	0.569770	-2.107594
Mg3	-1.592155	1.829012	0.960367
Mg4	3.178863	0.705558	2.682687
Mg5	-1.350538	-2.411360	-2.433115
Mg6	0.634382	3.340305	-0.695766
Mg7	0.052335	-0.073953	2.935941
Mg8	-0.857289	-1.850176	0.467323
Mg9	2.277095	-2.065657	1.584172
Mg10	-3.232432	-0.254941	-0.863773

Mg11	2.688300	1.058387	-2.291024
Mg12	-5.401098	-1.775413	1.156711
Mg13	-3.618074	-3.337018	-0.677239
Mg14	-3.030325	-0.386859	2.382948
Mg15	-2.657761	2.767371	-1.718471
Mg16	4.289904	-0.530769	-0.359389
Mg17	1.741765	-1.899641	-1.548416
Mg18	4.204641	-3.639611	-0.287435
Mg19	-1.939845	4.938884	0.200658
Mg20	3.763796	2.464351	0.277971

@mg20-isomer44 bp86/6-31G(d) Etot=-4001.816294 Eb=-13.25

Mg1	-1.995090	1.353288	-1.486124
Mg2	0.047882	0.661395	0.964046
Mg3	1.047965	-2.275885	1.083932
Mg4	2.165018	3.061114	0.839625
Mg5	-4.991703	1.629510	-0.542709
Mg6	-2.695765	1.647235	1.560254
Mg7	-0.666109	3.752128	0.062699
Mg8	1.092280	1.526532	-1.859630
Mg9	-0.472918	-1.203784	-1.674770
Mg10	4.042878	1.600106	-0.964386
Mg11	-3.458735	-1.373573	-1.042013
Mg12	5.921798	0.216973	1.173058
Mg13	-4.999366	-0.440041	1.670896
Mg14	-1.495769	-3.686869	-0.202290
Mg15	2.491009	-1.172156	-1.480775
Mg16	-1.970745	-1.408381	1.722777
Mg17	-6.610329	-0.831048	-0.845483
Mg18	2.836652	0.256069	1.733549
Mg19	4.100895	-2.353798	0.803229
Mg20	5.610150	-0.958816	-1.515883

@mg20-isomer45 bp86/6-31G(d) Etot=-4001.816188 Eb=-13.25

Mg1	-0.280708	0.047702	0.300651
Mg2	-2.385477	-1.089589	-1.741946
Mg3	2.593940	-0.447398	-1.013651
Mg4	-4.770250	-1.788042	0.065918
Mg5	-0.734822	2.701951	1.688272
Mg6	3.439797	-3.353373	-0.388506
Mg7	2.108135	0.893273	1.995124
Mg8	-1.920839	-2.419140	0.950961
Mg9	4.626071	1.447420	0.385714
Mg10	-1.632297	2.168202	-1.494578
Mg11	1.555914	2.493495	-0.683965
Mg12	1.354327	-2.222090	1.581307
Mg13	0.213418	0.175260	-2.767306
Mg14	5.662601	-1.209261	-0.820830
Mg15	-3.196733	3.977799	0.473346
Mg16	4.326043	-1.290519	1.818918
Mg17	-7.582734	-3.133843	0.606416
Mg18	-0.396122	4.876741	-0.386926
Mg19	0.358896	-2.655306	-1.298664
Mg20	-3.339161	0.826718	0.729747

@mg20-isomer46 bp86/6-31G(d) Etot=-4001.807850 Eb=-12.99

Mg1	-0.084941	0.497370	1.086698
Mg2	0.510722	-1.566533	3.229061
Mg3	-3.022798	-0.874361	-0.270732
Mg4	-1.143549	-2.772205	0.923793
Mg5	-1.186602	1.889053	-1.354342
Mg6	-2.549045	-0.652679	2.758051
Mg7	1.769001	-2.211120	0.469035
Mg8	1.990594	0.892180	-1.086484

Mg9	-0.313115	-1.179039	-1.765880
Mg10	4.641645	-0.800541	-0.478313
Mg11	-4.250625	2.289557	-0.981187
Mg12	-3.100358	0.262615	-3.059776
Mg13	2.877946	0.237994	1.970432
Mg14	4.442538	2.146950	0.256295
Mg15	-5.119120	0.667540	1.521439
Mg16	6.079779	4.841663	0.043891
Mg17	-2.523503	2.308030	1.486355
Mg18	4.074567	-3.824707	-0.747391
Mg19	-5.782846	-0.305634	-1.382982
Mg20	2.689711	-1.846131	-2.617962

@mg20-isomer47 bp86/6-31G(d) Etot=-4001.798590 Eb=-12.70

Mg1	-1.974705	1.160667	1.213794
Mg2	0.234960	1.941835	-1.304038
Mg3	-1.800254	-2.139047	1.534939
Mg4	0.832084	-0.447227	1.149818
Mg5	-2.645395	-3.544292	-1.035169
Mg6	3.022161	1.563599	-0.162957
Mg7	0.831412	-3.026075	2.789395
Mg8	-1.151204	-0.928127	-1.250069
Mg9	-1.225206	4.414124	-0.042201
Mg10	-5.101454	1.770248	0.588911
Mg11	1.822082	-0.914763	-1.762154
Mg12	2.198724	-3.218995	0.103265
Mg13	0.734163	2.704064	1.596030
Mg14	-4.082532	-0.858932	-0.231750
Mg15	-2.945273	1.938771	-1.544181
Mg16	-0.404175	-4.783577	0.593512
Mg17	-4.125077	4.537217	0.091200
Mg18	6.125635	1.699871	-0.076868
Mg19	9.447927	1.716154	-0.072808
Mg20	0.206127	-3.585515	-2.178669

@mg20-isomer48 bp86/6-31G(d) Etot=-4001.783450 Eb=-12.22

Mg1	-0.392885	0.736069	-1.041952
Mg2	2.183223	1.748577	0.359967
Mg3	2.158805	-1.258056	-0.931606
Mg4	0.519980	-0.604248	1.659247
Mg5	3.640920	-0.693821	1.667251
Mg6	-2.462027	-0.402552	1.026566
Mg7	-3.754790	-2.845689	-0.391279
Mg8	-5.268810	0.055315	-0.495376
Mg9	-0.957151	2.208141	1.546335
Mg10	5.081232	0.779050	-0.580883
Mg11	0.351319	3.938939	-0.642077
Mg12	7.795429	-0.697972	-1.295691
Mg13	-6.854620	-2.663437	-0.180166
Mg14	6.897675	-0.800160	1.536781
Mg15	-3.132885	2.251204	-0.932580
Mg16	5.287409	-2.292786	-0.610971
Mg17	-0.730024	-2.394861	-0.715286
Mg18	-5.155977	-1.546527	2.153089
Mg19	-2.373426	4.941482	0.222669
Mg20	-2.833397	-0.458667	-2.354039

@mg20-isomer49 bp86/6-31G(d) Etot=-4001.749968 Eb=-11.17

Mg1	-3.174221	0.349478	0.667590
Mg2	-5.674209	2.134658	-0.009544
Mg3	-0.621599	-1.407913	0.706040
Mg4	-5.810162	-0.721201	1.735020
Mg5	-0.802711	1.543564	2.164429
Mg6	-5.197075	-0.625043	-1.571822

Mg7	-3.594254	-2.689240	0.359234
Mg8	1.842301	0.474227	1.148636
Mg9	-2.159342	-1.094507	-1.993870
Mg10	-0.496726	1.323312	-0.898885
Mg11	4.808474	0.071873	1.018695
Mg12	7.556225	1.300242	-0.242049
Mg13	7.531530	-0.455892	2.417353
Mg14	-6.629873	-3.055416	-0.043443
Mg15	9.046238	-0.139207	-2.876771
Mg16	7.131619	-1.583764	-0.536266
Mg17	10.109233	-0.568500	0.067825
Mg18	-3.312037	1.762836	-2.210579
Mg19	-2.625506	3.365921	0.308120
Mg20	-7.927904	0.014572	-0.209714

@mg21-isomer01 bp86/6-31G(d) Etot=-4201.993305 Eb=-15.83

Mg1	1.730810	-2.719828	0.457744
Mg2	4.514103	-1.911424	-0.849535
Mg3	2.850347	0.475722	-1.797853
Mg4	-0.786286	-2.605670	-1.378611
Mg5	-0.000744	-0.072586	-3.028442
Mg6	1.997999	-2.365062	-2.556811
Mg7	3.240531	-0.136370	1.230455
Mg8	1.990341	2.564617	0.372522
Mg9	-2.919320	-0.524688	-2.172100
Mg10	-5.722907	-0.156563	-0.248936
Mg11	1.047699	2.759848	-2.603852
Mg12	-1.097178	-2.311915	1.708889
Mg13	0.287041	0.003196	0.129135
Mg14	-2.707326	0.233589	0.940175
Mg15	-1.105258	0.128165	3.565969
Mg16	1.524139	1.506109	3.240059
Mg17	-1.690116	2.076261	-1.364381
Mg18	-0.148645	4.556752	-0.523846
Mg19	-0.850677	2.556605	1.657958
Mg20	1.412293	-1.504845	3.278933
Mg21	-3.566847	-2.551913	-0.057472

@mg21-isomer02 bp86/6-31G(d) Etot=-4201.988802 Eb=-15.69

Mg1	-5.039308	0.457066	-0.000021
Mg2	-2.403090	2.626748	-0.000109
Mg3	0.002182	2.280191	1.928628
Mg4	-0.000012	-0.136803	3.711616
Mg5	-2.475556	0.419823	-2.047581
Mg6	2.806465	-1.830794	0.000073
Mg7	0.004380	4.586680	-0.000146
Mg8	0.000023	-0.137095	-3.711615
Mg9	-1.515856	-2.447592	2.644080
Mg10	1.513180	-2.450152	2.645197
Mg11	-2.809813	-1.825798	0.000053
Mg12	-0.000877	-0.115639	-0.000012
Mg13	-0.001989	-3.137352	0.000106
Mg14	0.002219	2.280052	-1.928772
Mg15	-2.475573	0.419960	2.047487
Mg16	2.474633	0.415649	-2.045943
Mg17	5.038232	0.452841	-0.000047
Mg18	2.408751	2.624618	-0.000007
Mg19	-1.515803	-2.447764	-2.643928
Mg20	1.513204	-2.450349	-2.645020
Mg21	2.474608	0.415709	2.045963

@mg21-isomer03 bp86/6-31G(d) Etot=-4201.987752 Eb=-15.66

Mg1	0.333704	-2.584803	-2.618813
Mg2	-0.718930	0.002743	-3.685996

Mg3	-2.654190	-1.969897	2.693559
Mg4	1.931338	-0.080317	-2.143524
Mg5	0.320962	-2.571173	2.632234
Mg6	-2.880066	1.026253	1.740814
Mg7	-2.319901	3.449457	-0.012172
Mg8	2.196688	2.021788	0.000947
Mg9	-0.132064	2.348007	1.939314
Mg10	-0.463233	-0.080908	0.000493
Mg11	-2.870920	1.017976	-1.756859
Mg12	-0.123292	2.339719	-1.949343
Mg13	7.294143	-0.395095	-0.000168
Mg14	-0.736967	0.020709	3.685675
Mg15	0.452599	4.576369	-0.009314
Mg16	-1.198105	-3.005579	0.004266
Mg17	4.133872	-0.420630	0.013306
Mg18	-2.640685	-1.983287	-2.695525
Mg19	1.921416	-0.069982	2.155369
Mg20	-3.682999	-1.298207	-0.004630
Mg21	1.836629	-2.343144	0.010366

@mg21-isomer04 bp86/6-31G(d) Etot=-4201.985672 Eb=-15.60

Mg1	3.460604	2.430991	0.004828
Mg2	0.430435	3.160128	0.003365
Mg3	-1.589510	1.932883	-1.908751
Mg4	-0.601981	-0.243490	-3.675420
Mg5	1.532623	1.342438	2.155620
Mg6	-2.009165	-3.133229	-0.004423
Mg7	-2.571131	4.021013	0.001112
Mg8	-0.607490	-0.249393	3.675058
Mg9	1.868733	-1.599625	-2.643014
Mg10	-0.811151	-3.003679	-2.713446
Mg11	2.922101	-0.510446	0.002903
Mg12	-0.284882	-0.158746	-0.000937
Mg13	0.983282	-2.920968	0.000300
Mg14	-1.592755	1.930793	1.910520
Mg15	1.537931	1.347038	-2.151276
Mg16	-2.888670	-0.794721	1.702034
Mg17	6.166420	0.430531	-0.001753
Mg18	-4.105060	1.423504	-0.001906
Mg19	1.865177	-1.605088	2.645974
Mg20	-0.817395	-3.006504	2.708660
Mg21	-2.888117	-0.793432	-1.709447

@mg21-isomer05 bp86/6-31G(d) Etot=-4201.982209 Eb=-15.50

Mg1	0.589644	-2.297217	-2.122997
Mg2	0.885127	-2.674812	1.090304
Mg3	2.231164	1.433980	3.596396
Mg4	5.394008	-0.096745	-0.860310
Mg5	-1.837760	3.065638	-2.981256
Mg6	-0.579012	0.330977	-3.125193
Mg7	-2.357673	-1.761293	-1.502101
Mg8	-3.085236	1.058756	-1.130390
Mg9	0.990440	2.850214	-2.253659
Mg10	-2.095764	-2.220523	1.707105
Mg11	-1.157506	-4.229001	-0.424346
Mg12	2.756033	-0.395619	1.298196
Mg13	2.321171	0.228238	-1.893070
Mg14	3.302436	-2.510498	-0.902613
Mg15	-4.694450	-1.038425	0.588391
Mg16	-0.417691	2.527015	2.987222
Mg17	-0.030059	-0.517869	3.182944
Mg18	-0.227015	0.053028	0.034444
Mg19	1.790506	2.364545	0.623285
Mg20	-2.610823	0.777256	1.984143

Mg21	-1.167539	3.052357	0.103505
@mg21-isomer06 bp86/6-31G(d) Etot=-4201.979379 Eb=-15.41			
Mg1	2.795142	1.984461	0.152376
Mg2	2.917701	-0.852721	0.960148
Mg3	-2.725934	-1.871183	-1.642517
Mg4	-1.303058	2.162846	2.502312
Mg5	-3.847477	0.908273	-2.065530
Mg6	0.140285	0.118701	0.155867
Mg7	0.194935	-2.141973	-2.044513
Mg8	-1.356449	-2.552086	1.073526
Mg9	0.698836	3.810155	1.113508
Mg10	-0.982400	0.561594	-2.793716
Mg11	-2.843014	0.056432	0.900331
Mg12	-1.772420	2.557945	-0.483385
Mg13	4.902571	0.226192	-1.235715
Mg14	1.407529	1.061182	2.917845
Mg15	3.197299	-2.310320	-1.812748
Mg16	0.813742	3.076677	-1.900867
Mg17	2.002327	0.359111	-2.450813
Mg18	1.117406	-2.088670	3.088878
Mg19	1.439945	-3.435990	0.406328
Mg20	-5.540319	-1.043399	-0.409905
Mg21	-1.256645	-0.587228	3.568590
@mg21-isomer07 bp86/6-31G(d) Etot=-4201.977037 Eb=-15.34			
Mg1	-0.142556	-1.555191	2.802321
Mg2	2.379756	-0.050428	-2.923282
Mg3	2.378046	-2.560279	-1.419210
Mg4	-0.145135	-3.202154	0.054607
Mg5	0.766753	-0.000065	0.000007
Mg6	2.379010	2.559133	1.419415
Mg7	-0.143564	3.201937	-0.054604
Mg8	3.726943	-0.000919	0.000127
Mg9	-0.142382	-1.649929	-2.747748
Mg10	2.379052	2.509262	-1.505669
Mg11	2.379580	0.049289	2.923439
Mg12	2.377917	-2.510416	1.505806
Mg13	-0.141512	1.555718	-2.803442
Mg14	-0.141698	1.650443	2.748769
Mg15	-2.639802	-0.051065	-3.032812
Mg16	-2.642502	-2.651584	-1.472172
Mg17	-2.641072	2.652619	1.471962
Mg18	-2.063248	0.000284	-0.000050
Mg19	-2.640972	2.600955	-1.561715
Mg20	-2.640011	0.052329	3.032652
Mg21	-2.642603	-2.599937	1.561600
@mg21-isomer08 bp86/6-31G(d) Etot=-4201.974772 Eb=-15.27			
Mg1	1.783923	-1.617926	3.665347
Mg2	-2.297763	1.359160	2.064835
Mg3	0.679063	1.206130	3.053138
Mg4	-2.398891	3.133416	-0.636429
Mg5	0.951186	0.135611	-3.433858
Mg6	0.428065	2.798525	-1.875450
Mg7	2.155782	2.475299	0.643742
Mg8	3.165142	1.136336	-1.809860
Mg9	2.823602	-0.429121	1.069336
Mg10	-2.380708	-1.326447	0.771726
Mg11	5.715374	-0.727649	-0.824360
Mg12	-1.857581	-4.094434	-0.188870
Mg13	-4.281035	0.737853	-0.360401
Mg14	0.566777	-2.541436	0.951242
Mg15	2.423873	-1.793313	-1.611048

Mg16	0.014901	0.359724	-0.014231
Mg17	-0.523173	-2.060034	-2.028374
Mg18	-1.103071	-1.205248	3.413508
Mg19	-1.863403	0.697721	-2.399412
Mg20	-3.536701	-1.857366	-1.966787
Mg21	-0.465363	3.613200	1.516204

@mg21-isomer09 bp86/6-31G(d) Etot=-4201.974282 Eb=-15.26

Mg1	2.274546	-0.227268	-1.431292
Mg2	3.353898	-0.534939	1.433867
Mg3	-0.478340	0.075597	-0.072673
Mg4	-3.539944	1.630526	-0.849188
Mg5	-0.183248	-2.038125	-2.346106
Mg6	-3.159273	-1.245462	-0.134813
Mg7	-1.143328	-3.155777	0.955146
Mg8	0.611349	-1.145150	2.572751
Mg9	-0.224383	-4.806623	-1.358102
Mg10	-3.665221	1.223913	2.059128
Mg11	-2.427875	-1.308485	2.936011
Mg12	-1.293435	2.842452	0.769907
Mg13	1.713120	-2.773698	0.088439
Mg14	-2.444331	-0.190270	-2.973873
Mg15	-1.026248	1.335249	3.494521
Mg16	-1.516220	2.878375	-2.605046
Mg17	0.316675	0.745137	-3.500607
Mg18	1.437638	1.815821	1.866467
Mg19	1.132657	2.630131	-1.161648
Mg20	3.832518	2.099228	0.100412
Mg21	6.429446	0.149367	0.156700

@mg21-isomer10 bp86/6-31G(d) Etot=-4201.971977 Eb=-15.19

Mg1	1.492270	2.577289	0.916974
Mg2	0.359702	2.156779	-2.069677
Mg3	-0.595144	-1.213624	2.931784
Mg4	-1.434395	3.033917	0.395850
Mg5	-0.898305	-1.071087	-2.667475
Mg6	3.310866	1.917742	-1.470912
Mg7	1.401581	-2.621794	-1.337949
Mg8	-2.324211	-1.869940	0.130691
Mg9	-0.592563	1.971626	3.167774
Mg10	1.883658	0.477921	3.513133
Mg11	0.209496	-0.004646	0.089750
Mg12	-0.174704	-3.659576	1.116312
Mg13	-5.650130	-0.454360	0.583623
Mg14	-1.244539	-3.998101	-1.687494
Mg15	1.934218	-0.169918	-3.153524
Mg16	-2.254932	3.464456	-2.632544
Mg17	3.906757	-1.009584	-1.028277
Mg18	2.230969	-1.793638	1.488067
Mg19	-2.721135	0.827369	-1.300299
Mg20	-2.741072	0.627118	1.725660
Mg21	3.901612	0.812051	1.288532

@mg21-isomer11 bp86/6-31G(d) Etot=-4201.968955 Eb=-15.10

Mg1	-0.596829	-0.147602	0.050960
Mg2	-1.641310	-1.636242	-2.739619
Mg3	1.660070	1.350300	1.810089
Mg4	0.665073	2.568074	-0.776666
Mg5	0.893605	0.357660	-2.917524
Mg6	-0.477674	0.000979	3.660265
Mg7	-3.653194	-0.313237	-1.025873
Mg8	2.215138	-1.282321	-0.749759
Mg9	-1.395391	-2.695276	2.654560
Mg10	0.003662	-3.205514	-0.360685

Mg11	3.401199	1.426586	-0.975803
Mg12	-1.708045	4.297725	-0.713750
Mg13	1.029429	-2.647458	-3.274963
Mg14	1.403892	-1.782722	2.082027
Mg15	-3.048491	-0.197962	2.006286
Mg16	4.073778	-0.288912	1.617420
Mg17	-1.825752	1.639212	-2.430276
Mg18	-3.603603	2.287098	0.283482
Mg19	-2.854695	-2.917325	-0.001885
Mg20	-1.070023	2.461672	1.854100
Mg21	6.529164	0.725266	-0.052386

@mg21-isomer12 bp86/6-31G(d) Etot=-4201.968532 Eb=-15.09

Mg1	-0.240325	0.804861	-2.837155
Mg2	2.163052	0.439558	-0.903702
Mg3	-0.538712	-0.526189	-0.033451
Mg4	-3.583357	2.520334	0.809205
Mg5	1.220300	3.180523	-1.413946
Mg6	-2.387302	0.207449	2.313448
Mg7	2.398506	2.537696	1.365119
Mg8	3.802562	-0.182279	2.017495
Mg9	-3.074184	0.416911	-1.445688
Mg10	4.990344	1.503810	-0.254523
Mg11	1.419629	-2.196287	-2.213743
Mg12	-3.108199	-2.237339	0.211620
Mg13	-0.851858	-2.544994	2.296547
Mg14	-1.559766	-2.083361	-2.578424
Mg15	-0.604661	2.527444	1.086368
Mg16	-0.427789	-3.825360	-0.440673
Mg17	1.887894	-2.309693	0.891735
Mg18	-5.116238	-0.078587	0.866086
Mg19	-1.788801	3.161586	-1.680813
Mg20	4.523019	-1.537446	-0.678867
Mg21	0.875885	0.221362	2.623362

@mg21-isomer13 bp86/6-31G(d) Etot=-4201.966855 Eb=-15.04

Mg1	-0.749434	-0.148583	-0.005231
Mg2	1.483043	1.565109	-2.936869
Mg3	-1.596494	2.262693	1.875202
Mg4	1.305287	1.031031	1.971939
Mg5	-1.597428	-2.489637	-1.656877
Mg6	2.821655	2.593688	-0.208743
Mg7	4.505680	-2.206298	0.734578
Mg8	-3.369536	-2.179240	0.869822
Mg9	-4.102324	0.601096	1.516438
Mg10	-0.785336	-3.486727	1.293852
Mg11	-3.150994	2.357129	-0.743507
Mg12	0.871397	4.008333	1.703817
Mg13	1.620608	-2.014442	2.009766
Mg14	5.252867	0.705387	0.304242
Mg15	2.341286	-0.348268	-0.622511
Mg16	0.869263	-1.437985	-3.111169
Mg17	1.410142	-3.253763	-0.723003
Mg18	-1.403230	-0.803003	2.848425
Mg19	-0.206039	2.893867	-0.886495
Mg20	-1.516149	0.755951	-2.840645
Mg21	-4.004263	-0.406339	-1.393031

@mg21-isomer14 bp86/6-31G(d) Etot=-4201.965640 Eb=-15.00

Mg1	-0.815718	-0.123867	-0.036084
Mg2	-1.628535	2.883809	-0.677444
Mg3	-1.361068	1.777978	2.429537
Mg4	2.109863	0.121291	-1.305404
Mg5	2.840770	-1.117000	1.564778

Mg6	-1.731186	-3.048713	0.410341
Mg7	5.376493	-0.393594	-0.311252
Mg8	3.447329	-2.692127	-0.904660
Mg9	-2.950141	-1.064972	2.398194
Mg10	0.108590	-1.228779	2.872198
Mg11	-0.400597	1.081220	-2.877459
Mg12	0.202792	4.150681	1.315090
Mg13	-3.422659	0.847606	-2.188745
Mg14	-2.198692	-1.861183	-2.497689
Mg15	-3.893669	1.334841	0.731906
Mg16	1.486854	1.517668	1.467275
Mg17	1.292595	3.076928	-1.347607
Mg18	-4.260742	-1.486964	-0.312959
Mg19	0.560947	-2.535981	-1.657395
Mg20	1.109012	-3.513919	1.151227
Mg21	4.127762	2.275077	-0.223849

@mg21-isomer15 bp86/6-31G(d) Etot=-4201.964283 Eb=-14.96

Mg1	-0.829380	2.722324	0.014438
Mg2	-2.340429	-0.716600	-2.539248
Mg3	1.563833	0.221974	-0.938092
Mg4	0.166021	1.008004	2.484530
Mg5	-1.914270	-1.165197	3.021237
Mg6	-1.167229	-0.288139	0.040287
Mg7	1.128657	2.837916	-2.401633
Mg8	2.563470	2.486237	3.415326
Mg9	-2.087122	-3.038333	0.459347
Mg10	3.138472	-0.040374	1.677489
Mg11	0.341255	0.235683	-3.813671
Mg12	-3.620891	1.487193	-0.661583
Mg13	0.275349	-2.355284	-2.241679
Mg14	5.272858	-0.436865	-0.833797
Mg15	2.823053	-2.466811	-0.402421
Mg16	0.747649	-1.981422	1.781434
Mg17	-2.842035	1.648139	2.325416
Mg18	2.262192	2.777007	0.456535
Mg19	-1.770258	2.265400	-2.965561
Mg20	-4.268760	-0.771258	1.237311
Mg21	0.557565	-4.429595	-0.115664

@mg21-isomer16 bp86/6-31G(d) Etot=-4201.963199 Eb=-14.93

Mg1	-0.358460	0.198651	0.252329
Mg2	-4.392715	0.145533	0.618543
Mg3	-2.228042	1.427708	2.316405
Mg4	-0.057935	-0.889729	3.284438
Mg5	1.571229	-0.742606	-1.896112
Mg6	-2.284612	-2.008191	1.518893
Mg7	0.429120	-3.367758	1.804621
Mg8	2.216428	-3.347382	-0.590941
Mg9	4.635343	-1.592637	-1.037817
Mg10	0.761889	1.985626	3.015842
Mg11	2.252568	2.370887	0.466854
Mg12	-2.608297	2.281035	-0.730292
Mg13	0.254236	2.440279	-1.870500
Mg14	-0.439202	3.655632	0.849500
Mg15	3.250321	1.832902	-2.286687
Mg16	-4.553948	0.553959	-2.315037
Mg17	2.409924	-0.830133	1.275930
Mg18	-0.705738	-2.817650	-1.048818
Mg19	-1.567273	-0.207056	-2.492116
Mg20	5.027346	1.049337	0.071498
Mg21	-3.612182	-2.138406	-1.206533

@mg21-isomer17 bp86/6-31G(d) Etot=-4201.962577 Eb=-14.91

Mg1	-1.004608	-0.854405	-2.608186
Mg2	-3.886370	-1.426470	-1.408148
Mg3	-3.182595	1.310838	-2.488712
Mg4	1.863592	-0.005086	-1.756282
Mg5	-1.605038	-3.366943	-0.956219
Mg6	-0.363480	2.311607	-1.888984
Mg7	-4.507432	0.719543	0.449219
Mg8	1.320387	-2.881754	-1.207833
Mg9	2.428695	2.582653	-0.257149
Mg10	-2.709195	-1.683314	1.461366
Mg11	-0.098309	-3.533189	1.605213
Mg12	-0.077473	3.420182	1.065591
Mg13	-0.507923	0.097881	0.204809
Mg14	4.344052	-1.707646	-0.921873
Mg15	4.862444	1.125931	-1.745489
Mg16	-2.113100	1.392214	2.384532
Mg17	-2.717305	2.986089	-0.073047
Mg18	2.098833	-1.428833	1.299225
Mg19	1.600745	1.367391	2.488026
Mg20	-0.251782	-1.078282	3.238911
Mg21	4.505862	0.651593	1.115029

@mg21-isomer18 bp86/6-31G(d) Etot=-4201.962552 Eb=-14.91

Mg1	-0.747752	0.701094	-2.440919
Mg2	1.285395	3.184777	1.209690
Mg3	-1.294904	2.914747	-0.485219
Mg4	1.330347	0.206966	-0.108012
Mg5	-3.665930	1.280872	-1.768000
Mg6	-0.151730	-2.140391	-1.552018
Mg7	-2.998129	-1.624751	-2.324637
Mg8	1.509143	2.863776	-1.841627
Mg9	-3.900020	1.845936	1.141045
Mg10	3.246525	0.385139	-2.510250
Mg11	-2.353205	-2.983746	0.421401
Mg12	0.931727	0.623109	2.887982
Mg13	0.645157	-3.987361	0.604195
Mg14	-0.412128	-2.119221	2.656818
Mg15	-4.708536	-0.956568	0.089543
Mg16	-1.555828	-0.063275	0.695558
Mg17	2.525174	-1.911069	1.862721
Mg18	2.773468	-2.446263	-1.162190
Mg19	3.957762	2.176865	0.055522
Mg20	-1.311763	2.656105	2.567341
Mg21	4.895226	-0.606741	0.001057

@mg21-isomer19 bp86/6-31G(d) Etot=-4201.961105 Eb=-14.86

Mg1	-2.635843	2.361683	-2.222793
Mg2	0.118157	2.967122	-0.949004
Mg3	-2.403923	2.535326	0.737545
Mg4	2.830551	2.138674	3.589834
Mg5	2.873858	2.362627	0.466197
Mg6	-0.251766	0.496350	-2.913495
Mg7	2.553330	1.769530	-2.437341
Mg8	-5.155559	1.347967	-0.142078
Mg9	0.208028	2.322881	2.165849
Mg10	0.664084	0.020082	0.001017
Mg11	4.254438	-0.147113	-0.843608
Mg12	-2.434803	-0.362494	-0.934238
Mg13	-4.978738	-1.377697	0.978484
Mg14	3.034453	-0.446603	1.975314
Mg15	2.310039	-1.307551	-2.920619
Mg16	-1.790679	-0.104121	2.164034
Mg17	-0.279403	-2.447982	-1.824039
Mg18	-2.217014	-2.842240	0.768905

Mg19	0.514246	-2.212149	2.198767
Mg20	2.559690	-2.565157	-0.138280
Mg21	0.226854	-4.509133	0.279550

@mg21-isomer20 bp86/6-31G(d) Etot=-4201.958806 Eb=-14.80

Mg1	-1.288073	2.835494	2.131331
Mg2	-0.848920	0.364552	0.069413
Mg3	1.094957	3.053230	0.336060
Mg4	-3.758247	1.819063	0.546274
Mg5	0.380745	1.854002	-2.410842
Mg6	3.472475	1.383745	1.247344
Mg7	-2.410256	-0.303404	2.513590
Mg8	-2.697004	0.814825	-2.317687
Mg9	0.802798	0.683244	2.734429
Mg10	5.154102	-0.187701	-0.662954
Mg11	-4.517967	-0.967518	0.128756
Mg12	-0.569955	-1.565148	-2.249701
Mg13	3.697052	-2.816147	-1.032908
Mg14	2.621888	-1.588091	1.737178
Mg15	-1.614328	3.431242	-0.883511
Mg16	-0.150414	-2.392018	2.693813
Mg17	1.908551	-0.357475	-0.967918
Mg18	-3.434481	-2.345597	-2.288996
Mg19	0.826860	-3.275057	-0.112586
Mg20	3.397290	2.332026	-1.606209
Mg21	-2.067075	-2.773267	0.395123

@mg21-isomer21 bp86/6-31G(d) Etot=-4201.958787 Eb=-14.80

Mg1	0.022138	1.653550	-2.333676
Mg2	-1.043332	0.000256	0.026223
Mg3	-3.106923	-2.644613	1.340390
Mg4	-2.565323	0.002698	-2.770793
Mg5	-2.824136	-0.000253	2.607186
Mg6	0.019617	-1.652531	-2.335419
Mg7	-0.239670	-1.725688	2.452045
Mg8	1.935117	1.649238	0.170124
Mg9	2.634084	-0.001175	-2.290311
Mg10	5.102103	-1.488764	-0.952400
Mg11	1.932678	-1.652425	0.168371
Mg12	-0.489369	-3.595813	0.015491
Mg13	5.172123	0.001653	1.679449
Mg14	-4.227859	0.002083	-0.159944
Mg15	2.303668	-0.003126	2.711235
Mg16	-0.237672	1.722174	2.453731
Mg17	-2.952438	-2.660706	-1.594840
Mg18	-2.949497	2.665415	-1.592560
Mg19	5.103182	1.487408	-0.955814
Mg20	-0.484822	3.594937	0.018888
Mg21	-3.103669	2.645681	1.342623

@mg21-isomer22 bp86/6-31G(d) Etot=-4201.958439 Eb=-14.79

Mg1	0.940288	0.271750	-2.441578
Mg2	2.218357	1.628812	-0.029361
Mg3	3.898529	0.130847	-2.262976
Mg4	-0.829502	-0.017220	0.168590
Mg5	5.527584	-1.499741	-0.228908
Mg6	5.678702	1.445520	-0.157085
Mg7	-3.638734	-2.096031	-1.344790
Mg8	-0.510934	2.807099	-1.231781
Mg9	1.241614	-0.099230	2.452933
Mg10	-3.169056	-1.994187	1.685427
Mg11	-2.188489	-4.302012	0.020858
Mg12	-0.088920	-2.750455	1.509733
Mg13	-3.563804	2.934147	-1.688845

Mg14	0.048399	2.671520	1.822279
Mg15	-0.508210	-2.444848	-1.736263
Mg16	4.200130	-0.023658	2.048928
Mg17	-2.226193	0.689698	2.702597
Mg18	-4.087425	0.574680	0.218705
Mg19	-2.229914	0.313904	-2.444675
Mg20	-2.856465	3.272499	1.141903
Mg21	2.144044	-1.513094	-0.205692

@mg21-isomer23 bp86/6-31G(d) Etot=-4201.958285 Eb=-14.78

Mg1	3.081378	-1.968296	-1.039347
Mg2	4.008672	-1.798851	1.845522
Mg3	1.994799	2.962782	1.633766
Mg4	-1.647795	-1.161063	-1.111686
Mg5	1.148585	-2.555689	1.325327
Mg6	-4.172448	-1.796786	0.637962
Mg7	-1.035917	1.766633	-2.199863
Mg8	0.958349	-0.567708	-2.871852
Mg9	-3.978846	0.648665	-2.112267
Mg10	0.447972	-3.288188	-1.598018
Mg11	3.736453	0.843606	0.269787
Mg12	-5.940494	0.462906	0.146168
Mg13	1.831388	2.567328	-1.589166
Mg14	1.792132	0.183134	2.867028
Mg15	-0.529084	3.649215	0.079392
Mg16	0.575771	0.414051	0.112049
Mg17	-0.622261	2.150748	2.773948
Mg18	-2.588775	1.422818	0.542101
Mg19	3.897289	0.448684	-2.678056
Mg20	-1.617483	-3.525155	0.756154
Mg21	-1.339687	-0.858833	2.211051

@mg21-isomer24 bp86/6-31G(d) Etot=-4201.957314 Eb=-14.75

Mg1	-1.681883	-0.234169	0.132440
Mg2	2.512617	0.624952	-2.290681
Mg3	0.724508	-3.141651	0.728083
Mg4	-1.759528	-2.239122	2.390175
Mg5	-2.157892	-3.148328	-0.487755
Mg6	0.187669	-1.710923	-1.899272
Mg7	-4.671182	-1.017558	-0.226024
Mg8	3.824712	1.869040	0.399585
Mg9	0.949379	-1.269496	3.179413
Mg10	-0.585869	1.381886	-2.290991
Mg11	1.137539	0.427700	0.440969
Mg12	1.395694	3.285924	-1.096544
Mg13	1.159651	3.123444	1.931605
Mg14	3.337948	-1.449954	1.348360
Mg15	-2.764620	-1.077582	-2.697417
Mg16	2.980003	-2.460246	-1.409160
Mg17	-3.892073	1.544479	1.347483
Mg18	5.182378	-0.418650	-0.849732
Mg19	-3.559544	1.721155	-1.591454
Mg20	-1.333764	3.025827	0.207232
Mg21	-0.985744	1.163273	2.733685

@mg21-isomer25 bp86/6-31G(d) Etot=-4201.956783 Eb=-14.74

Mg1	3.259409	0.733013	-0.362920
Mg2	1.499376	0.362313	-2.999805
Mg3	0.154788	0.043478	-0.016444
Mg4	-1.111634	1.519371	2.892243
Mg5	-3.162933	-0.383731	1.854295
Mg6	-2.479348	2.083029	0.235839
Mg7	0.324509	3.275918	0.652027
Mg8	-0.162526	-2.236610	-2.412756

Mg9	2.690607	-2.038406	-1.588615
Mg10	-5.310541	1.060301	-0.374573
Mg11	1.895357	1.359761	2.399249
Mg12	-5.110993	-1.875200	-0.372066
Mg13	3.395817	3.510246	0.885648
Mg14	-1.927401	-2.421858	0.057659
Mg15	2.568747	-1.503523	1.672154
Mg16	-2.554460	-0.161830	-1.810470
Mg17	2.115869	3.150667	-1.848844
Mg18	4.135855	-3.752321	0.445012
Mg19	-0.700187	2.366651	-2.206287
Mg20	0.854636	-3.505590	0.306981
Mg21	-0.374948	-1.585676	2.591673

@mg21-isomer26 bp86/6-31G(d) Etot=-4201.956605 Eb=-14.73

Mg1	2.882846	0.830180	1.727553
Mg2	2.727103	2.545459	-0.915195
Mg3	5.250164	0.936731	-0.264274
Mg4	1.398681	-2.023485	1.754024
Mg5	4.108225	-1.793711	0.233565
Mg6	1.021564	3.250605	1.708565
Mg7	-1.440188	-2.067485	2.760222
Mg8	1.679605	-2.931434	-1.309885
Mg9	-3.444979	-2.286799	0.308483
Mg10	-4.617503	0.645926	0.738878
Mg11	-0.299487	2.948511	-0.931465
Mg12	1.049507	-0.007953	-0.819157
Mg13	-1.271546	0.869196	-2.786013
Mg14	-2.004538	2.698755	1.609111
Mg15	-1.213738	-2.070101	-1.854620
Mg16	0.044345	0.611441	2.845103
Mg17	-1.591602	0.058273	0.371294
Mg18	-3.980136	-0.441409	-1.999666
Mg19	-0.664404	-3.850483	0.500621
Mg20	3.621903	-0.423783	-2.431962
Mg21	-3.255822	2.501566	-1.245183

@mg21-isomer27 bp86/6-31G(d) Etot=-4201.954838 Eb=-14.68

Mg1	-0.952851	-0.250630	0.083190
Mg2	-1.541064	3.134065	-0.170376
Mg3	1.447718	1.804659	-0.946512
Mg4	0.820702	4.206777	1.079806
Mg5	-0.254941	-0.262684	-2.934660
Mg6	0.132007	-2.500591	2.097376
Mg7	0.035397	-2.959352	-1.191923
Mg8	-0.198529	1.578873	2.234182
Mg9	2.544671	-3.317606	0.319582
Mg10	2.153011	-0.435159	1.207918
Mg11	5.139652	-1.827537	-0.158506
Mg12	-3.126990	1.115139	-1.800019
Mg13	-3.476198	1.594427	1.456873
Mg14	2.423383	-1.080835	-1.828252
Mg15	-2.441376	-3.156399	0.746656
Mg16	-4.517007	-0.941119	0.413574
Mg17	-2.718343	-1.886831	-1.953235
Mg18	3.012926	2.381194	1.829726
Mg19	4.687837	1.048639	-0.275724
Mg20	-2.467344	-0.954801	2.809358
Mg21	-0.702661	2.709770	-3.019034

@mg21-isomer28 bp86/6-31G(d) Etot=-4201.948791 Eb=-14.50

Mg1	0.898525	0.717510	-2.344879
Mg2	2.242845	1.449579	0.352876
Mg3	3.854327	0.615140	-2.226593

Mg4	-0.914748	-0.174467	0.231939
Mg5	5.430614	-1.292930	-0.325324
Mg6	5.623372	1.633578	0.080056
Mg7	-3.688287	-1.593953	-0.816142
Mg8	-0.298171	2.883815	-0.530536
Mg9	1.426290	-0.925976	2.192010
Mg10	-2.684389	-2.777156	1.817843
Mg11	-2.402873	-4.245064	-0.792538
Mg12	0.095268	-3.220061	0.628267
Mg13	-3.085487	3.513298	-1.524288
Mg14	-0.138281	1.815229	2.389389
Mg15	-0.626005	-2.061128	-2.143769
Mg16	4.329803	-0.096462	2.236100
Mg17	-2.955562	0.244404	2.451089
Mg18	-4.374935	1.238921	-0.086518
Mg19	-2.253384	0.696503	-2.343459
Mg20	-2.669769	3.120452	1.526040
Mg21	2.190847	-1.541233	-0.771564

@mg21-isomer29 bp86/6-31G(d) Etot=-4201.944715 Eb=-14.38

Mg1	-2.362012	2.092601	1.423513
Mg2	-4.190844	1.217660	-1.288132
Mg3	-4.778423	-1.598242	-0.190613
Mg4	-1.524584	-0.166005	-0.361552
Mg5	3.703185	-3.103640	1.071741
Mg6	-2.113539	-3.110201	-0.086580
Mg7	-4.979730	0.607357	1.695175
Mg8	-2.448619	-1.136093	2.321258
Mg9	0.086705	-2.230229	-2.114505
Mg10	1.810585	3.425775	-1.558661
Mg11	3.097426	-1.878973	-1.629300
Mg12	-1.146868	2.599871	-1.458975
Mg13	3.022028	1.856678	0.923093
Mg14	0.812166	-2.120088	0.868951
Mg15	0.302643	3.736844	1.100335
Mg16	0.340647	0.729574	2.027122
Mg17	2.934883	-0.697742	2.622449
Mg18	5.017739	-0.466973	0.424160
Mg19	-3.005030	-1.319461	-2.657187
Mg20	1.284346	0.417696	-1.221469
Mg21	4.137295	1.143591	-1.910820

@mg21-isomer30 bp86/6-31G(d) Etot=-4201.944048 Eb=-14.36

Mg1	0.506938	4.003913	0.034461
Mg2	-2.301025	3.060666	-0.307761
Mg3	-0.627363	2.332780	2.217625
Mg4	-3.257350	0.724066	1.883475
Mg5	-0.613650	-0.323342	0.693305
Mg6	1.999351	1.319329	1.088130
Mg7	-2.790848	-2.882227	-1.144052
Mg8	-0.300835	-1.497440	-2.232306
Mg9	2.064781	-3.285585	-1.248166
Mg10	4.488734	-0.235966	2.434988
Mg11	1.918068	-1.775990	1.486610
Mg12	-5.006850	1.845380	-0.338072
Mg13	-0.342496	-3.597928	0.518860
Mg14	-2.797232	-2.328591	1.869230
Mg15	2.396812	-0.235695	-1.643709
Mg16	2.865049	2.938773	-1.505716
Mg17	4.580888	-1.869616	-0.121794
Mg18	4.892786	1.173611	-0.292871
Mg19	-4.926487	-1.175651	0.122774
Mg20	-0.019762	1.609913	-1.863363
Mg21	-2.729510	0.199600	-1.651646

@mg21-isomer31 bp86/6-31G(d) Etot=-4201.942982 Eb=-14.32

Mg1	-1.502825	-0.220018	-0.662050
Mg2	-4.375943	-0.772031	-1.922947
Mg3	1.492897	-0.690429	-1.320252
Mg4	0.394651	-0.235064	1.773613
Mg5	0.079155	-3.016316	0.288922
Mg6	-2.098445	-2.171115	2.198495
Mg7	-2.372243	1.004878	2.128610
Mg8	4.645201	-1.367225	-1.374990
Mg9	-1.305593	3.062597	-0.200818
Mg10	1.781221	2.144432	0.109088
Mg11	3.075092	-1.648060	1.304530
Mg12	-4.656094	-1.089227	1.061895
Mg13	-2.545389	1.822244	-2.700026
Mg14	-2.888237	-3.144274	-0.525799
Mg15	4.821032	0.921585	0.544372
Mg16	-4.236281	1.620617	-0.139691
Mg17	0.386532	1.943628	-2.535978
Mg18	2.934276	1.193768	2.800595
Mg19	2.662880	-3.591312	-1.055166
Mg20	3.572034	1.373697	-2.241376
Mg21	0.136078	2.857625	2.468972

@mg21-isomer32 bp86/6-31G(d) Etot=-4201.941740 Eb=-14.29

Mg1	0.006590	3.234934	-2.101760
Mg2	-2.691581	1.851041	-1.232394
Mg3	-2.568871	-3.608440	0.404186
Mg4	5.304996	-2.785943	-0.392471
Mg5	2.695001	1.847001	-1.216180
Mg6	-3.132971	2.191701	1.732072
Mg7	2.731481	-1.279662	-1.695404
Mg8	1.652157	4.345945	0.247056
Mg9	3.117014	2.184465	1.751160
Mg10	1.628275	-0.564249	1.215249
Mg11	-2.728026	-1.298847	-1.689111
Mg12	-0.007869	1.971764	1.411039
Mg13	-0.000833	-3.072650	1.960371
Mg14	-1.650441	4.344755	0.239445
Mg15	4.689521	0.037817	0.340101
Mg16	-5.288915	-2.796118	-0.365343
Mg17	-4.699434	0.044023	0.316418
Mg18	-0.004909	0.278197	-1.459739
Mg19	-1.647830	-0.570017	1.218688
Mg20	2.587881	-3.573387	0.416307
Mg21	0.008762	-2.782328	-1.099691

@mg21-isomer33 bp86/6-31G(d) Etot=-4201.936022 Eb=-14.12

Mg1	0.213425	0.502514	0.205363
Mg2	0.129817	-0.869254	-2.641130
Mg3	2.397223	-1.673128	-0.778017
Mg4	-2.113659	-0.340059	1.826042
Mg5	-0.931680	2.230321	-1.974242
Mg6	-2.544156	-0.321000	-1.429211
Mg7	-3.729744	-2.857181	-0.054212
Mg8	2.356157	1.191522	-1.926074
Mg9	4.384883	3.104351	-0.457915
Mg10	1.369856	3.446205	0.038547
Mg11	-4.054542	2.171333	2.299786
Mg12	5.021166	0.068756	-0.575476
Mg13	4.120969	-1.837464	1.676169
Mg14	-1.404830	2.975818	1.054357
Mg15	1.106363	-1.278530	2.381398
Mg16	-3.913312	2.376030	-0.734648

Mg17	-0.566039	-2.533491	0.203769
Mg18	1.960381	-3.984009	1.255550
Mg19	-1.813943	-3.327203	-2.425876
Mg20	2.980347	1.103156	1.457520
Mg21	-4.968682	-0.148688	0.598299

@mg21-isomer34 bp86/6-31G(d) Etot=-4201.934740 Eb=-14.08

Mg1	-1.930897	0.960935	1.465355
Mg2	1.475607	0.983388	1.085582
Mg3	0.913669	-1.195926	-1.770535
Mg4	4.256181	2.425021	0.278303
Mg5	1.591763	1.864418	-1.795902
Mg6	-0.557069	3.300133	-0.198696
Mg7	-1.467661	0.735069	-1.612328
Mg8	0.059271	-1.039475	2.797750
Mg9	-3.706222	2.653098	-0.344561
Mg10	4.181208	-0.113217	2.008573
Mg11	3.888251	-0.184699	-1.245529
Mg12	-4.426283	-2.299497	0.014798
Mg13	-3.165996	-1.577345	2.665856
Mg14	3.261246	-3.112248	-1.929896
Mg15	-2.636898	-1.869492	-2.492868
Mg16	-5.025950	0.384516	1.304498
Mg17	2.037744	-2.176177	0.890054
Mg18	-4.714259	0.203381	-1.757095
Mg19	5.123020	-2.489141	0.353605
Mg20	2.162258	4.509015	0.083655
Mg21	-1.318984	-1.961757	0.199381

@mg21-isomer35 bp86/6-31G(d) Etot=-4201.932840 Eb=-14.02

Mg1	1.635657	-1.866072	-0.998873
Mg2	-1.517343	0.209971	2.743562
Mg3	-0.783035	0.070363	-0.231014
Mg4	1.968767	1.219099	-0.844503
Mg5	0.286889	2.531522	1.611662
Mg6	4.609125	-2.923579	-0.699669
Mg7	-4.603149	0.335312	2.347673
Mg8	-3.329061	-1.829890	0.644712
Mg9	-1.428184	-2.443392	-1.737835
Mg10	-3.015307	2.166350	0.438846
Mg11	-0.621883	2.947251	-1.414381
Mg12	4.419294	-0.201580	-2.045293
Mg13	-5.280849	0.346919	-0.622434
Mg14	-0.333560	-2.613907	1.276955
Mg15	-2.796666	0.787274	-2.386575
Mg16	1.995817	4.175324	-0.255293
Mg17	1.443041	-0.190344	2.047337
Mg18	2.675335	-2.979411	1.736641
Mg19	4.346104	-0.375687	0.991992
Mg20	-4.285329	-1.884569	-2.367520
Mg21	4.614336	2.519046	-0.235991

@mg21-isomer36 bp86/6-31G(d) Etot=-4201.929553 Eb=-13.92

Mg1	-0.428028	0.272467	-1.239725
Mg2	-3.063586	-1.053292	0.944200
Mg3	1.540893	2.798489	-0.575530
Mg4	-2.008829	-2.483814	-1.556546
Mg5	1.728151	-0.396385	0.798387
Mg6	1.107383	-2.429929	-1.567136
Mg7	0.918883	-1.848226	3.453100
Mg8	1.937342	2.114068	2.506716
Mg9	2.263539	-3.371172	1.196423
Mg10	-5.598057	0.769444	0.010134
Mg11	2.362754	0.456410	-2.350084

Mg12	-1.239798	3.185428	-1.536254
Mg13	-5.064126	-1.947654	-1.192974
Mg14	-2.833133	1.994586	0.717433
Mg15	-0.717449	0.535744	2.360028
Mg16	4.201638	1.440140	0.330329
Mg17	-0.434211	3.636001	1.564611
Mg18	5.329045	0.440825	-2.317161
Mg19	-3.296370	0.627289	-2.028658
Mg20	-0.729382	-2.917596	1.233032
Mg21	4.023344	-1.822823	-0.750324

@mg21-isomer37 bp86/6-31G(d) Etot=-4201.918604 Eb=-13.60

Mg1	0.323746	-0.381640	-2.658373
Mg2	-0.242650	0.154010	0.403216
Mg3	-2.010931	-1.799239	2.010554
Mg4	-2.353595	1.121494	-1.551818
Mg5	-1.835972	-1.929190	-1.200214
Mg6	1.281973	-2.371179	-0.473135
Mg7	2.169109	1.347362	1.794444
Mg8	-3.867993	-3.620459	0.131026
Mg9	-0.372339	3.161639	0.561364
Mg10	-3.159856	3.939043	0.040593
Mg11	1.165916	-1.519713	2.494317
Mg12	3.261394	-0.608315	-2.110432
Mg13	6.238531	-0.687748	-1.361874
Mg14	-4.612042	-1.003532	-1.803993
Mg15	-2.763842	1.260607	1.756030
Mg16	3.771132	-1.209949	0.933563
Mg17	1.739636	1.928114	-1.237767
Mg18	-4.782510	-0.935783	1.245807
Mg19	-5.159277	1.590174	-0.271055
Mg20	4.652351	1.596034	-0.205168
Mg21	6.557220	-0.031729	1.502915

@mg21-isomer38 bp86/6-31G(d) Etot=-4201.918173 Eb=-13.58

Mg1	0.173985	0.013054	-2.295980
Mg2	-1.554760	0.524111	0.525778
Mg3	3.070705	-0.028886	-1.567073
Mg4	-4.021628	-1.418265	0.006735
Mg5	1.720422	-2.575349	-1.972659
Mg6	3.680362	-2.272647	0.420204
Mg7	-4.901054	1.488025	-1.436102
Mg8	5.874771	-0.043682	-0.238689
Mg9	-2.054468	2.605964	-1.511116
Mg10	1.111452	2.023475	-0.204120
Mg11	3.568018	0.779508	1.747715
Mg12	6.227234	2.330720	1.629659
Mg13	0.882954	-3.682984	0.890901
Mg14	4.252902	2.738617	-0.646261
Mg15	-3.653699	-0.021087	2.778755
Mg16	1.081717	-0.762993	1.190262
Mg17	-1.545100	-2.151741	1.976332
Mg18	-2.863717	-0.334412	-2.578788
Mg19	-6.105407	0.604231	1.243386
Mg20	-3.746050	2.617401	1.122036
Mg21	-1.198640	-2.433061	-1.080975

@mg21-isomer39 bp86/6-31G(d) Etot=-4201.909859 Eb=-13.33

Mg1	-2.808814	-0.582412	0.352850
Mg2	-0.045904	0.775117	-0.417510
Mg3	0.893222	-4.017903	0.664615
Mg4	-0.242995	-1.515872	1.826759
Mg5	-2.456634	2.948591	0.097299
Mg6	-5.575494	-0.211889	-1.122045

Mg7	-3.503465	-2.352429	-1.989069
Mg8	4.664832	0.136235	-2.182623
Mg9	-5.176222	2.729520	-1.249645
Mg10	2.532390	-1.672234	-0.627749
Mg11	-4.819705	1.462744	1.523006
Mg12	4.784392	-0.134997	0.841284
Mg13	2.001188	0.798936	1.908884
Mg14	5.963610	2.394737	-0.644130
Mg15	1.642422	0.135747	-2.814888
Mg16	-1.461066	1.275726	2.361672
Mg17	2.849972	2.200727	-0.692499
Mg18	-0.435730	-2.025619	-1.542809
Mg19	0.499753	3.404379	1.021252
Mg20	2.838468	-2.118930	2.227493
Mg21	-2.144222	-3.630176	0.457853

@mg22-isomer01 bp86/6-31G(d) Etot=-4402.087956 Eb=-15.82

Mg1	-0.513652	-0.008016	-0.171898
Mg2	2.200145	-0.382779	1.406166
Mg3	-0.384133	0.416361	2.977123
Mg4	1.763182	2.479251	1.982681
Mg5	-1.184687	2.781730	1.206849
Mg6	-0.547280	-2.214094	-3.080480
Mg7	-0.203167	-3.077366	-0.140530
Mg8	0.558697	-2.565929	2.749614
Mg9	0.980625	4.347093	-0.215469
Mg10	1.986248	-1.450654	-1.594111
Mg11	-2.247460	-1.869026	1.905021
Mg12	-2.879310	-1.877821	-1.070147
Mg13	5.018185	-1.320310	-0.205493
Mg14	-4.974676	-0.800454	0.860101
Mg15	2.002917	1.580627	-1.076910
Mg16	-0.803160	2.568362	-1.927764
Mg17	4.706892	1.550463	0.611426
Mg18	0.691473	0.471476	-3.638852
Mg19	-3.339018	1.342226	-0.524562
Mg20	2.764214	-3.260761	0.720258
Mg21	-3.340341	1.059702	2.495519
Mg22	-2.255695	0.229920	-3.268541

@mg22-isomer02 bp86/6-31G(d) Etot=-4402.087345 Eb=-15.80

Mg1	-1.592319	2.963478	0.697065
Mg2	0.757244	-2.195073	-1.846272
Mg3	-0.700393	0.983442	3.003798
Mg4	0.964765	0.864852	-2.749531
Mg5	0.415617	3.546815	-1.503839
Mg6	-0.503922	-0.052585	0.080462
Mg7	-1.975887	1.726809	-2.103168
Mg8	-1.297584	-3.081626	0.357855
Mg9	1.707718	-2.855136	1.081475
Mg10	-1.324752	-0.804735	-3.712558
Mg11	-0.416398	-2.024100	3.056764
Mg12	-1.842143	-3.548260	-2.603018
Mg13	1.393662	2.192629	1.045004
Mg14	-3.584150	1.869533	2.850797
Mg15	-4.173485	1.387120	-0.009113
Mg16	2.568976	-0.269417	-0.374558
Mg17	2.060645	-0.368537	2.694855
Mg18	3.255862	2.475655	-1.453167
Mg19	-3.204540	-1.155722	-1.274493
Mg20	5.654062	0.685063	-0.545117
Mg21	-3.007144	-0.912352	1.809305
Mg22	4.844165	-1.427854	1.497453

@mg22-isomer03 bp86/6-31G(d) Etot=-4402.086815 Eb=-15.79

Mg1	0.303716	-3.347116	-0.099312
Mg2	2.348267	-0.005054	-3.243142
Mg3	-1.962296	-1.580495	1.152727
Mg4	-2.504804	3.117181	-1.361665
Mg5	-2.396864	0.001152	-1.504156
Mg6	4.436686	-0.003226	-1.000004
Mg7	-4.989624	-1.475072	-0.106111
Mg8	-0.919618	0.004381	3.506161
Mg9	0.552658	-0.004403	0.048282
Mg10	0.311990	3.343782	-0.105029
Mg11	2.739374	-2.472489	-1.656471
Mg12	2.045274	0.001610	3.626930
Mg13	-0.086444	-1.650457	-2.547988
Mg14	0.513253	2.504052	2.763723
Mg15	-1.954881	1.585379	1.147501
Mg16	0.510977	-2.497514	2.763744
Mg17	2.744960	2.464816	-1.665165
Mg18	-4.985791	1.481272	-0.108915
Mg19	2.942222	1.609813	1.144689
Mg20	2.945988	-1.607987	1.149877
Mg21	-0.081956	1.645074	-2.550850
Mg22	-2.513086	-3.114700	-1.354827

@mg22-isomer04 bp86/6-31G(d) Etot=-4402.086250 Eb=-15.77

Mg1	-2.605316	-3.451683	0.016126
Mg2	0.125923	-3.662187	-1.235992
Mg3	-0.000288	-2.589987	1.613508
Mg4	2.642329	-2.482221	-0.028706
Mg5	1.309411	-1.269033	-2.665074
Mg6	-1.749593	-1.319300	-1.902676
Mg7	2.227826	-0.637560	2.574581
Mg8	4.925160	-0.695874	1.131830
Mg9	-4.865862	-1.227829	-0.613117
Mg10	-2.335541	-0.684410	1.198508
Mg11	4.003112	-0.329282	-1.606096
Mg12	0.463909	0.051357	0.089718
Mg13	-0.650766	0.874472	-3.635919
Mg14	-2.047989	1.604370	-0.897854
Mg15	-4.833391	1.343030	1.069054
Mg16	-0.625035	-0.201156	3.602456
Mg17	1.886501	1.815339	-2.181218
Mg18	3.091186	1.695596	0.692735
Mg19	1.033017	2.161950	2.998566
Mg20	-0.509084	3.656683	-2.607326
Mg21	-1.869251	2.183955	2.141736
Mg22	0.383740	3.163769	0.245160

@mg22-isomer05 bp86/6-31G(d) Etot=-4402.083745 Eb=-15.70

Mg1	-0.750731	1.657748	-2.729319
Mg2	0.004246	-2.514488	1.741264
Mg3	-0.128758	3.174525	-0.096453
Mg4	0.936289	-2.425915	-1.264894
Mg5	1.050083	-0.609808	-3.687806
Mg6	-0.613656	0.124252	0.166072
Mg7	-1.667704	-1.297962	-2.523006
Mg8	-2.159865	-0.420057	2.813133
Mg9	0.822647	-0.104359	3.462857
Mg10	-1.719423	-3.642889	-0.582867
Mg11	-0.787308	2.330093	2.698752
Mg12	-2.900968	-3.282844	2.183536
Mg13	1.890744	1.120045	-1.209564
Mg14	-2.750949	3.698689	-1.444350
Mg15	-3.683731	0.922558	-2.087802

Mg16	2.485013	-0.877218	0.950000
Mg17	2.057574	2.097457	1.831584
Mg18	3.569555	-1.288803	-2.152788
Mg19	-3.547167	-1.185559	0.052079
Mg20	6.020931	-0.499394	-0.588013
Mg21	-3.150398	1.805230	0.847399
Mg22	5.023576	1.218699	1.620186

@mg22-isomer06 bp86/6-31G(d) Etot=-4402.079507 Eb=-15.58

Mg1	0.679279	0.021695	-0.115351
Mg2	-1.698044	1.635189	-1.764130
Mg3	1.119188	2.724819	-1.436165
Mg4	-1.225857	3.864262	0.175331
Mg5	0.981520	2.502776	1.748277
Mg6	-0.232980	-2.955744	-0.293435
Mg7	1.129855	-2.069450	-2.883208
Mg8	0.312563	0.627429	-3.782863
Mg9	-1.902931	2.196459	2.530597
Mg10	-3.295697	-2.931893	-0.292621
Mg11	2.981219	0.274266	-2.194499
Mg12	2.775421	-2.206587	-0.280291
Mg13	-5.090872	-0.530795	-0.543412
Mg14	5.103065	-0.390810	0.223171
Mg15	-2.105596	-0.251193	0.680194
Mg16	-0.078550	-0.121823	3.047129
Mg17	-4.023410	2.164427	0.189885
Mg18	-1.618869	-2.731443	2.410748
Mg19	2.904425	-0.001626	2.349511
Mg20	-1.712093	-1.281917	-2.394201
Mg21	3.626050	2.155700	0.283603
Mg22	1.372313	-2.693743	2.341730

@mg22-isomer07 bp86/6-31G(d) Etot=-4402.078828 Eb=-15.56

Mg1	-0.492671	0.000218	-0.084448
Mg2	-2.617774	-2.123836	-1.101348
Mg3	0.053899	-2.427246	-2.662187
Mg4	-1.777098	2.072217	1.897211
Mg5	-0.259650	3.738341	-0.096680
Mg6	0.051718	2.415370	-2.673757
Mg7	1.770184	-0.004674	-2.128001
Mg8	2.473856	-2.681818	-0.735706
Mg9	-1.620945	-0.007302	-3.199882
Mg10	-1.774263	-2.064272	1.905566
Mg11	-3.738929	0.000289	0.798873
Mg12	-2.618913	2.118326	-1.110038
Mg13	5.275838	1.516051	-0.031794
Mg14	-4.497441	-0.005717	-2.143320
Mg15	-0.257219	-3.739781	-0.080348
Mg16	0.156686	0.008414	3.271395
Mg17	5.278254	-1.512338	-0.036413
Mg18	-2.806434	0.007751	3.867697
Mg19	2.470897	2.678549	-0.748124
Mg20	1.271958	2.550406	2.101037
Mg21	1.272643	-2.540901	2.112527
Mg22	2.385402	0.001953	0.877738

@mg22-isomer08 bp86/6-31G(d) Etot=-4402.077009 Eb=-15.51

Mg1	0.817818	-0.004090	-0.186688
Mg2	0.826385	-0.645684	3.455454
Mg3	-0.894498	1.286072	2.032841
Mg4	-2.858293	2.856780	0.403792
Mg5	-3.613423	-0.013441	2.079119
Mg6	0.112605	3.849115	0.945582
Mg7	-1.393042	-2.558964	-1.729628

Mg8	-0.442541	2.477606	-1.696866
Mg9	-2.157186	0.201507	-0.816713
Mg10	1.215163	-2.033675	-3.191897
Mg11	1.820337	0.963215	-3.115121
Mg12	-1.242466	-1.930766	1.302260
Mg13	-0.992542	-0.076662	-3.543387
Mg14	1.282955	-3.011004	-0.307291
Mg15	2.146637	1.807294	2.108189
Mg16	1.073564	-3.471941	2.651682
Mg17	2.483944	2.802928	-0.714166
Mg18	3.173419	-1.268909	1.656090
Mg19	-4.258203	-2.095475	-0.218686
Mg20	3.499629	-1.063280	-1.288526
Mg21	4.706498	1.137705	0.443995
Mg22	-5.306761	0.791668	-0.270033

@mg22-isomer09 bp86/6-31G(d) Etot=-4402.078301 Eb=-15.54

Mg1	-0.037006	-0.136730	-0.084691
Mg2	-0.673928	1.102657	2.783573
Mg3	-3.440611	1.875134	1.639030
Mg4	2.164031	-0.008101	2.095445
Mg5	-0.936805	2.999476	0.450730
Mg6	-0.798401	2.854090	-2.584030
Mg7	-3.013721	-0.873537	3.029189
Mg8	1.753176	2.538966	-0.944953
Mg9	-2.772065	0.789797	-1.109310
Mg10	-1.395448	-1.813451	-2.355244
Mg11	-0.226882	-2.027896	2.318470
Mg12	-2.657655	-2.141691	0.354816
Mg13	-0.217295	-3.818196	-0.129385
Mg14	1.510503	-2.590796	-2.190693
Mg15	2.421047	-2.725226	0.794249
Mg16	4.397753	1.906653	0.709578
Mg17	-5.081691	-0.443330	0.766648
Mg18	-1.860143	0.571874	-4.190796
Mg19	3.011074	-0.213362	-1.010665
Mg20	5.247504	-1.119218	0.746869
Mg21	1.712653	2.951127	2.033435
Mg22	0.893910	0.321760	-3.122263

@mg22-isomer10 bp86/6-31G(d) Etot=-4402.076253 Eb=-15.49

Mg1	2.789219	0.146400	2.713959
Mg2	-2.270116	-1.409802	2.301321
Mg3	5.007585	-0.657060	0.240945
Mg4	-3.222077	1.588625	2.174115
Mg5	1.492260	0.774951	-3.104704
Mg6	-3.875697	2.152968	-0.768849
Mg7	-2.926258	-2.492806	-0.775439
Mg8	1.860756	2.764536	1.390872
Mg9	-1.236567	2.057047	-2.526434
Mg10	-0.279178	0.936544	2.681141
Mg11	3.954621	1.823259	-0.844315
Mg12	1.297323	3.340044	-1.524762
Mg13	-1.049752	3.040613	0.377678
Mg14	0.639494	-1.874950	3.250583
Mg15	-0.133886	-2.631095	0.443498
Mg16	-0.961728	-0.996040	-3.037270
Mg17	-4.798542	-0.424242	0.511841
Mg18	1.319555	0.171295	-0.045704
Mg19	1.799162	-2.096690	-1.936482
Mg20	-0.609486	-3.871998	-2.311901
Mg21	-1.572697	0.105175	-0.240345
Mg22	2.776007	-2.446776	1.030253

@mg22-isomer11 bp86/6-31G(d) Etot=-4402.074804 Eb=-15.44

Mg1	5.129485	-1.628579	0.125383
Mg2	3.282458	1.437596	0.364092
Mg3	2.412344	-1.239039	1.881386
Mg4	6.382812	1.205634	0.020397
Mg5	1.410257	1.411146	2.708336
Mg6	2.167794	-1.107177	-1.131429
Mg7	0.233362	-3.065693	0.960449
Mg8	-0.521987	-0.869272	2.980019
Mg9	0.885457	3.428529	0.656125
Mg10	1.168325	1.753543	-1.858319
Mg11	-0.019544	-3.019516	-2.006919
Mg12	0.655290	-0.615197	-3.753439
Mg13	-2.379488	-3.212402	2.597835
Mg14	-0.459157	-0.022973	-0.014282
Mg15	-1.484227	2.042785	2.137441
Mg16	-2.513738	-2.377345	-0.297973
Mg17	-3.353652	-0.384488	1.877194
Mg18	-1.723357	3.092406	-0.737535
Mg19	-2.186019	-1.371452	-3.150857
Mg20	-1.485663	1.511624	-3.299935
Mg21	-3.349199	0.477293	-1.048264
Mg22	-4.251553	2.552577	0.990298

@mg22-isomer12 bp86/6-31G(d) Etot=-4402.074108 Eb=-15.42

Mg1	-1.567128	-0.188984	2.790349
Mg2	3.624290	-2.431383	0.739715
Mg3	-3.977148	-1.591567	1.200767
Mg4	0.729198	2.138190	-1.798410
Mg5	3.667990	0.150209	2.402620
Mg6	-1.433571	-3.099430	1.834408
Mg7	2.059596	-0.505512	-1.103057
Mg8	-4.082635	1.401523	1.361855
Mg9	-2.065271	2.577163	-0.769795
Mg10	-0.042550	-2.044022	-3.012513
Mg11	-3.835356	0.069816	-1.244028
Mg12	3.301100	2.298370	0.012878
Mg13	0.770928	-3.191684	-0.281927
Mg14	-1.562797	0.626773	-3.251235
Mg15	0.487912	4.047918	0.451112
Mg16	1.157448	-1.736747	2.306407
Mg17	-1.577967	2.836942	2.251102
Mg18	-2.269478	-2.751188	-1.118795
Mg19	-0.857599	-0.267524	-0.184758
Mg20	0.943171	1.285986	1.607829
Mg21	1.251629	0.348321	-4.127649
Mg22	5.278238	0.026831	-0.066875

@mg22-isomer13 bp86/6-31G(d) Etot=-4402.072442 Eb=-15.38

Mg1	0.106471	-2.451748	-2.030588
Mg2	5.080641	-0.823711	0.663443
Mg3	-2.659689	-2.442868	-0.690677
Mg4	-1.193621	3.707337	0.083114
Mg5	4.460213	-1.059198	-2.241777
Mg6	-0.246577	-3.611163	0.645578
Mg7	2.096264	0.491341	1.350408
Mg8	-4.700709	-0.661725	-2.089880
Mg9	-3.168060	1.695655	-1.020790
Mg10	-0.124431	0.328163	3.756830
Mg11	-4.262535	-0.436765	0.820196
Mg12	1.676030	2.955930	-0.473378
Mg13	1.147424	-2.106370	2.728161
Mg14	-2.349565	1.622687	2.031064
Mg15	-0.518060	2.324710	-2.444297

Mg16	2.377289	-2.262489	-0.070442
Mg17	-1.790554	-0.338925	-2.979094
Mg18	-1.937037	-1.757375	2.372519
Mg19	-0.631232	-0.036821	0.030781
Mg20	1.662011	0.283179	-1.960684
Mg21	0.467564	2.889802	2.384232
Mg22	4.508164	1.690355	-0.864721

@mg22-isomer14 bp86/6-31G(d) Etot=-4402.071630 Eb=-15.35

Mg1	4.250363	3.817977	-0.236103
Mg2	1.113905	2.550102	-0.411530
Mg3	-0.784999	3.318958	1.892640
Mg4	-2.018562	2.583266	-0.815054
Mg5	-0.174946	2.137893	-3.162999
Mg6	3.422269	0.610477	0.232370
Mg7	1.231680	1.102972	2.364255
Mg8	-1.818985	0.571726	2.732580
Mg9	-3.632611	0.153449	0.270719
Mg10	1.791875	-0.028149	-2.211056
Mg11	-3.805963	2.823427	1.661082
Mg12	-0.507518	-0.171919	0.022233
Mg13	-2.290956	-0.066702	-2.495522
Mg14	3.176813	-1.258965	2.575777
Mg15	-0.081512	-0.506336	-4.561598
Mg16	5.048581	-2.366059	0.211144
Mg17	0.169296	-1.816240	2.590129
Mg18	-2.807917	-2.274325	2.010446
Mg19	1.819772	-2.238457	-0.005973
Mg20	-0.286650	-2.425907	-2.210852
Mg21	-3.062423	-2.655481	-0.950659
Mg22	-0.751514	-3.861705	0.497971

@mg22-isomer15 bp86/6-31G(d) Etot=-4402.069879 Eb=-15.30

Mg1	-1.669508	-2.621776	1.928248
Mg2	1.470743	0.042573	-4.247267
Mg3	-2.015898	2.592222	-1.178968
Mg4	3.371059	0.032587	-1.832355
Mg5	-4.251634	-1.567532	0.679894
Mg6	-0.526615	-0.024491	3.224503
Mg7	0.888228	-1.720970	-1.750580
Mg8	-1.989893	-2.592936	-1.213635
Mg9	0.476010	-3.778893	0.278706
Mg10	-1.348179	0.013490	-3.057212
Mg11	-4.277482	1.535830	0.687281
Mg12	1.282375	-2.459207	2.800754
Mg13	0.862035	1.742702	-1.705121
Mg14	3.207181	2.471241	0.230047
Mg15	0.436578	3.799428	0.327696
Mg16	4.995503	0.014659	0.626390
Mg17	-4.032172	-0.008064	-1.855096
Mg18	3.243989	-2.454012	0.191180
Mg19	1.575785	-0.012125	0.914214
Mg20	-1.262092	-0.007970	0.176553
Mg21	1.258283	2.425683	2.818010
Mg22	-1.694297	2.577561	1.956757

@mg22-isomer16 bp86/6-31G(d) Etot=-4402.068387 Eb=-15.26

Mg1	0.662923	-2.430861	1.546676
Mg2	-2.494462	-2.350033	-2.284397
Mg3	-1.163642	-0.056824	0.005170
Mg4	3.319924	-0.956412	2.139391
Mg5	-3.546457	0.587273	-1.753663
Mg6	5.729675	0.650940	0.991349
Mg7	-2.131180	-1.265923	2.543916

Mg8	-4.401337	0.916965	1.396224
Mg9	-0.009175	2.891493	0.488303
Mg10	-1.810300	-3.650296	0.489970
Mg11	-1.317725	2.635915	-2.301393
Mg12	-3.062630	3.177273	0.051812
Mg13	2.783385	1.898987	0.850774
Mg14	-0.357459	-0.302945	-2.913630
Mg15	-1.970612	2.015375	2.645489
Mg16	1.601477	2.043705	-2.058758
Mg17	1.853372	-0.659472	-0.685299
Mg18	4.496478	0.911035	-1.785447
Mg19	-4.069846	-1.722971	0.159372
Mg20	0.264832	-3.049389	-1.545017
Mg21	4.955041	-1.806442	-0.472712
Mg22	0.667717	0.522608	2.491869

@mg22-isomer17 bp86/6-31G(d) Etot=-4402.063020 Eb=-15.11

Mg1	0.471979	-2.319988	2.114051
Mg2	-0.682925	0.640285	2.757733
Mg3	-2.451815	-1.840555	2.467612
Mg4	3.423957	-2.755281	0.770649
Mg5	-1.433102	3.048809	0.911200
Mg6	-1.484821	2.371399	-2.126576
Mg7	3.972089	2.450498	0.970495
Mg8	-1.039573	-0.184026	-0.109431
Mg9	5.157837	-0.277333	0.258157
Mg10	-1.613055	-3.800978	0.367921
Mg11	0.938450	0.086234	-2.338811
Mg12	1.949814	0.051712	0.798109
Mg13	-1.885464	-2.181592	-2.190165
Mg14	3.640461	1.386969	-1.751730
Mg15	-4.085649	3.087143	-0.732392
Mg16	-4.126330	-2.048865	-0.079644
Mg17	1.228588	2.897090	2.347530
Mg18	-3.811454	0.323986	-1.931617
Mg19	1.140573	2.786290	-0.717006
Mg20	3.512450	-1.675199	-1.990051
Mg21	-3.681637	0.732492	1.169292
Mg22	0.859625	-2.779090	-0.965325

@mg22-isomer18 bp86/6-31G(d) Etot=-4402.061796 Eb=-15.07

Mg1	-1.216377	0.967146	2.768372
Mg2	0.567268	-1.931597	2.029400
Mg3	-2.475186	-2.109571	2.226755
Mg4	-0.851801	1.340405	-2.233444
Mg5	0.415611	3.121870	1.332451
Mg6	-2.445834	-1.528935	-2.617975
Mg7	-4.342318	0.336642	1.568498
Mg8	-4.192950	0.738722	-1.414047
Mg9	4.304391	1.310942	0.404952
Mg10	2.239204	-2.760070	-0.495887
Mg11	-4.294395	-2.073385	-0.268896
Mg12	-0.992010	-3.211835	-0.447632
Mg13	-0.520899	4.198194	-1.311831
Mg14	1.869549	1.013564	2.859854
Mg15	1.296047	0.193939	0.016351
Mg16	3.558968	-1.299736	1.918623
Mg17	2.018120	2.599957	-1.446378
Mg18	-1.577880	-0.329788	0.061316
Mg19	0.537009	-1.569529	-2.595118
Mg20	3.243095	-0.224335	-2.268011
Mg21	5.307496	-1.339798	-0.491282
Mg22	-2.447108	2.557198	0.403929

@mg22-isomer19 bp86/6-31G(d) Etot=-4402.059200 Eb=-15.00

Mg1	0.499176	-3.136260	1.255040
Mg2	1.734842	-0.656817	-3.048214
Mg3	-1.284263	-1.342594	3.179768
Mg4	-2.278173	2.711832	-1.517472
Mg5	-3.536693	-0.596880	-2.095714
Mg6	4.563168	-1.440027	-1.813197
Mg7	-5.624562	-1.489733	0.042720
Mg8	-0.098425	1.434250	3.411578
Mg9	0.642730	-0.164969	0.593608
Mg10	2.735244	3.901253	-0.166842
Mg11	2.135638	-3.110578	-1.284890
Mg12	2.565169	1.713591	2.022980
Mg13	-0.655674	-2.727160	-2.050122
Mg14	0.007739	2.929919	0.626182
Mg15	-2.197667	0.992365	1.138038
Mg16	1.602673	-1.045122	3.564246
Mg17	0.897858	2.584176	-2.338643
Mg18	-5.067696	1.524439	-0.181696
Mg19	3.114052	1.040613	-0.920491
Mg20	3.294503	-1.460408	1.006591
Mg21	-0.788313	0.221656	-1.828959
Mg22	-2.261328	-1.883546	0.405491

@mg22-isomer20 bp86/6-31G(d) Etot=-4402.055118 Eb=-14.88

Mg1	-0.132550	1.083265	2.620105
Mg2	0.697676	-1.918686	2.921975
Mg3	0.047485	-3.649775	0.489346
Mg4	-0.981935	3.310393	0.649164
Mg5	1.918425	-2.744560	-1.699391
Mg6	0.393732	2.624909	-1.960382
Mg7	1.936717	2.728213	0.800961
Mg8	3.930811	-0.605452	-0.804809
Mg9	0.801364	-0.125431	-0.067115
Mg10	3.379916	2.174822	-2.051204
Mg11	-1.024315	-1.894280	-1.855851
Mg12	2.984898	0.095603	2.149302
Mg13	-1.832315	-1.307738	1.218222
Mg14	2.968602	-2.840535	1.151183
Mg15	-2.894928	-4.011631	-0.432683
Mg16	-4.136909	-1.479225	-1.291913
Mg17	-3.056638	1.428541	1.944058
Mg18	1.576497	0.021968	-3.047480
Mg19	-5.426228	0.863208	-0.066350
Mg20	-3.933494	3.444508	-0.214293
Mg21	4.840565	1.941280	0.589618
Mg22	-2.057375	0.860603	-1.042461

@mg22-isomer21 bp86/6-31G(d) Etot=-4402.050093 Eb=-14.74

Mg1	-1.667349	1.750950	2.054990
Mg2	2.009338	0.247371	0.458429
Mg3	-0.077797	3.776800	0.400966
Mg4	-2.506857	-1.273714	2.607709
Mg5	3.433548	1.071884	-2.230567
Mg6	-4.181294	0.316165	0.703935
Mg7	5.185715	1.109532	0.097345
Mg8	-2.398688	2.408087	-0.959119
Mg9	1.323505	2.322188	2.623827
Mg10	1.254596	-1.056036	-2.347264
Mg11	-5.393718	1.909559	-1.487372
Mg12	0.518608	1.980903	-1.869467
Mg13	-0.432893	-3.128032	1.219330
Mg14	-3.485339	-2.562316	0.031615
Mg15	0.420458	-0.627973	2.867573

Mg16	-0.903781	-0.266850	-0.179115
Mg17	2.543787	-2.507011	1.730423
Mg18	1.715622	-3.585975	-0.881924
Mg19	4.093347	-1.651268	-0.803846
Mg20	2.887813	3.148968	-0.060153
Mg21	-3.232136	-0.423827	-2.227331
Mg22	-1.106485	-2.959406	-1.749982

@mg22-isomer22 bp86/6-31G(d) Etot=-4402.046991 Eb=-14.65

Mg1	-4.818496	-2.285286	0.515561
Mg2	-3.171670	-1.520971	-1.951991
Mg3	0.122226	-0.828690	2.236435
Mg4	-3.022345	-0.154276	2.119257
Mg5	-2.790235	1.593577	-2.264868
Mg6	3.366922	-1.326967	1.678769
Mg7	4.544135	1.495211	0.723080
Mg8	-1.283786	0.086413	-0.256581
Mg9	-3.379045	2.739481	0.854220
Mg10	-1.901898	-2.929833	0.751734
Mg11	1.003986	-3.457307	0.911340
Mg12	5.008182	-0.925467	-0.972625
Mg13	0.355951	1.370641	-2.423475
Mg14	-0.189638	-2.526445	-1.725750
Mg15	1.703992	-0.288247	-0.464085
Mg16	3.500222	1.400785	-2.144976
Mg17	1.889371	2.984248	0.060438
Mg18	2.353699	1.354328	2.651445
Mg19	-4.870990	0.482523	-0.338345
Mg20	3.044216	-3.099415	-1.216173
Mg21	-0.950093	3.663223	-0.666997
Mg22	-0.514705	2.172472	1.923587

@mg22-isomer23 bp86/6-31G(d) Etot=-4402.044991 Eb=-14.59

Mg1	3.297512	-2.937488	2.089228
Mg2	-4.528559	-1.864544	-0.760956
Mg3	-1.107547	-0.519366	1.743258
Mg4	-3.043586	1.766662	2.233374
Mg5	1.910747	4.772819	1.056444
Mg6	-4.241187	-1.035673	2.239272
Mg7	4.826515	-0.523659	0.868434
Mg8	1.534556	-1.762680	-2.641716
Mg9	3.727924	-2.701572	-0.891828
Mg10	0.708497	3.271156	-1.360098
Mg11	-3.698377	0.353407	-2.647730
Mg12	-1.469965	-1.426093	-1.453125
Mg13	0.139983	2.323415	1.542316
Mg14	-0.297107	1.024038	-3.110796
Mg15	2.067181	-0.234042	2.311674
Mg16	4.003160	0.219787	-1.970331
Mg17	-2.370141	-3.137657	0.938035
Mg18	-1.936763	1.708261	-0.578368
Mg19	3.415374	2.124463	0.535078
Mg20	-5.039437	1.010234	0.057322
Mg21	1.242432	0.279327	-0.525588
Mg22	0.858787	-2.710795	0.326100

@mg22-isomer24 bp86/6-31G(d) Etot=-4402.042760 Eb=-14.53

Mg1	2.168567	1.144842	-1.534202
Mg2	-2.473987	-2.838196	-1.905879
Mg3	3.305243	3.183959	0.643318
Mg4	2.412773	-1.735900	-0.703325
Mg5	-0.333200	0.095864	0.114247
Mg6	0.770570	3.940928	-1.286510
Mg7	-2.795442	0.241084	-1.766901

Mg8	-2.137497	1.412741	2.252369
Mg9	0.133681	-1.297469	-2.684354
Mg10	-0.447680	1.800305	-2.885246
Mg11	0.143700	-3.611826	-0.672749
Mg12	5.484143	-2.274488	-0.656874
Mg13	-4.751021	-1.611175	-0.307854
Mg14	0.760711	-2.251044	1.976421
Mg15	-2.146607	-2.357108	1.152968
Mg16	-2.037937	2.985895	-0.402559
Mg17	2.018184	0.573874	1.933793
Mg18	-4.559145	1.497004	0.399385
Mg19	3.803357	-1.865426	2.025338
Mg20	4.710887	0.592341	0.264824
Mg21	0.330615	3.032692	1.522190
Mg22	-4.359917	-0.658898	2.521599

@mg22-isomer25 bp86/6-31G(d) Etot=-4402.038587 Eb=-14.41

Mg1	0.089462	-1.223671	0.270807
Mg2	1.707642	1.182717	1.304687
Mg3	0.089729	-3.195069	-2.233942
Mg4	-0.003823	-0.121920	-2.560433
Mg5	5.051553	2.979513	0.005040
Mg6	-4.485527	-0.149801	0.450566
Mg7	2.342320	4.103689	0.160533
Mg8	-0.165491	3.685298	1.819408
Mg9	-5.538880	2.549718	-0.296151
Mg10	1.744164	-4.220440	0.082212
Mg11	-1.602821	0.941852	1.417785
Mg12	-2.721301	1.159690	-1.691044
Mg13	-0.108527	2.504821	-0.999524
Mg14	0.174333	-3.273674	2.587932
Mg15	-1.417871	-4.392505	0.129075
Mg16	-2.565555	-2.056238	1.759845
Mg17	2.769066	-1.806918	1.675189
Mg18	2.667498	1.415814	-1.671152
Mg19	-2.611777	-1.953514	-1.331752
Mg20	-2.823737	3.578789	0.324846
Mg21	2.757753	-1.750333	-1.448182
Mg22	4.651790	0.042183	0.244257

@mg22-isomer26 bp86/6-31G(d) Etot=-4402.037938 Eb=-14.39

Mg1	1.721386	-1.446980	0.185454
Mg2	-0.826246	0.199634	0.648821
Mg3	-1.174811	-2.800979	-0.224581
Mg4	-0.096183	-0.748731	-2.365994
Mg5	-3.018548	-0.641277	-1.643198
Mg6	3.752919	-1.516049	2.417458
Mg7	1.864945	0.950436	2.098298
Mg8	1.598857	1.452532	-1.038156
Mg9	-4.248082	-3.141072	-0.172444
Mg10	-0.211536	3.144420	1.250807
Mg11	-2.833344	-1.408940	2.120919
Mg12	4.399848	0.667281	0.215269
Mg13	-1.502567	2.238372	-1.487607
Mg14	4.644661	-2.341558	-0.398883
Mg15	3.056226	3.560087	0.649752
Mg16	-4.609926	1.952582	-1.207576
Mg17	-5.297479	-0.391091	0.552408
Mg18	-3.248351	1.708082	1.538956
Mg19	3.253330	-0.732335	-2.472557
Mg20	1.702224	-3.361442	-2.058273
Mg21	0.834273	4.452871	-1.275510
Mg22	0.238406	-1.795843	2.666635

@mg22-isomer27 bp86/6-31G(d) Etot=-4402.037712 Eb=-14.39

Mg1	-0.925327	-3.084383	1.159534
Mg2	-2.106238	-4.285390	-1.309445
Mg3	-3.781836	0.523846	0.136376
Mg4	7.408636	-2.381131	-0.230329
Mg5	0.297020	-2.551777	-1.547675
Mg6	4.684244	2.075700	-0.735095
Mg7	-2.833034	1.462190	-2.699137
Mg8	4.879499	-0.692908	0.498333
Mg9	2.850583	1.253186	1.623399
Mg10	-0.771135	0.005000	-0.023982
Mg11	1.074186	-1.118602	2.089022
Mg12	-1.913046	3.069321	-0.257208
Mg13	-2.559397	-1.440980	-2.245062
Mg14	-2.463499	-0.951390	2.643516
Mg15	-0.582334	3.258447	-3.086003
Mg16	1.235173	2.314904	-0.945130
Mg17	0.092397	0.240285	-3.046981
Mg18	-2.739390	2.092206	2.641971
Mg19	-3.884742	-2.467704	0.347890
Mg20	-0.451920	0.677266	4.143017
Mg21	0.139187	2.471333	1.864061
Mg22	2.350973	-0.469419	-1.021071

@mg22-isomer28 bp86/6-31G(d) Etot=-4402.036925 Eb=-14.36

Mg1	-0.529800	-2.371882	1.193771
Mg2	2.393615	-1.663099	-2.233390
Mg3	-1.690467	0.497338	3.599899
Mg4	-2.095434	1.369036	-2.655647
Mg5	-3.061879	-1.525446	-1.680720
Mg6	4.817955	-2.315258	-0.377375
Mg7	-5.942635	-1.508392	-0.096018
Mg8	0.935649	2.090816	3.901418
Mg9	0.556726	0.594014	1.403327
Mg10	3.153575	3.474274	-1.603177
Mg11	1.875111	-3.947415	-0.289619
Mg12	1.503193	3.313941	0.970777
Mg13	-0.468956	-3.182681	-1.986352
Mg14	0.027145	3.328613	-1.699237
Mg15	-1.779441	2.190421	0.445820
Mg16	0.903102	-1.059734	4.002945
Mg17	1.629945	1.235642	-3.086768
Mg18	-4.683970	1.182161	-0.914195
Mg19	3.130365	0.767772	-0.302596
Mg20	2.483808	-1.651673	1.473126
Mg21	-0.112318	-0.295748	-1.214534
Mg22	-3.045290	-0.522699	1.148544

@mg22-isomer29 bp86/6-31G(d) Etot=-4402.033904 Eb=-14.28

Mg1	1.373763	-3.303077	-1.747487
Mg2	1.282552	-0.425180	-0.636794
Mg3	0.793533	4.232157	-1.007670
Mg4	-3.332839	-2.346128	0.357701
Mg5	-1.146726	0.002726	1.047366
Mg6	-1.876695	3.092191	0.422920
Mg7	-0.084951	-2.924206	1.064405
Mg8	1.585368	-0.640980	2.379319
Mg9	-1.264780	-1.535931	-1.970599
Mg10	-5.825850	-0.578405	0.176657
Mg11	3.113161	-2.820870	0.637764
Mg12	1.087850	2.206091	1.195588
Mg13	3.954987	0.774673	0.557702
Mg14	2.750806	1.862889	-1.993379
Mg15	4.545052	-1.233475	2.810989

Mg16	3.787133	-1.192979	-1.890978
Mg17	-3.246131	0.580760	-1.119543
Mg18	-0.491229	1.634954	-1.989838
Mg19	-3.920512	0.523451	2.140830
Mg20	-4.946906	2.688835	0.380936
Mg21	-1.680407	-4.526634	-0.955808
Mg22	3.542823	3.929139	0.139919

@mg22-isomer30 bp86/6-31G(d) Etot=-4402.025428 Eb=-14.04

Mg1	-0.346338	-1.445725	-0.410259
Mg2	1.928559	0.074180	1.366192
Mg3	-3.055955	-0.576272	1.071879
Mg4	-0.560253	-1.034120	2.725056
Mg5	-2.151918	0.657206	-1.825968
Mg6	-2.588002	4.311896	0.498576
Mg7	2.402732	-2.196800	-1.401170
Mg8	2.526431	2.898527	-0.053262
Mg9	4.172152	0.557986	-1.301269
Mg10	0.402316	4.598879	1.129931
Mg11	-4.338967	2.052139	-0.081307
Mg12	5.324804	-2.190230	-2.078626
Mg13	-0.814225	1.582653	0.933276
Mg14	-5.000779	-0.622254	-1.323693
Mg15	-1.765621	-3.507989	1.287149
Mg16	1.108669	0.721564	-1.768404
Mg17	4.612103	1.323179	1.584339
Mg18	1.570752	-2.954542	1.567842
Mg19	-2.754417	-2.639364	-1.695657
Mg20	4.440311	-1.762313	0.903333
Mg21	-4.731633	-3.279181	0.443507
Mg22	-0.380719	3.430581	-1.571464

@mg22-isomer31 bp86/6-31G(d) Etot=-4402.023235 Eb=-13.97

Mg1	-0.722867	-0.051552	0.530206
Mg2	2.254128	-0.018853	-0.048102
Mg3	-2.308578	-1.341453	-1.679054
Mg4	3.313962	-2.889678	-0.411528
Mg5	-4.902468	0.099987	-0.973044
Mg6	2.763937	2.543294	-1.405150
Mg7	-3.748446	0.968889	1.716664
Mg8	-7.928838	0.248558	-1.591518
Mg9	4.876849	1.757579	0.697618
Mg10	5.296970	-0.526194	-1.180685
Mg11	-1.272825	-3.188971	0.752603
Mg12	2.906988	-0.853060	-2.928560
Mg13	-1.665885	-0.864246	3.111904
Mg14	1.402022	-1.951609	1.991196
Mg15	0.050409	3.712303	-0.529440
Mg16	-3.953900	-1.917633	1.023318
Mg17	0.576430	-2.355731	-1.504132
Mg18	4.398099	-1.013573	1.811161
Mg19	-2.399958	1.878875	-0.998055
Mg20	0.262661	0.786910	-2.156412
Mg21	1.876990	2.432632	1.634368
Mg22	-1.075680	2.543526	2.136641

@mg22-isomer32 bp86/6-31G(d) Etot=-4402.016849 Eb=-13.79

Mg1	-0.480891	0.373725	0.525629
Mg2	2.918702	-0.219927	1.183152
Mg3	0.669069	-0.119816	3.278730
Mg4	-1.236092	3.313093	0.170619
Mg5	1.386066	2.189012	-1.172436
Mg6	-2.481752	0.928253	-1.706778
Mg7	-2.085334	-1.363168	2.542308

Mg8	3.371647	-2.739664	-0.475659
Mg9	4.178256	2.499323	0.510908
Mg10	6.177439	-1.865695	-0.984155
Mg11	1.372627	2.571189	1.781039
Mg12	1.039412	-0.900592	-1.743822
Mg13	-4.157447	3.359914	-0.729317
Mg14	6.595651	1.133188	-0.671260
Mg15	-3.325007	1.272350	1.413946
Mg16	-5.716812	0.800817	-0.733216
Mg17	-1.763101	-2.043876	-1.384873
Mg18	-4.291158	-1.638794	0.427769
Mg19	0.610667	-2.471000	1.025124
Mg20	-2.148210	-3.943221	0.949695
Mg21	-4.513865	-1.341462	-2.556874
Mg22	3.880134	0.206349	-1.650529

@mg22-isomer33 bp86/6-31G(d) Etot=-4402.003922 Eb=-13.42

Mg1	1.322082	0.280495	1.752782
Mg2	2.798010	-2.422815	1.229606
Mg3	-0.803470	0.523677	-0.407747
Mg4	4.253560	-2.543435	-1.635598
Mg5	-1.039776	2.956454	-2.275556
Mg6	5.916076	-2.363252	0.807664
Mg7	1.769428	1.988250	-1.482167
Mg8	3.953933	0.360007	-0.055749
Mg9	-4.254972	0.108412	0.417371
Mg10	-1.970693	0.302420	2.522076
Mg11	-0.147735	2.779926	2.510748
Mg12	-0.322863	-2.272942	1.235131
Mg13	6.565789	-0.533661	-1.609821
Mg14	2.640967	2.932548	1.251314
Mg15	-2.394147	-2.076417	-1.110279
Mg16	-2.561111	2.800878	0.454452
Mg17	-3.231100	-2.389367	2.024284
Mg18	0.228649	4.378005	-0.042343
Mg19	-5.645692	-2.930284	0.256838
Mg20	-5.374560	-1.299529	-2.247142
Mg21	1.419531	-1.233357	-1.199148
Mg22	-3.121904	0.653985	-2.396715

@mg22-isomer34 bp86/6-31G(d) Etot=-4401.997161 Eb=-13.23

Mg1	-0.361302	1.638755	-1.613946
Mg2	2.209799	0.101138	-1.409514
Mg3	-1.144656	3.600344	0.666554
Mg4	-0.376189	-1.551109	-1.573839
Mg5	0.685120	-2.051984	1.334957
Mg6	-1.430304	0.199422	1.128610
Mg7	1.361492	1.747659	0.994935
Mg8	-4.136702	1.805332	0.782911
Mg9	-3.177607	-0.107084	-1.406265
Mg10	-1.778634	-2.235526	3.126817
Mg11	5.287459	-1.117442	-1.032929
Mg12	-4.220431	-1.020958	1.766228
Mg13	-2.907760	-3.021950	-2.496917
Mg14	-2.974844	3.215347	-1.828792
Mg15	2.709924	-2.920317	-0.832154
Mg16	-2.221934	-3.157162	0.410850
Mg17	4.423664	1.922951	0.012853
Mg18	-5.179623	-2.492414	-0.599181
Mg19	6.476965	0.167716	1.685717
Mg20	-3.965644	4.834977	0.496969
Mg21	3.410280	-0.790533	1.325115
Mg22	7.310927	1.232837	-0.938978

@mg22-isomer35 bp86/6-31G(d) Etot=-4401.983668 Eb=-12.85

Mg1	0.767351	-0.218980	-0.000362
Mg2	-1.554314	-0.750019	1.913950
Mg3	2.897579	-2.597632	0.028148
Mg4	-4.241137	-1.230315	0.015886
Mg5	-1.234457	2.024223	-0.027194
Mg6	3.350772	0.393315	-1.618217
Mg7	3.350401	0.430431	1.604711
Mg8	1.355983	-1.779012	2.526962
Mg9	4.568157	-2.174730	2.517638
Mg10	1.836680	2.724190	-0.030308
Mg11	1.354894	-1.839389	-2.485365
Mg12	-1.556313	-0.799709	-1.897462
Mg13	-4.500282	-1.053679	2.975317
Mg14	-6.824027	0.337695	-1.503310
Mg15	-3.820013	1.525758	1.574556
Mg16	4.565573	-2.235958	-2.470163
Mg17	-6.823213	0.378730	1.498450
Mg18	3.831754	5.083369	-0.042691
Mg19	-3.820394	1.485902	-1.613993
Mg20	-4.503431	-1.130176	-2.945668
Mg21	5.789798	-0.850217	0.007539
Mg22	5.208640	2.276202	-0.028425

@mg23-isomer01 bp86/6-31G(d) Etot=-4602.187622 Eb=-15.95

Mg1	-4.806432	1.641478	0.296251
Mg2	-4.542206	-0.653192	-1.700810
Mg3	-2.276659	3.474421	0.845489
Mg4	-4.449412	-1.145858	1.399712
Mg5	0.467559	3.027328	-0.573283
Mg6	-2.024902	1.305522	-1.270771
Mg7	0.220038	2.935958	2.473777
Mg8	0.135027	1.658325	-3.331612
Mg9	-1.793152	0.681916	1.875539
Mg10	-1.320228	-1.013847	-3.140690
Mg11	2.811318	2.072534	1.249308
Mg12	-1.914035	-1.730271	-0.247941
Mg13	2.817366	1.515080	-1.861367
Mg14	0.642281	-0.015886	-0.156163
Mg15	1.138011	0.076979	3.012220
Mg16	-1.096130	-2.054856	2.759216
Mg17	1.666598	-0.861280	-3.506486
Mg18	5.210055	0.837559	-0.182642
Mg19	0.642989	-2.832222	-1.474803
Mg20	3.381387	-1.430072	-0.889706
Mg21	4.053033	-0.640171	2.066257
Mg22	-0.668238	-4.316183	0.852080
Mg23	1.705730	-2.533262	1.506426

@mg23-isomer02 bp86/6-31G(d) Etot=-4602.182782 Eb=-15.82

Mg1	1.111677	-0.205406	0.011666
Mg2	0.132295	2.565792	1.079550
Mg3	3.513954	-1.880420	-0.553747
Mg4	-0.640255	0.009453	2.897788
Mg5	2.077593	1.117636	3.008589
Mg6	4.445789	-0.280376	1.873219
Mg7	2.508899	0.779686	-2.418513
Mg8	0.773147	3.183904	-1.821584
Mg9	-2.706437	2.232823	1.953144
Mg10	-1.686753	0.085069	0.006067
Mg11	5.210291	0.601746	-0.819756
Mg12	1.694355	-2.003366	2.325207
Mg13	3.001329	2.301799	0.325431
Mg14	1.162446	-1.933947	-2.904809

Mg15	-3.557235	-0.666259	2.461415
Mg16	-2.120880	2.764303	-1.188630
Mg17	-3.478822	0.103393	-2.415448
Mg18	-1.491250	-2.377311	-1.807051
Mg19	-4.187422	-1.896099	-0.212087
Mg20	-4.807969	1.036494	0.090092
Mg21	0.868590	-3.532161	-0.340325
Mg22	-1.342934	-2.608045	1.386851
Mg23	-0.480409	0.601290	-2.937069

@mg23-isomer03 bp86/6-31G(d) Etot=-4602.182553 Eb=-15.81

Mg1	1.689928	0.107520	0.425719
Mg2	-1.167672	-1.987485	2.240856
Mg3	1.757958	-1.631478	2.974480
Mg4	4.302066	-0.255602	-1.784659
Mg5	4.716492	0.848560	0.985727
Mg6	-2.998834	0.722219	2.302383
Mg7	0.248935	2.688809	-0.828422
Mg8	-1.422324	1.446493	-3.069165
Mg9	3.774116	-2.094045	0.586476
Mg10	1.464813	0.613601	-2.848893
Mg11	-1.061279	-0.082323	-0.193838
Mg12	-0.040427	0.733514	2.948173
Mg13	-2.815811	2.345270	-0.473975
Mg14	-1.075782	3.259360	1.877524
Mg15	0.961882	-3.703747	0.976460
Mg16	-1.421153	-2.981696	-0.774674
Mg17	1.972348	2.755852	1.752700
Mg18	-0.825393	-1.398612	-3.418873
Mg19	3.255376	2.488271	-1.128719
Mg20	1.455857	-2.127903	-1.594002
Mg21	-3.555105	-0.588104	-1.982311
Mg22	-5.256567	0.671516	0.234747
Mg23	-3.959424	-1.829990	0.792284

@mg23-isomer04 bp86/6-31G(d) Etot=-4602.181850 Eb=-15.79

Mg1	1.981587	1.519174	2.917978
Mg2	-3.106639	1.330888	1.749722
Mg3	-1.327796	2.969219	-0.642979
Mg4	-1.977155	1.149917	-3.037892
Mg5	0.945315	1.653751	-2.519452
Mg6	-0.460372	-0.230193	2.942185
Mg7	-3.402591	-1.274323	-1.678176
Mg8	1.674343	0.051139	-0.067925
Mg9	-1.308365	-3.313557	-0.615207
Mg10	1.634534	-2.886685	-0.562760
Mg11	3.969025	1.438350	-1.639673
Mg12	-2.810396	-1.846784	1.656877
Mg13	4.492802	-1.486860	-0.486933
Mg14	4.509481	0.878386	1.295238
Mg15	2.684772	-0.975845	-2.958823
Mg16	-4.280968	1.708029	-1.057069
Mg17	-1.132285	-0.012057	-0.063615
Mg18	-0.525924	2.828276	2.292443
Mg19	-0.246148	-1.326083	-2.631757
Mg20	-5.276458	-0.512469	0.572019
Mg21	2.370473	-1.478473	2.272431
Mg22	1.682843	2.998394	0.168647
Mg23	-0.090078	-3.182196	2.094721

@mg23-isomer05 bp86/6-31G(d) Etot=-4602.179565 Eb=-15.73

Mg1	-1.179436	2.389489	-0.724705
Mg2	0.136526	4.208359	1.408140
Mg3	0.560578	1.012489	-2.989477

Mg4	-1.394609	1.925137	2.519958
Mg5	-2.397232	0.344308	-2.674508
Mg6	-5.314291	0.209275	-1.448860
Mg7	1.814299	2.933122	-0.778044
Mg8	-4.930933	-1.080038	1.220930
Mg9	-3.350082	-2.223496	-1.238598
Mg10	3.678015	1.203468	-2.460947
Mg11	2.358222	-1.403492	-2.848900
Mg12	1.119419	0.033798	-0.089729
Mg13	4.107572	1.413884	0.580165
Mg14	-4.089442	1.873745	0.726247
Mg15	1.606579	1.764239	2.438359
Mg16	-0.482187	-1.918031	-2.069633
Mg17	-1.846321	-0.257517	0.544041
Mg18	-0.004043	-0.772133	2.984236
Mg19	4.422219	-1.224685	-0.639564
Mg20	-0.994217	-3.051257	0.827917
Mg21	1.893960	-2.909965	-0.214026
Mg22	3.027801	-1.027557	2.109055
Mg23	1.257603	-3.443143	2.817944

@mg23-isomer06 bp86/6-31G(d) Etot=-4602.179487 Eb=-15.73

Mg1	0.796469	0.117889	-0.144657
Mg2	-0.906494	-3.497880	0.290892
Mg3	3.584806	2.011986	-1.352315
Mg4	-5.345043	-0.332593	0.596173
Mg5	-2.154797	-0.649566	-0.460336
Mg6	3.125444	1.307934	1.530802
Mg7	2.535380	-0.145034	-3.253415
Mg8	-1.405542	2.165376	-1.307743
Mg9	1.856000	-2.662927	1.259987
Mg10	4.538271	-1.494545	2.230419
Mg11	-2.815332	1.012432	1.985521
Mg12	-0.470171	-0.214143	-3.059867
Mg13	1.094044	2.504142	-2.991145
Mg14	-0.755328	-1.236656	2.293455
Mg15	3.749155	-0.990436	-0.602203
Mg16	-1.731662	-2.951047	-2.491109
Mg17	1.156191	3.273485	0.040680
Mg18	1.928448	-0.588134	3.579888
Mg19	-1.686695	3.725641	1.168847
Mg20	-4.375389	2.469053	-0.190943
Mg21	0.160709	1.712455	2.538089
Mg22	1.215410	-2.530571	-1.758405
Mg23	-4.093873	-3.006860	0.097385

@mg23-isomer07 bp86/6-31G(d) Etot=-4602.179418 Eb=-15.73

Mg1	1.191346	0.074228	3.345452
Mg2	4.241918	-0.804804	1.937751
Mg3	4.947171	0.300974	-0.770964
Mg4	2.099009	-0.414201	-2.029110
Mg5	1.997183	1.087577	0.637380
Mg6	-1.693017	2.709185	0.149650
Mg7	-3.410253	-1.316600	1.243445
Mg8	-0.644969	-0.211948	-0.036035
Mg9	-5.181093	-0.591566	-1.190369
Mg10	-1.162147	-3.279490	0.593362
Mg11	-2.519844	-2.109647	-1.795842
Mg12	-1.843408	0.887064	2.753692
Mg13	1.524521	-2.081448	1.208816
Mg14	0.070838	1.991200	-2.266767
Mg15	-2.792408	1.002677	-2.159917
Mg16	0.938416	4.041674	-0.297094
Mg17	0.335250	2.888556	2.435381

Mg18	-0.529707	-0.705909	-3.504906
Mg19	-0.897807	-1.953914	3.245164
Mg20	3.096725	2.468253	-1.835973
Mg21	3.918802	-2.522926	-0.703047
Mg22	-4.427355	1.508500	0.755385
Mg23	0.740826	-2.967435	-1.715454

@mg23-isomer08 bp86/6-31G(d) Etot=-4602.178732 Eb=-15.71

Mg1	-1.332689	2.074178	-1.055182
Mg2	-2.618077	-0.552071	-1.801085
Mg3	2.203196	-2.746714	0.269063
Mg4	0.823485	-0.016087	0.168242
Mg5	2.002554	-2.379946	-2.812487
Mg6	3.081871	0.470283	-2.136942
Mg7	3.930405	-0.174683	0.855100
Mg8	2.599736	2.479134	0.165877
Mg9	-5.277857	-0.374947	1.555887
Mg10	-5.781973	-0.953988	-1.316673
Mg11	-0.018572	2.498657	1.815046
Mg12	0.101587	-0.036765	-2.933404
Mg13	-3.131768	-2.513007	0.468697
Mg14	1.207751	2.776407	-2.661537
Mg15	0.344364	4.537216	-0.398992
Mg16	-4.567442	1.741189	-0.528978
Mg17	4.636689	-2.014733	-1.484925
Mg18	-2.049426	0.224976	1.327736
Mg19	-0.419073	-2.342363	1.881910
Mg20	2.325225	-1.559599	3.045964
Mg21	-0.071811	0.093356	3.697382
Mg22	2.562647	1.426221	3.057681
Mg23	-0.550824	-2.656715	-1.178381

@mg23-isomer09 bp86/6-31G(d) Etot=-4602.178241 Eb=-15.69

Mg1	3.599968	-1.685351	1.364596
Mg2	0.140681	-1.307676	-2.316354
Mg3	4.912086	0.260010	-0.649984
Mg4	0.654325	-2.573365	2.509177
Mg5	-1.511080	0.107772	-0.080202
Mg6	0.887290	0.416961	3.156204
Mg7	-4.178148	1.097439	1.479170
Mg8	-2.920930	-1.792836	-2.301125
Mg9	1.297118	-3.566972	-0.203694
Mg10	0.348445	2.113794	-1.767723
Mg11	3.179548	2.742132	-0.853206
Mg12	3.628905	1.327949	1.802710
Mg13	3.190909	-1.927163	-1.745864
Mg14	-1.812297	-0.909607	2.687381
Mg15	-1.482697	2.186827	2.708446
Mg16	0.855098	2.876905	1.151222
Mg17	-1.489971	-2.912266	0.216042
Mg18	-4.695121	0.670718	-1.441057
Mg19	2.661912	0.673538	-2.957536
Mg20	-4.341682	-1.662072	0.448022
Mg21	1.422710	-0.091754	0.134441
Mg22	-2.153953	1.025685	-3.032072
Mg23	-2.193115	2.929333	-0.308594

@mg23-isomer10 bp86/6-31G(d) Etot=-4602.177266 Eb=-15.67

Mg1	0.979349	-0.338632	3.567829
Mg2	-3.212065	0.728884	1.016437
Mg3	5.211759	0.724831	0.089704
Mg4	2.713759	0.103447	-1.577117
Mg5	2.082663	1.231993	1.228780
Mg6	-1.956334	3.219385	-0.215712

Mg7	-2.769524	-2.293811	0.820678
Mg8	-0.377117	-0.302101	0.005749
Mg9	-4.456302	-0.969617	-1.308059
Mg10	-0.199555	-3.646410	-0.095847
Mg11	-1.808458	-2.275807	-2.247645
Mg12	-1.986958	-0.612581	3.432107
Mg13	2.080436	-1.863972	0.977390
Mg14	0.563335	2.215365	-1.607133
Mg15	-2.223510	0.880359	-2.258277
Mg16	0.850377	4.090194	0.687729
Mg17	-0.690199	1.956352	2.325332
Mg18	0.280336	-0.388210	-3.308424
Mg19	-0.306887	-2.931548	2.814369
Mg20	3.682127	3.246287	-0.386617
Mg21	4.608277	-2.174702	-0.779262
Mg22	-4.755386	2.133483	-1.060816
Mg23	1.689876	-2.733187	-2.121196

@mg23-isomer11 bp86/6-31G(d) Etot=-4602.176338 Eb=-15.64

Mg1	-0.485114	2.315630	2.714473
Mg2	1.841153	2.119652	0.675893
Mg3	1.457251	0.269532	3.297535
Mg4	-5.177184	1.035194	-0.934437
Mg5	-0.599335	0.186401	0.001381
Mg6	4.393368	0.353408	1.888523
Mg7	1.977666	-1.111465	0.601977
Mg8	1.918471	-2.267784	-2.245903
Mg9	-0.841976	3.452186	0.035022
Mg10	0.590362	2.821324	-2.420598
Mg11	-0.338378	-0.155903	-3.059330
Mg12	-2.382736	1.941945	-2.059224
Mg13	2.418664	0.638474	-1.989830
Mg14	0.691572	-3.816115	0.088755
Mg15	-3.091441	1.700922	1.154129
Mg16	-3.116519	-0.985519	-1.695444
Mg17	-1.958372	-2.509166	0.713895
Mg18	4.862588	1.937033	-0.634927
Mg19	-4.550743	-0.987234	1.164495
Mg20	0.316447	-2.464458	2.785804
Mg21	-1.743270	-0.376234	3.021792
Mg22	-0.980766	-3.002818	-2.226712
Mg23	4.798295	-1.095006	-0.877270

@mg23-isomer12 bp86/6-31G(d) Etot=-4602.175521 Eb=-15.62

Mg1	4.807794	2.462791	-0.397677
Mg2	1.838992	3.362898	0.550881
Mg3	-1.033956	3.350396	1.222644
Mg4	-0.119282	2.783773	-1.742323
Mg5	3.526130	1.222271	1.993206
Mg6	4.964323	-0.668074	0.098632
Mg7	0.535386	1.185547	2.566714
Mg8	-2.479289	0.955602	2.528441
Mg9	2.114315	0.732013	-1.032502
Mg10	-2.181967	1.157869	-3.254312
Mg11	-3.128796	2.204746	-0.460614
Mg12	-5.149388	0.687130	1.225428
Mg13	1.902171	-1.215843	1.311100
Mg14	-0.733851	0.088969	-0.113997
Mg15	3.766448	-3.361136	-0.085227
Mg16	-0.796391	-1.725812	2.570518
Mg17	0.603324	0.312913	-3.619274
Mg18	-3.673440	-1.865300	1.780100
Mg19	1.084788	-2.170793	-1.608010
Mg20	-3.567950	-0.748420	-1.055841

Mg21	-1.671886	-2.980710	-0.275838
Mg22	-1.439685	-1.784242	-3.144901
Mg23	0.832212	-3.986589	0.942852

@mg23-isomer13 bp86/6-31G(d) Etot=-4602.175070 Eb=-15.61

Mg1	-3.097872	-2.785199	0.041936
Mg2	-2.937508	-0.678996	2.260954
Mg3	-3.085804	1.364552	-2.388893
Mg4	-0.009377	0.086342	3.117574
Mg5	2.249968	-1.583715	1.882663
Mg6	1.886081	-1.112182	-1.242399
Mg7	-2.336905	1.888056	3.699008
Mg8	-0.961058	-0.098866	-0.080090
Mg9	-0.547204	-2.860701	-1.571991
Mg10	4.755376	-0.097046	0.117162
Mg11	-0.659669	2.744022	-1.437081
Mg12	-0.335187	2.952631	1.669665
Mg13	-3.060162	-1.587935	-2.786486
Mg14	1.814642	1.118009	0.743694
Mg15	-0.439763	0.008192	-3.143664
Mg16	-0.543456	-2.678435	1.718521
Mg17	2.057881	1.696785	-2.379294
Mg18	-4.528982	-0.284150	-0.384533
Mg19	4.587164	2.801740	-0.434849
Mg20	1.811308	3.975848	-0.403135
Mg21	1.718736	-3.922900	0.098019
Mg22	-3.076904	2.134700	0.588063
Mg23	4.738697	-3.080751	0.315155

@mg23-isomer14 bp86/6-31G(d) Etot=-4602.174711 Eb=-15.60

Mg1	-1.232211	0.359446	3.515174
Mg2	-3.600038	0.088191	1.591797
Mg3	-3.722974	-2.508556	0.002588
Mg4	-1.445237	-2.239645	2.036634
Mg5	-1.861011	2.708318	1.750370
Mg6	-1.374643	-4.482709	0.006124
Mg7	-4.393048	2.642606	-0.002695
Mg8	1.142666	1.923029	2.706164
Mg9	1.301752	-1.062863	2.668624
Mg10	-3.602604	0.084467	-1.591252
Mg11	-0.872296	0.101766	-0.001632
Mg12	0.936760	-2.486772	0.002890
Mg13	-1.445765	-2.246686	-2.032800
Mg14	0.532441	3.081421	-0.003422
Mg15	4.039186	0.378445	2.367053
Mg16	-1.862149	2.704927	-1.755513
Mg17	2.058109	0.497564	0.000710
Mg18	-1.234039	0.351798	-3.513107
Mg19	4.334365	-1.881840	0.000553
Mg20	1.300792	-1.070099	-2.665945
Mg21	5.823317	0.763878	-0.002884
Mg22	1.141532	1.915844	-2.709630
Mg23	4.035094	0.377468	-2.369803

@mg23-isomer15 bp86/6-31G(d) Etot=-4602.174125 Eb=-15.58

Mg1	-1.533451	2.595170	-2.001471
Mg2	1.302180	3.091005	-1.355025
Mg3	4.150386	2.183132	-1.144266
Mg4	0.457223	0.291514	-2.776926
Mg5	-3.819630	0.364720	-1.888997
Mg6	-1.367094	-0.051478	-0.120323
Mg7	2.471835	2.395384	1.561215
Mg8	-0.660030	2.987823	0.892797
Mg9	5.140550	-0.011190	0.585092

Mg10	3.771576	-0.756060	-2.063187
Mg11	-3.752504	2.729855	0.060876
Mg12	-1.666066	-1.919099	-2.632935
Mg13	-3.895848	-2.313995	-0.400603
Mg14	1.084846	-2.556074	-1.573514
Mg15	1.690721	0.070571	-0.063037
Mg16	-4.813203	0.063168	1.016581
Mg17	0.160928	0.502187	2.592374
Mg18	3.091250	-0.508360	2.675672
Mg19	-2.681156	1.419995	2.576665
Mg20	3.664388	-2.618489	0.449263
Mg21	-1.261586	-3.721075	-0.132650
Mg22	0.751489	-2.456024	1.576765
Mg23	-2.286803	-1.782678	2.165637

@mg23-isomer16 bp86/6-31G(d) Etot=-4602.172961 Eb=-15.55

Mg1	2.853818	-3.015680	1.278708
Mg2	4.033465	-2.885048	-1.441610
Mg3	0.948440	-3.046551	-1.159552
Mg4	3.915422	-0.262797	0.222441
Mg5	-0.113575	-2.544640	1.744276
Mg6	2.085145	-0.512312	2.788814
Mg7	2.401424	-0.644765	-2.600254
Mg8	-0.502543	-0.848847	4.259379
Mg9	0.721900	-0.019777	0.002232
Mg10	-1.883150	-1.721709	-0.720641
Mg11	2.667557	2.200422	1.672410
Mg12	-0.361059	-1.453521	-3.350079
Mg13	-2.475087	-0.579807	2.050203
Mg14	2.870425	2.079950	-1.483640
Mg15	-5.082526	-1.648952	0.247836
Mg16	2.985994	4.651585	-0.004787
Mg17	-2.704542	0.321627	-2.979667
Mg18	-0.263293	1.657865	2.484739
Mg19	0.058936	1.575654	-2.616712
Mg20	-2.074413	1.477736	-0.207610
Mg21	-5.362637	0.774011	-1.534794
Mg22	0.306100	3.288912	-0.074158
Mg23	-5.025803	1.156643	1.422467

@mg23-isomer17 bp86/6-31G(d) Etot=-4602.172633 Eb=-15.54

Mg1	-4.815998	-0.801928	-0.102826
Mg2	-2.792101	-0.298677	2.092039
Mg3	-2.901749	1.411601	-1.056105
Mg4	4.528353	-1.494268	0.679918
Mg5	0.973430	3.365022	1.800034
Mg6	2.302752	-1.615750	-1.327998
Mg7	2.338577	-1.326283	2.955853
Mg8	-1.925620	2.680155	1.528834
Mg9	-4.943051	1.986218	1.138126
Mg10	-0.325875	-2.375831	2.034276
Mg11	0.321170	-1.492671	-3.632768
Mg12	2.259574	-3.565392	0.920559
Mg13	-0.428868	-0.165734	-0.192721
Mg14	1.820962	1.102488	-2.503414
Mg15	0.032082	0.633957	2.870128
Mg16	-2.952973	-2.996085	0.530856
Mg17	-0.989957	1.121669	-3.428489
Mg18	-0.209234	-3.210862	-0.951621
Mg19	2.233643	0.720839	0.719773
Mg20	2.947705	3.464121	-0.606233
Mg21	5.076251	1.384889	-0.224732
Mg22	-0.108997	2.868910	-0.995563
Mg23	-2.440076	-1.396387	-2.247925

@mg23-isomer18 bp86/6-31G(d) Etot=-4602.171137 Eb=-15.50

Mg1	-4.694637	-1.500324	-0.903265
Mg2	-4.855209	1.365717	-0.096398
Mg3	-2.439165	-2.727465	-2.526725
Mg4	-4.260657	-0.810024	2.071410
Mg5	-1.855268	-2.039121	0.425141
Mg6	0.888065	-2.662057	1.478947
Mg7	-1.193798	-0.974290	3.229567
Mg8	-1.811435	0.254511	-1.856985
Mg9	0.413094	-2.322919	-1.845775
Mg10	0.909324	0.298183	-3.252997
Mg11	-1.932908	1.140047	1.206732
Mg12	3.383986	-0.883965	-2.024907
Mg13	1.745889	-0.566282	3.504277
Mg14	2.603066	2.157796	-1.470765
Mg15	2.847952	-3.515120	-0.725564
Mg16	0.750467	0.102970	0.063436
Mg17	-2.464311	3.141580	-0.955125
Mg18	-0.035665	3.023824	-2.557501
Mg19	3.615622	-1.234595	1.157656
Mg20	0.135680	1.901177	3.234532
Mg21	5.053377	0.887224	-0.275311
Mg22	0.373445	3.220157	0.451773
Mg23	2.823085	1.742977	1.667846

@mg23-isomer19 bp86/6-31G(d) Etot=-4602.169299 Eb=-15.45

Mg1	1.641333	-0.617074	-0.934116
Mg2	3.722441	-3.017775	-0.247111
Mg3	-1.019608	-1.871845	-2.272604
Mg4	-1.826309	-3.094105	0.359167
Mg5	-1.051278	0.269683	0.164997
Mg6	-1.105637	3.538862	0.941758
Mg7	-1.887769	3.170251	-1.873294
Mg8	0.854042	-3.828378	-0.953701
Mg9	1.220932	1.766564	1.691688
Mg10	-1.488556	1.651248	3.236863
Mg11	-0.134985	0.958685	-2.879599
Mg12	-1.869560	-1.310401	2.839896
Mg13	3.251506	-0.505643	1.705312
Mg14	-4.013167	-0.860119	0.611073
Mg15	1.081841	3.057630	-1.072019
Mg16	0.756619	-0.215775	3.973464
Mg17	3.139305	1.378544	-2.618917
Mg18	-4.018083	-2.685341	-1.747791
Mg19	-3.764476	2.148848	0.311997
Mg20	0.738085	-2.157771	1.577762
Mg21	3.939575	2.256981	0.101999
Mg22	-3.191653	0.364514	-2.127793
Mg23	5.025400	-0.397582	-0.789031

@mg23-isomer20 bp86/6-31G(d) Etot=-4602.169068 Eb=-15.44

Mg1	0.917934	2.510002	2.815879
Mg2	-3.283473	3.682638	-0.304364
Mg3	2.876468	2.372638	0.428951
Mg4	2.657952	-0.076391	2.677856
Mg5	-1.928435	1.710746	1.728898
Mg6	-0.307746	-0.033067	3.521068
Mg7	0.726296	-2.583349	2.596666
Mg8	-0.140716	3.583519	0.272693
Mg9	4.406094	-0.209830	0.116487
Mg10	1.269708	2.781071	-2.168369
Mg11	3.234175	-2.789671	0.930697
Mg12	0.996254	0.029337	0.060953

Mg13	3.759261	1.119471	-2.382418
Mg14	-1.611675	-1.160169	0.912674
Mg15	-4.766211	1.134069	-0.002487
Mg16	-1.371365	1.194370	-1.352808
Mg17	0.507042	-3.556245	-0.203313
Mg18	2.586605	-1.829134	-1.876848
Mg19	-4.913118	-1.878012	0.527580
Mg20	1.073413	0.220452	-3.574582
Mg21	-3.569021	-0.897207	-1.924967
Mg22	-0.608130	-1.743268	-2.181650
Mg23	-2.511313	-3.581968	-0.618596

@mg23-isomer21 bp86/6-31G(d) Etot=-4602.168628 Eb=-15.43

Mg1	-5.125820	0.776902	-0.128304
Mg2	-3.359061	3.156835	0.351468
Mg3	-4.718365	-2.054960	0.835223
Mg4	-2.581175	0.220436	1.424441
Mg5	-0.374359	2.209279	1.702247
Mg6	-0.319093	-0.346290	3.370069
Mg7	-1.781910	-2.638855	2.132874
Mg8	-0.594310	4.173896	-0.465587
Mg9	-1.494083	1.262017	-1.466499
Mg10	-2.147815	-1.714640	-0.957219
Mg11	2.321590	0.774778	2.251679
Mg12	0.493915	-0.467499	0.112692
Mg13	2.131130	3.750568	1.107419
Mg14	1.649987	-2.413366	2.330051
Mg15	-0.002092	-3.630142	0.017590
Mg16	1.496118	2.151189	-1.298707
Mg17	4.244695	1.840609	0.111862
Mg18	2.878791	-3.071613	-0.473848
Mg19	4.367430	-1.087115	1.014610
Mg20	-1.743970	-0.798051	-3.814438
Mg21	3.107654	-0.369319	-1.799193
Mg22	0.695667	-2.261281	-2.630752
Mg23	0.855076	0.536624	-3.727677

@mg23-isomer22 bp86/6-31G(d) Etot=-4602.167657 Eb=-15.40

Mg1	3.615428	-3.687559	-0.369811
Mg2	3.785344	-0.722064	-0.152651
Mg3	2.669743	-2.088171	-2.761274
Mg4	2.057636	-2.208056	1.892595
Mg5	3.962691	2.256101	-0.012272
Mg6	0.604809	-2.985263	-0.692846
Mg7	2.635444	0.734465	2.357113
Mg8	2.342661	0.835788	-2.339417
Mg9	0.150761	-0.718311	3.934230
Mg10	-0.961746	-2.570071	1.974257
Mg11	0.597314	0.028586	0.125425
Mg12	-0.256122	-1.027822	-2.923152
Mg13	1.884876	3.641973	1.587533
Mg14	1.482132	3.523191	-1.323666
Mg15	-2.182416	-1.687143	-0.618424
Mg16	-0.166214	1.916642	2.771922
Mg17	-0.401340	1.990759	-2.999828
Mg18	-1.169616	2.406209	-0.074904
Mg19	-2.297090	0.138657	1.815686
Mg20	-2.852742	0.618999	-2.300697
Mg21	-5.134446	-1.122142	1.445556
Mg22	-4.871452	1.575196	0.144979
Mg23	-5.495655	-0.849964	-1.480355

@mg23-isomer23 bp86/6-31G(d) Etot=-4602.167594 Eb=-15.40

Mg1	1.195686	-0.067536	0.012146
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Mg2	0.090285	1.520710	-2.370746
Mg3	4.533850	1.340086	0.303337
Mg4	3.187084	0.007664	-2.242670
Mg5	0.156788	1.385838	2.656426
Mg6	-2.853624	-2.262228	0.966344
Mg7	-0.175471	-1.682349	2.269765
Mg8	-1.838930	0.851405	0.419149
Mg9	0.586178	-1.426838	-3.126918
Mg10	-2.186422	-0.822532	-2.064295
Mg11	4.434886	-1.607902	0.137373
Mg12	2.184870	-3.128115	1.282657
Mg13	-5.087353	-0.081596	1.482930
Mg14	-5.009156	-1.575690	-1.082590
Mg15	0.091925	3.167054	0.154252
Mg16	2.574559	2.987861	1.874926
Mg17	-4.638972	1.403594	-1.244523
Mg18	-2.445328	3.350187	-1.604276
Mg19	-2.591932	-0.047450	3.264510
Mg20	2.582970	2.890359	-1.292158
Mg21	2.861561	-0.165917	2.502260
Mg22	2.608170	-3.079301	-1.738455
Mg23	-0.261624	-2.957305	-0.559444

@mg23-isomer24 bp86/6-31G(d) Etot=-4602.165707 Eb=-15.35

Mg1	1.429568	0.005057	-0.476634
Mg2	2.781830	2.689629	0.442496
Mg3	-0.903648	0.755129	-2.729696
Mg4	4.465000	0.633787	-1.580911
Mg5	0.210033	1.608649	2.137623
Mg6	-1.511722	-0.109930	0.062332
Mg7	2.971549	-2.243469	-1.956751
Mg8	1.981054	1.971058	-2.721011
Mg9	1.583427	-2.875730	0.784989
Mg10	2.670936	-0.275331	2.385498
Mg11	-0.083416	2.952898	-0.582507
Mg12	5.180358	1.172515	1.320511
Mg13	4.599341	-1.637281	0.425689
Mg14	-2.714839	0.209825	2.758952
Mg15	-0.112945	-2.397727	-1.759697
Mg16	-0.161746	-1.492213	2.817994
Mg17	-2.289026	3.118490	1.446361
Mg18	-2.928683	2.655536	-1.459988
Mg19	-3.941313	-0.118613	-1.978459
Mg20	-4.646859	1.386231	0.685393
Mg21	-1.420599	-3.379266	0.890071
Mg22	-2.999113	-3.012575	-1.663169
Mg23	-4.159187	-1.616667	0.750914

@mg23-isomer25 bp86/6-31G(d) Etot=-4602.165529 Eb=-15.35

Mg1	-1.745809	0.177864	-0.862769
Mg2	-1.125107	-2.438514	0.923193
Mg3	-4.867063	1.267243	1.136627
Mg4	1.728430	-2.438301	2.355651
Mg5	1.350860	-0.400387	-0.032273
Mg6	-0.051254	-2.164539	-2.182998
Mg7	2.634527	3.163529	-1.495640
Mg8	-2.918064	-0.293528	2.746820
Mg9	1.184061	0.764759	-2.715819
Mg10	4.265341	0.560433	-1.011398
Mg11	-0.402394	3.033931	-1.316550
Mg12	1.270242	2.692727	1.244982
Mg13	3.015227	-1.915698	-2.210041
Mg14	-3.623925	2.726157	-1.187749
Mg15	1.567347	-3.825085	-0.251591

Mg16	-4.828288	0.010146	-1.628333
Mg17	-3.065621	-2.454095	-1.804122
Mg18	4.164601	-2.216096	0.520102
Mg19	3.354637	0.281241	2.136946
Mg20	0.034673	0.145077	2.509011
Mg21	4.326496	2.858258	0.969774
Mg22	-4.386347	-1.860675	0.758255
Mg23	-1.882570	2.325552	1.397922

@mg23-isomer26 bp86/6-31G(d) Etot=-4602.165521 Eb=-15.35

Mg1	-1.253929	0.167984	0.395377
Mg2	1.710692	-0.203628	0.292482
Mg3	-3.974442	1.376266	1.175426
Mg4	4.021632	1.211844	1.628960
Mg5	3.200981	-2.397790	-1.779529
Mg6	4.779129	0.053235	-1.210124
Mg7	0.703728	1.165569	2.824641
Mg8	0.306082	2.620808	-1.174764
Mg9	0.085922	-2.153599	-1.674622
Mg10	1.888195	0.327742	-2.674850
Mg11	-1.290823	-3.562502	0.652656
Mg12	1.694261	-3.495338	0.564627
Mg13	-3.054133	-1.484461	2.089778
Mg14	4.267185	-1.838562	1.068970
Mg15	-1.477092	0.342139	-2.648568
Mg16	-5.432362	-1.131589	0.368648
Mg17	-2.724796	2.902942	-1.144848
Mg18	-2.976854	-1.913524	-1.246078
Mg19	0.155506	-1.826419	2.558967
Mg20	-4.495969	0.638333	-1.888390
Mg21	1.781382	3.474515	1.376520
Mg22	3.308532	2.580549	-1.029731
Mg23	-1.222827	3.145488	1.474451

@mg23-isomer27 bp86/6-31G(d) Etot=-4602.165376 Eb=-15.34

Mg1	2.379750	0.182325	1.043208
Mg2	0.111275	3.142005	-1.186371
Mg3	-0.436397	0.916472	-3.238069
Mg4	-2.689699	1.652015	-1.259470
Mg5	2.032279	-1.683514	-1.571474
Mg6	-2.847506	-0.039447	1.830901
Mg7	1.238343	3.053602	1.604726
Mg8	4.587292	-2.013558	0.232507
Mg9	2.249106	1.227551	-2.038521
Mg10	1.800328	-1.581952	3.567483
Mg11	-0.025994	-2.002827	-3.810015
Mg12	5.027890	0.941743	-0.269278
Mg13	-4.943565	-0.423524	-0.322748
Mg14	-3.356521	-2.826222	0.504793
Mg15	1.908314	-3.188966	1.006503
Mg16	-0.334432	0.038851	-0.154296
Mg17	-4.697784	2.316353	0.950739
Mg18	-0.505541	-3.164963	-0.823027
Mg19	-2.443587	-1.226415	-2.095553
Mg20	-0.753124	-2.324495	2.139906
Mg21	-1.684762	2.877868	1.329874
Mg22	3.464799	3.485706	-0.357288
Mg23	-0.080462	0.641392	2.915470

@mg23-isomer28 bp86/6-31G(d) Etot=-4602.165194 Eb=-15.34

Mg1	1.749345	-1.108017	-1.372295
Mg2	4.401783	-2.012662	0.316221
Mg3	2.079144	-0.177109	1.830905
Mg4	1.288004	-2.950668	0.989526

Mg5	-1.078620	0.288286	3.329387
Mg6	-1.011003	0.127116	-2.822383
Mg7	-2.628112	2.199455	-0.822868
Mg8	4.989150	-0.084855	-1.952051
Mg9	-4.176105	-0.021884	-1.827266
Mg10	-0.759501	-0.006448	0.219568
Mg11	-3.739455	0.068497	1.297987
Mg12	0.257392	2.610329	-1.531571
Mg13	-2.864182	-2.231156	-3.318013
Mg14	-1.713884	-2.461057	1.861810
Mg15	0.495024	2.391710	1.657558
Mg16	-2.617827	2.702660	2.317288
Mg17	-0.808889	-2.746952	-1.193888
Mg18	-3.753305	-2.544105	-0.337942
Mg19	5.427743	0.686454	0.941848
Mg20	2.879465	1.785546	-0.406817
Mg21	0.612370	-2.117597	3.778963
Mg22	2.124367	1.067360	-3.337561
Mg23	-1.152904	4.535097	0.381595

@mg23-isomer29 bp86/6-31G(d) Etot=-4602.164401 Eb=-15.32

Mg1	1.562279	-3.519915	0.277338
Mg2	3.283873	-1.346420	1.720302
Mg3	4.472957	-2.610912	-0.773153
Mg4	0.226760	-1.528717	2.299489
Mg5	-1.341861	-3.522903	0.742601
Mg6	-0.539104	-2.814828	-2.073733
Mg7	1.529739	0.992511	1.134174
Mg8	4.628434	1.453106	2.211295
Mg9	-2.917839	-1.291500	2.171245
Mg10	-3.505561	-2.329674	-0.861366
Mg11	1.766397	-0.971026	-1.287721
Mg12	4.517623	0.570179	-0.631582
Mg13	3.328313	3.280047	0.177523
Mg14	-1.011182	-0.096152	-0.244599
Mg15	1.658453	1.955946	-2.017486
Mg16	-3.197441	0.341376	-2.377531
Mg17	-0.204970	-0.003414	-3.506918
Mg18	-4.818601	0.103083	0.211538
Mg19	-4.165653	1.474098	2.759780
Mg20	-1.225962	1.377677	2.433257
Mg21	0.013301	3.368494	0.170318
Mg22	-1.166138	2.656017	-2.572931
Mg23	-2.893816	2.462927	0.038160

@mg23-isomer30 bp86/6-31G(d) Etot=-4602.162446 Eb=-15.26

Mg1	-0.849740	0.963752	-3.600893
Mg2	-1.678049	2.471841	-1.003290
Mg3	0.213094	3.725946	-3.056475
Mg4	2.057826	1.556958	-2.383621
Mg5	0.730590	-1.292898	-2.492894
Mg6	1.008841	3.464246	0.074495
Mg7	-4.195759	1.882388	0.567267
Mg8	-2.225646	-0.552986	-1.203791
Mg9	-3.874928	-3.271238	-0.808326
Mg10	-1.185684	2.412583	2.012654
Mg11	-0.726663	-3.510082	-1.054889
Mg12	0.466655	0.394352	0.159201
Mg13	3.346141	-0.627035	-0.839348
Mg14	3.679990	2.067480	0.490010
Mg15	-5.197702	-0.948719	0.346581
Mg16	2.328209	-3.587804	-1.364031
Mg17	1.750722	2.325696	2.849042
Mg18	-3.074079	0.155208	2.649672

Mg19	-1.689733	-2.063385	1.359806
Mg20	0.064052	-0.166119	3.169945
Mg21	1.283064	-2.350843	1.144112
Mg22	3.171651	-0.288953	2.301972
Mg23	4.597149	-2.760387	0.682803

@mg23-isomer31 bp86/6-31G(d) Etot=-4602.161463 Eb=-15.24

Mg1	5.224842	-2.849672	1.229560
Mg2	2.835195	-1.288667	-0.601842
Mg3	-1.497356	3.910232	0.226865
Mg4	0.249378	0.386606	0.016939
Mg5	0.391324	-2.757752	0.795355
Mg6	-0.249421	-1.220857	3.315699
Mg7	2.599478	-1.317102	2.363867
Mg8	-3.472395	1.624447	-0.041095
Mg9	2.913263	-1.148491	-3.592610
Mg10	1.215858	3.113403	-1.300720
Mg11	-2.075507	-3.456370	-0.821283
Mg12	-2.357242	-1.118174	1.114371
Mg13	-1.624881	2.470768	-2.271331
Mg14	-5.924710	-0.093507	0.329694
Mg15	3.551705	1.403120	-2.128028
Mg16	-5.003407	-2.889539	-0.031803
Mg17	0.983981	3.285126	1.703844
Mg18	0.393592	-2.238275	-2.163039
Mg19	-1.365662	1.507551	2.313340
Mg20	0.591093	0.687595	-3.072097
Mg21	1.596620	1.134811	3.650506
Mg22	-2.127408	-0.512618	-1.906525
Mg23	3.151660	1.367365	0.870332

@mg23-isomer32 bp86/6-31G(d) Etot=-4602.161219 Eb=-15.23

Mg1	-1.750963	1.670135	-1.079560
Mg2	-0.064172	-0.242770	-2.741709
Mg3	-1.590537	0.021310	1.693535
Mg4	-0.060666	-2.733029	1.413025
Mg5	-4.875896	1.535259	-0.840573
Mg6	1.201348	2.485517	-1.856099
Mg7	3.052180	-0.253566	-2.164193
Mg8	-3.416149	-0.150725	-2.853045
Mg9	1.124647	0.034114	0.116043
Mg10	-1.839189	-1.862304	-0.953972
Mg11	-3.251053	2.686202	1.475011
Mg12	1.947296	-0.780603	2.794222
Mg13	-3.375782	-2.602656	1.652061
Mg14	2.918193	-3.306090	1.329143
Mg15	4.299542	-2.838793	-1.230068
Mg16	-4.974128	-1.566939	-0.714385
Mg17	1.182066	-2.788553	-1.427221
Mg18	0.056760	2.756271	1.237905
Mg19	4.236502	2.144988	-0.788993
Mg20	2.444288	4.289141	0.234916
Mg21	-4.673487	0.088351	1.868052
Mg22	4.356786	-0.566093	0.816748
Mg23	3.052416	1.980832	2.019157

@mg23-isomer33 bp86/6-31G(d) Etot=-4602.156566 Eb=-15.10

Mg1	-1.597715	-3.143644	1.360310
Mg2	-1.320867	-0.030018	0.852196
Mg3	-4.156135	-1.317816	0.920112
Mg4	-1.131294	-0.001216	-2.319799
Mg5	-3.571989	1.406791	2.190679
Mg6	2.309866	-0.934811	-2.814094
Mg7	1.029128	-1.631821	2.254292

Mg8	-2.768836	-2.654213	-1.381302
Mg9	-0.070575	2.745993	-1.565298
Mg10	-2.888029	2.098276	-0.891374
Mg11	1.495969	0.281448	-0.195068
Mg12	4.719080	-0.166505	-1.139528
Mg13	4.358377	2.162644	0.722674
Mg14	1.128735	1.428391	2.610514
Mg15	1.244318	-4.319693	1.137807
Mg16	-1.067810	3.127311	1.486630
Mg17	1.755252	3.632580	0.585949
Mg18	2.966334	2.222397	-2.038193
Mg19	-4.275793	-0.242610	-2.218552
Mg20	3.912581	-0.633305	1.828719
Mg21	3.274122	-2.674307	-0.355830
Mg22	0.298297	-2.550667	-1.100134
Mg23	-5.643015	1.194794	0.069290

@mg23-isomer34 bp86/6-31G(d) Etot=-4602.155792 Eb=-15.08

Mg1	1.516497	-3.133339	-1.452776
Mg2	1.676251	-0.180967	-0.320832
Mg3	4.231237	-1.500931	-1.544684
Mg4	1.886356	-0.583079	2.642020
Mg5	4.040286	1.540283	-1.251262
Mg6	-3.972615	0.100067	2.396107
Mg7	-1.447534	-3.334131	-1.176872
Mg8	3.219617	-2.972689	1.071307
Mg9	0.535673	2.084844	1.728659
Mg10	3.558057	2.025813	1.703068
Mg11	-1.244246	-0.070515	0.618430
Mg12	-5.601546	-1.059598	0.236044
Mg13	-2.225583	1.632790	-2.683337
Mg14	0.861074	1.961303	-2.419174
Mg15	0.204807	-2.865226	1.341898
Mg16	2.081152	3.697873	-0.358024
Mg17	-1.023650	3.362706	-0.510923
Mg18	-2.432185	2.600154	2.069463
Mg19	4.888239	-0.575746	1.225396
Mg20	-3.346370	-0.974165	-1.684993
Mg21	-3.075229	-2.548714	1.242437
Mg22	-0.271067	-0.893352	-2.521917
Mg23	-4.059221	1.686620	-0.350034

@mg23-isomer35 bp86/6-31G(d) Etot=-4602.154048 Eb=-15.03

Mg1	-3.556561	-2.254689	-1.260642
Mg2	0.622064	-2.904122	1.500958
Mg3	-3.212203	0.908929	-1.692455
Mg4	-0.874775	2.018526	1.365241
Mg5	-0.145791	1.522136	-1.956768
Mg6	-0.811475	-3.651285	-1.183803
Mg7	-2.358735	-3.146234	1.410648
Mg8	1.729733	0.236569	1.168539
Mg9	-1.026084	-0.684766	-0.059555
Mg10	1.417090	3.350193	-0.014069
Mg11	-3.921871	-0.401150	1.072669
Mg12	4.581494	0.089880	2.535088
Mg13	3.584865	-2.502795	1.242167
Mg14	1.588289	-1.605380	-1.360234
Mg15	4.328295	2.413256	0.599279
Mg16	5.136420	-0.466874	-0.290876
Mg17	-1.092363	-0.768818	2.931767
Mg18	-4.055219	2.618673	0.608750
Mg19	-3.061903	1.554725	3.306290
Mg20	2.870589	1.133426	-1.724520
Mg21	-1.205247	-1.325172	-3.107184

Mg22	1.209947	0.128794	-4.171314
Mg23	-1.746559	3.736176	-0.919978

@mg23-isomer36 bp86/6-31G(d) Etot=-4602.153228 Eb=-15.01

Mg1	-3.890338	0.751213	1.623321
Mg2	-3.445469	2.712709	-0.849444
Mg3	0.614310	-1.858771	-1.926691
Mg4	2.883993	-3.078032	-0.066062
Mg5	-0.852909	4.050717	-1.404797
Mg6	-0.960380	2.691042	1.307102
Mg7	3.113547	-1.174538	2.460129
Mg8	-1.532984	-0.038682	-0.137126
Mg9	3.552288	-1.659147	-2.655845
Mg10	1.768259	3.125560	-0.076092
Mg11	3.468977	1.184903	-1.764799
Mg12	-4.589027	-0.102606	-1.391698
Mg13	1.505538	2.077769	2.854256
Mg14	0.223622	-2.811826	1.169506
Mg15	-2.131039	-2.947164	-0.938867
Mg16	-2.058894	-0.666862	-3.026839
Mg17	0.252730	1.410084	-2.184818
Mg18	-2.593089	-2.234325	1.966556
Mg19	1.503209	-0.012017	0.303621
Mg20	4.111801	1.531030	1.178435
Mg21	4.990999	-1.010757	-0.042336
Mg22	-5.349036	-1.897525	0.811416
Mg23	-0.586105	-0.042773	2.791071

@mg23-isomer37 bp86/6-31G(d) Etot=-4602.143997 Eb=-14.76

Mg1	-0.461943	0.962949	-0.172277
Mg2	0.359340	3.439427	1.632002
Mg3	2.262053	0.979677	1.663076
Mg4	-2.370134	-1.100939	1.242821
Mg5	1.710184	-3.279114	-1.422840
Mg6	-2.876751	1.908361	1.654403
Mg7	-1.875178	3.619402	-0.691300
Mg8	-3.008578	0.634332	-1.765321
Mg9	-0.432923	0.666697	2.919388
Mg10	0.675808	-1.676979	1.094690
Mg11	3.766474	-1.704753	0.423310
Mg12	-0.766661	-1.518719	-1.751823
Mg13	0.489121	-6.074426	-0.281820
Mg14	2.384402	-4.318860	1.247812
Mg15	2.092216	0.111322	-1.453053
Mg16	-1.468350	-3.929024	0.187987
Mg17	-5.145142	-0.058628	0.280977
Mg18	3.940093	2.821869	-2.282292
Mg19	-3.724800	-2.345583	-1.190562
Mg20	1.091822	3.224310	-1.360580
Mg21	4.807125	1.104317	-0.018888
Mg22	3.389693	3.737273	0.603128
Mg23	-4.837870	2.797088	-0.558837

@mg23-isomer38 bp86/6-31G(d) Etot=-4602.140266 Eb=-14.66

Mg1	0.633436	1.459602	-1.105375
Mg2	-1.360352	3.470049	0.105178
Mg3	2.537662	0.391540	1.308447
Mg4	4.023795	3.155914	0.624698
Mg5	3.396791	2.160715	-2.096171
Mg6	1.612875	4.471901	-0.744905
Mg7	-4.462465	2.718523	-0.342615
Mg8	-0.393942	-1.472706	-1.160475
Mg9	0.858513	-2.156866	1.551789
Mg10	-5.028252	-0.242368	0.634354

Mg11	1.246477	3.173637	1.909470
Mg12	-3.415551	-2.275016	-1.054884
Mg13	2.536925	-0.792254	-1.747861
Mg14	4.978960	0.286409	-0.315087
Mg15	-2.246486	0.707066	-0.852196
Mg16	-1.158824	-4.219704	0.196653
Mg17	3.670716	-2.647691	0.445015
Mg18	1.678753	-5.263647	0.946994
Mg19	-2.320132	-1.564067	1.606959
Mg20	-3.079074	1.591520	2.128855
Mg21	-0.324508	0.629687	1.780644
Mg22	-4.928149	0.177763	-2.328277
Mg23	1.542830	-3.760008	-1.491209

@mg23-isomer39 bp86/6-31G(d) Etot=-4602.137385 Eb=-14.58

Mg1	-0.316454	-0.000487	1.664138
Mg2	-2.961131	-1.553996	1.378277
Mg3	-0.281539	-3.104457	1.518159
Mg4	2.326585	-1.492309	1.575119
Mg5	2.325972	1.491610	1.574022
Mg6	-0.281850	3.103347	1.518508
Mg7	-2.961331	1.553073	1.379079
Mg8	2.721695	-4.628348	1.184137
Mg9	2.721447	4.627831	1.184667
Mg10	-5.716393	-0.001149	1.030637
Mg11	-1.916983	0.000300	-1.183655
Mg12	0.679628	1.470844	-1.100321
Mg13	0.680271	-1.469332	-1.099180
Mg14	-4.663630	1.515298	-1.288193
Mg15	-4.663287	-1.515645	-1.289253
Mg16	-2.009095	-3.177549	-0.990070
Mg17	0.761536	-4.586032	-0.940792
Mg18	3.570731	-2.730754	-0.959136
Mg19	3.091756	0.000521	-2.396648
Mg20	3.570490	2.731504	-0.959399
Mg21	0.760403	4.587393	-0.939473
Mg22	-2.010235	3.178075	-0.988948
Mg23	4.571416	0.000264	0.128325

@mg23-isomer40 bp86/6-31G(d) Etot=-4602.135899 Eb=-14.54

Mg1	0.866630	-0.441046	-0.117651
Mg2	0.012802	-0.288791	2.850141
Mg3	-1.732878	0.199327	-1.279662
Mg4	-2.663798	3.334401	-0.935041
Mg5	4.182714	-0.107478	-0.109991
Mg6	-0.492705	-2.989162	1.499997
Mg7	-4.395845	-1.102709	-2.151437
Mg8	-4.420053	1.175604	0.021595
Mg9	-0.329626	-2.748019	-1.613609
Mg10	2.516557	-1.729057	1.998037
Mg11	-3.023025	-3.101143	-0.265338
Mg12	-2.680356	-0.753260	1.797606
Mg13	2.043677	1.787617	1.523210
Mg14	0.442296	2.678724	-1.118038
Mg15	3.624499	2.768380	-0.842460
Mg16	2.164192	5.021368	0.454434
Mg17	1.802922	-4.387054	0.092654
Mg18	2.763089	-2.262625	-1.950951
Mg19	-5.539117	-1.598073	0.529044
Mg20	-1.304045	2.002374	1.362333
Mg21	4.595142	-3.175482	0.262087
Mg22	2.293671	0.635026	-2.526241
Mg23	-0.726743	5.081079	0.519281

@mg23-isomer41 bp86/6-31G(d) Etot=-4602.135047 Eb=-14.51

Mg1	0.857100	-0.050025	-1.484671
Mg2	-1.829925	-0.191784	0.019146
Mg3	3.055381	0.798174	2.295855
Mg4	1.036983	-1.408564	1.381566
Mg5	4.514351	1.999313	-0.077606
Mg6	3.972737	-1.032623	0.031662
Mg7	1.803839	2.804408	-1.383995
Mg8	-4.347702	1.278787	-1.398611
Mg9	-1.237698	2.219202	-1.769064
Mg10	3.612203	0.620504	-2.544388
Mg11	-2.239114	-0.606637	-2.761752
Mg12	-0.413631	4.398095	0.235223
Mg13	-4.812002	0.052544	1.341755
Mg14	-2.028781	0.034432	2.823090
Mg15	3.937370	-4.097442	0.492626
Mg16	0.979456	-4.514939	0.909693
Mg17	1.973010	-2.865611	-1.476074
Mg18	0.339124	1.550193	1.291977
Mg19	-4.635327	-1.714355	-1.065410
Mg20	-3.168137	-2.527576	1.454712
Mg21	-1.088683	-3.009592	-0.767580
Mg22	2.566179	3.669697	1.488472
Mg23	-2.846732	2.593798	0.963375

@mg23-isomer42 bp86/6-31G(d) Etot=-4602.123350 Eb=-14.20

Mg1	-0.052155	-1.997890	-2.030044
Mg2	-3.253259	-1.750779	-2.598081
Mg3	-3.270996	2.107659	0.448145
Mg4	3.020856	-2.213496	-1.450690
Mg5	-0.305550	3.096167	-0.544428
Mg6	-1.667791	0.633959	-1.727920
Mg7	-0.832641	-2.030396	2.968331
Mg8	-6.167853	0.900933	0.772885
Mg9	-5.287071	-1.714521	-0.308948
Mg10	1.585113	4.979973	0.776196
Mg11	4.169825	0.556958	0.700614
Mg12	1.927132	-0.736654	2.497641
Mg13	-2.153607	-2.153993	0.205587
Mg14	1.434832	0.304326	-0.844443
Mg15	6.026842	-1.376802	-0.753787
Mg16	-0.743854	0.604789	1.416131
Mg17	1.884410	2.272294	1.823974
Mg18	4.179883	0.571062	-2.417616
Mg19	-4.845953	0.821744	-2.034436
Mg20	1.004687	-2.986034	0.682671
Mg21	-3.652600	-0.385930	2.197663
Mg22	4.101299	-2.556172	1.366965
Mg23	2.898451	3.052802	-1.146409

@mg23-isomer43 bp86/6-31G(d) Etot=-4602.118420 Eb=-14.06

Mg1	0.163149	0.631233	1.688167
Mg2	-1.992056	-0.510205	-0.263995
Mg3	-2.580775	-0.535472	2.664016
Mg4	0.742095	-1.632361	-1.208652
Mg5	-5.797512	0.373482	-1.027952
Mg6	-3.924433	-1.483424	-2.410790
Mg7	3.053466	-0.452127	-2.726223
Mg8	2.646596	0.820510	-0.186863
Mg9	-5.097055	3.165521	-0.120379
Mg10	-5.095836	0.887842	1.801494
Mg11	-0.197303	-2.587709	1.470374
Mg12	-4.515697	-1.939937	0.593940
Mg13	3.640125	-2.402882	-0.272801

Mg14	-2.438832	2.229401	0.925055
Mg15	2.317416	-1.308230	2.377860
Mg16	5.790895	-0.394305	-1.176564
Mg17	5.404329	2.181103	0.506782
Mg18	4.617086	2.161664	-2.366984
Mg19	-1.783805	-3.444144	-1.037804
Mg20	-3.173321	1.601065	-1.996688
Mg21	5.139893	-0.607936	1.684930
Mg22	3.110262	1.763989	2.495431
Mg23	-0.028686	1.482920	-1.412353

@mg23-isomer44 bp86/6-31G(d) Etot=-4602.110301 Eb=-13.84

Mg1	-0.216124	-0.985039	-2.405034
Mg2	-0.894968	1.872285	-1.700000
Mg3	-1.326188	2.487180	1.521142
Mg4	2.133494	1.120451	-2.260757
Mg5	-2.462963	-0.363904	-0.109980
Mg6	2.539926	-1.778645	-1.140479
Mg7	-2.892988	-3.385194	1.091018
Mg8	-5.146819	-2.535874	-0.771634
Mg9	0.605657	0.268512	0.422076
Mg10	-4.358151	1.696301	2.134544
Mg11	5.131771	-2.122375	0.561206
Mg12	5.077680	-0.218716	2.961786
Mg13	4.939728	-0.176039	-2.116266
Mg14	1.612778	3.303223	0.006098
Mg15	-5.578563	0.499790	-0.382201
Mg16	-4.960460	-1.288342	1.940072
Mg17	-2.276813	-3.170148	-1.884023
Mg18	-1.062817	4.701923	-0.416302
Mg19	2.403298	-1.521337	1.976465
Mg20	-0.033028	-2.759406	0.202790
Mg21	3.634393	1.089418	0.428175
Mg22	-3.609119	2.928606	-0.486765
Mg23	6.740273	0.337332	0.428070

@mg23-isomer45 bp86/6-31G(d) Etot=-4602.108510 Eb=-13.79

Mg1	0.405196	-0.198541	2.363367
Mg2	3.279573	-1.243771	1.893279
Mg3	3.875409	-2.897308	-0.656562
Mg4	2.549977	1.789790	1.339863
Mg5	-0.345041	2.023252	0.273117
Mg6	1.365642	-1.052928	-0.717032
Mg7	-0.719494	0.229938	-2.427886
Mg8	1.816911	1.819099	-1.872180
Mg9	0.061418	-3.155671	1.390226
Mg10	-3.119729	1.625899	-1.003957
Mg11	-2.970012	3.798417	1.200630
Mg12	-3.504196	-1.271063	-2.190277
Mg13	-4.795514	-1.008814	0.777793
Mg14	-2.663809	1.015316	2.440719
Mg15	2.760165	-4.294214	1.838397
Mg16	4.305119	0.102941	-0.780968
Mg17	-5.904633	0.511917	-1.547167
Mg18	-0.798587	-2.909606	-1.880440
Mg19	-5.386411	1.905907	1.297578
Mg20	1.435216	-4.734760	-0.911966
Mg21	4.250564	3.131342	-0.735989
Mg22	5.846425	5.801254	-0.459337
Mg23	-1.744189	-0.988396	0.368794

@mg24-isomer01 bp86/6-31G(d) Etot=-4802.292625 Eb=-16.21

Mg1	-0.002104	-0.892736	-3.120981
Mg2	1.490059	1.722266	-2.745062

Mg3	2.975037	2.910681	-0.392152
Mg4	1.547342	1.997618	2.275021
Mg5	-1.505095	-0.019451	-0.092146
Mg6	-4.571422	1.208122	1.409212
Mg7	-4.309191	0.562499	-1.661475
Mg8	-2.982435	-0.802657	2.865860
Mg9	0.002065	2.879125	-0.256927
Mg10	1.506448	-0.018464	-0.089554
Mg11	-4.420556	-1.657979	0.378458
Mg12	0.000118	-0.703070	2.692061
Mg13	-1.542976	1.997074	2.274285
Mg14	2.983898	-0.805892	2.864395
Mg15	-2.661048	-2.007034	-2.057762
Mg16	-1.504297	-2.881834	1.100863
Mg17	4.309137	0.558902	-1.661976
Mg18	-2.970734	2.911850	-0.391222
Mg19	1.500261	-2.880805	1.098830
Mg20	-1.489059	1.725141	-2.745679
Mg21	-0.002811	-3.338010	-1.469108
Mg22	4.418967	-1.662036	0.375314
Mg23	4.572802	1.204415	1.407402
Mg24	2.655593	-2.007724	-2.057656

@mg24-isomer02 bp86/6-31G(d) Etot=-4802.291734 Eb=-16.18

Mg1	-1.505902	-0.032633	0.131969
Mg2	1.542312	1.761771	-2.453389
Mg3	1.546963	-3.019027	-0.710793
Mg4	0.156543	-0.398239	3.009046
Mg5	-2.987589	-1.148146	-2.714074
Mg6	4.580362	1.006887	-1.452245
Mg7	-0.019316	3.074479	-0.121686
Mg8	-1.535177	1.711011	-2.440779
Mg9	4.153063	0.705962	1.681237
Mg10	-0.010174	-3.132971	1.845183
Mg11	-4.266655	0.711179	1.631678
Mg12	-1.520928	-3.043044	-0.720992
Mg13	-3.029422	2.937502	0.027983
Mg14	-4.617588	0.989769	-1.495645
Mg15	-1.510904	2.110850	2.450040
Mg16	3.001641	-1.129625	-2.729627
Mg17	1.521840	0.043502	0.076269
Mg18	-4.478589	-1.765398	-0.177047
Mg19	-2.708212	-1.883253	2.229718
Mg20	3.018024	2.979389	0.033406
Mg21	2.726704	-1.963582	2.154928
Mg22	1.441868	2.311572	2.445764
Mg23	4.490284	-1.766084	-0.215178
Mg24	0.010851	-1.061873	-2.485766

@mg24-isomer03 bp86/6-31G(d) Etot=-4802.289018 Eb=-16.11

Mg1	1.444390	-0.032967	0.011247
Mg2	-1.445628	0.068333	0.031230
Mg3	4.593579	1.628801	0.348360
Mg4	3.624556	0.425460	-2.236810
Mg5	0.076607	-2.243518	1.760522
Mg6	-2.391596	-1.292190	3.208950
Mg7	2.636768	-2.983648	0.390120
Mg8	0.153174	0.499031	3.066633
Mg9	1.944152	2.871030	-0.869981
Mg10	-4.339615	-0.697999	-1.595327
Mg11	-2.547451	1.047177	-3.181119
Mg12	-0.961310	3.256436	-1.818968
Mg13	-0.439876	2.776754	1.026365
Mg14	0.445713	0.784136	-2.793427

Mg15	3.234386	-0.506294	2.374784
Mg16	-1.409678	-1.660394	-2.494422
Mg17	-4.607601	-0.362954	1.314472
Mg18	-3.552891	2.174373	-0.354498
Mg19	5.025092	-1.274080	-0.112145
Mg20	1.617935	-1.976672	-2.489809
Mg21	-2.741337	-2.634924	0.344482
Mg22	2.391910	2.363324	2.214650
Mg23	-2.675404	1.554549	2.627656
Mg24	-0.075874	-3.783765	-0.772966

@mg24-isomer04 bp86/6-31G(d) Etot=-4802.286775 Eb=-16.05

Mg1	-0.126497	2.640338	-2.950267
Mg2	2.477616	-2.485947	-1.279948
Mg3	-1.404899	1.524540	1.250271
Mg4	-4.443952	0.027092	-1.677091
Mg5	-2.856231	2.633114	-1.188805
Mg6	1.097181	-0.013418	0.035557
Mg7	-1.347535	0.040028	-1.832576
Mg8	-0.108016	-2.507953	-3.067017
Mg9	-0.128569	3.836548	-0.232263
Mg10	1.587216	-2.449315	1.776950
Mg11	-4.513277	1.493416	1.050860
Mg12	2.443372	2.545700	-1.161527
Mg13	4.413200	-1.500452	0.846521
Mg14	4.406453	1.493018	0.911260
Mg15	-4.505496	-1.545646	0.982683
Mg16	-1.398917	-1.610890	1.205624
Mg17	1.505279	0.073569	-3.067825
Mg18	-3.050513	-0.079017	3.300365
Mg19	2.998128	-0.057299	3.133438
Mg20	4.268870	0.052494	-1.775983
Mg21	-0.093956	-3.809873	-0.402561
Mg22	-2.836779	-2.586607	-1.295834
Mg23	0.054627	-0.084574	3.567200
Mg24	1.562693	2.371133	1.870969

@mg24-isomer05 bp86/6-31G(d) Etot=-4802.286619 Eb=-16.05

Mg1	1.627578	0.124784	-0.093080
Mg2	0.891254	2.837847	-1.252454
Mg3	-0.012626	0.309919	-2.763637
Mg4	2.197222	-1.949725	-2.271542
Mg5	-1.296745	0.228306	0.178508
Mg6	4.687051	-0.569293	-0.947627
Mg7	4.125685	0.434801	1.865908
Mg8	-0.789476	-2.607240	-2.887824
Mg9	-2.239138	2.297341	-1.705208
Mg10	-2.928849	-0.497159	-3.035357
Mg11	3.068436	-2.328520	0.938184
Mg12	3.892578	2.391850	-0.287504
Mg13	-4.531522	-0.846112	1.626739
Mg14	-1.113696	1.401403	3.052748
Mg15	-4.803079	0.493488	-1.023491
Mg16	2.955298	1.036470	-2.800787
Mg17	-0.976597	3.518281	0.967726
Mg18	1.098430	-0.556062	2.838262
Mg19	0.792546	-3.525288	2.717207
Mg20	-1.701568	-1.822588	2.360717
Mg21	-3.688894	2.048792	1.299053
Mg22	1.646935	2.439768	1.916179
Mg23	0.083217	-2.609067	-0.050949
Mg24	-2.984040	-2.251998	-0.641770

@mg24-isomer06 bp86/6-31G(d) Etot=-4802.285157 Eb=-16.01

Mg1	3.659910	2.391157	-1.695959
Mg2	1.585796	3.947694	-0.058858
Mg3	4.407322	-0.416617	-0.752312
Mg4	3.194041	1.656247	1.278380
Mg5	2.505311	-0.080709	-3.073436
Mg6	0.460585	2.083467	-1.997689
Mg7	3.954648	-1.194322	2.095193
Mg8	-0.505292	-0.309423	-3.394532
Mg9	0.191674	2.056027	1.775264
Mg10	-1.556052	3.506042	-0.208726
Mg11	0.917537	-2.670999	-2.433000
Mg12	2.720986	-2.947364	-0.002608
Mg13	1.188006	-0.305932	-0.064405
Mg14	-1.733769	0.268337	-0.586318
Mg15	1.321381	-2.704409	2.764715
Mg16	1.651951	0.157294	3.509695
Mg17	-2.165071	-2.418111	-2.171132
Mg18	-2.781498	1.848654	2.148108
Mg19	-0.376283	-2.977682	0.272051
Mg20	-4.396510	2.210110	-0.441212
Mg21	-1.059615	-0.732530	2.336370
Mg22	-4.775523	-0.698956	-1.455296
Mg23	-4.966646	-0.145338	1.496428
Mg24	-3.442889	-2.522637	0.659280

@mg24-isomer07 bp86/6-31G(d) Etot=-4802.284871 Eb=-16.01

Mg1	-1.009033	-0.005923	0.003765
Mg2	0.762731	2.868177	-0.564743
Mg3	2.074778	0.163612	-0.192844
Mg4	4.081062	2.631197	-0.413924
Mg5	0.908969	-2.695069	0.055312
Mg6	-3.533578	1.143190	1.417389
Mg7	-3.787421	-1.960169	2.001481
Mg8	-2.091821	-2.903639	-0.460080
Mg9	-0.630738	2.186553	2.203960
Mg10	-2.336553	-0.501445	-2.802854
Mg11	-0.124604	-2.658119	-2.805273
Mg12	-1.396256	2.470600	-2.717608
Mg13	-2.137166	3.454969	-0.041874
Mg14	1.030061	-0.473823	2.549776
Mg15	-4.125193	1.860179	-1.616727
Mg16	4.661369	0.328461	1.729917
Mg17	2.352649	2.331244	2.131520
Mg18	-1.824659	-0.215052	3.560315
Mg19	-4.451515	-0.954331	-0.681464
Mg20	2.758105	-1.935898	-2.321209
Mg21	4.031116	-2.422373	0.617536
Mg22	-0.958341	-2.820245	2.349892
Mg23	5.142127	-0.160488	-1.238797
Mg24	0.603908	0.268393	-2.763465

@mg24-isomer08 bp86/6-31G(d) Etot=-4802.284344 Eb=-15.99

Mg1	-2.032936	0.060056	3.058351
Mg2	3.286751	2.713789	0.434012
Mg3	0.659559	1.722958	2.635090
Mg4	1.104111	-0.429850	-3.571261
Mg5	3.971319	-2.287303	1.396868
Mg6	-0.068041	-2.267462	-1.507546
Mg7	-2.467749	2.476620	-1.050050
Mg8	4.941209	0.238530	-0.046321
Mg9	-3.111213	-2.539881	-1.453586
Mg10	0.684876	-1.286905	2.308110
Mg11	2.985285	-1.764056	-1.424078
Mg12	-1.804069	-0.162635	-2.918400

Mg13	1.302542	0.382176	-0.194520
Mg14	-4.321415	1.344625	1.195623
Mg15	0.328428	3.349718	0.013392
Mg16	-4.225959	-1.635384	1.174983
Mg17	-1.522217	-3.148082	1.103592
Mg18	-4.562956	0.091741	-1.438932
Mg19	3.301023	1.309743	-2.292138
Mg20	-1.889664	2.993147	1.991936
Mg21	1.423018	-3.718927	0.658326
Mg22	-1.526006	-0.102438	0.185160
Mg23	0.178739	2.259296	-2.795625
Mg24	3.365366	0.400525	2.537014

@mg24-isomer09 bp86/6-31G(d) Etot=-4802.284173 Eb=-15.99

Mg1	-0.704195	-1.237350	2.575057
Mg2	2.462026	-1.126115	2.600401
Mg3	0.746324	1.459079	2.626236
Mg4	-2.304469	1.317928	2.770125
Mg5	-3.769204	-2.328822	0.456476
Mg6	0.853119	-3.751825	2.376571
Mg7	-0.843794	3.643268	1.367514
Mg8	3.758845	1.442374	1.718734
Mg9	-4.836874	0.214368	1.500762
Mg10	-0.770240	-3.025035	-0.063233
Mg11	-2.575061	-2.137779	-2.369781
Mg12	1.362589	0.143681	-0.099015
Mg13	1.903273	3.217475	0.084227
Mg14	-1.590171	-0.010825	-0.077584
Mg15	-4.517655	0.075004	-1.578080
Mg16	4.206715	1.718668	-1.306505
Mg17	-3.458312	2.490676	-0.031080
Mg18	4.698198	-0.988784	0.360189
Mg19	2.247138	-2.803926	-0.198203
Mg20	0.439639	-1.637153	-2.545582
Mg21	-0.605941	2.593401	-1.366713
Mg22	-1.605507	0.485487	-3.284303
Mg23	3.431667	-0.935279	-2.382797
Mg24	1.471892	1.181484	-3.133415

@mg24-isomer10 bp86/6-31G(d) Etot=-4802.283252 Eb=-15.96

Mg1	-1.577315	1.282704	-1.597723
Mg2	0.447696	-2.801098	-2.552847
Mg3	-0.973150	-3.497872	0.018653
Mg4	4.045945	1.745975	-1.140549
Mg5	1.239451	0.692600	2.991954
Mg6	3.236367	-1.533388	2.417037
Mg7	-2.321154	-1.582725	-2.227118
Mg8	1.059738	0.022972	-0.094213
Mg9	0.292331	-2.211638	2.485600
Mg10	-0.734291	4.057124	-0.693686
Mg11	-1.694798	-0.723673	0.685343
Mg12	4.027287	1.202579	1.741999
Mg13	1.244079	2.291558	-2.332178
Mg14	4.655771	-1.087984	-0.179709
Mg15	-1.685444	-0.106846	3.621209
Mg16	2.770840	-0.680648	-2.498648
Mg17	1.799964	2.962908	0.654054
Mg18	-4.665894	0.163021	-1.234118
Mg19	2.095793	-2.888896	-0.020054
Mg20	-3.720709	2.810066	-0.016343
Mg21	0.015283	-0.131289	-3.668680
Mg22	-4.315989	0.350526	1.849628
Mg23	-1.033359	2.119662	1.558817
Mg24	-4.208446	-2.455639	0.231573

@mg24-isomer11 bp86/6-31G(d) Etot=-4802.283222 Eb=-15.96

Mg1	0.470279	2.840856	1.126479
Mg2	3.982018	-1.395748	1.640135
Mg3	3.136349	1.613952	2.239763
Mg4	-3.773126	-2.826073	0.331159
Mg5	-1.753957	-2.268484	2.430663
Mg6	-4.235508	2.183726	-0.149528
Mg7	5.086567	1.004471	0.039471
Mg8	-2.324646	2.440355	2.137527
Mg9	-2.530280	-2.166141	-2.393553
Mg10	-0.635088	-3.171484	-0.284898
Mg11	-3.996442	-0.144073	1.887758
Mg12	1.526616	0.000764	0.189942
Mg13	2.320336	-2.812970	-0.876311
Mg14	3.190507	0.357494	-2.345151
Mg15	1.157396	-2.497521	2.077181
Mg16	0.460068	2.017746	-2.006594
Mg17	-2.444414	1.188195	-2.594116
Mg18	-4.708632	-0.501365	-1.256072
Mg19	3.067325	3.005115	-0.624661
Mg20	0.228855	-1.092937	-2.445716
Mg21	-0.112851	0.361710	2.784170
Mg22	-1.667480	3.571695	-0.736762
Mg23	5.066791	-1.733478	-1.193323
Mg24	-1.510683	0.024196	0.022438

@mg24-isomer12 bp86/6-31G(d) Etot=-4802.281137 Eb=-15.91

Mg1	-1.581084	0.028647	-0.335637
Mg2	1.395430	0.216462	-0.051848
Mg3	-0.108434	-0.663762	-2.989650
Mg4	-3.054841	-2.264995	1.413223
Mg5	1.656340	-2.557110	-1.276968
Mg6	3.882551	1.825678	-1.075535
Mg7	2.951483	-0.331999	-2.941221
Mg8	4.330653	0.591268	1.770470
Mg9	2.779075	-2.042005	1.739897
Mg10	-1.727485	1.907590	-2.870758
Mg11	-4.831982	0.116276	1.134092
Mg12	-1.341952	-2.894578	-1.286522
Mg13	-2.979580	2.529318	0.939047
Mg14	-0.380216	2.843172	2.655205
Mg15	-4.423900	1.402579	-1.599966
Mg16	-0.136999	-1.829506	1.831506
Mg17	-4.199853	-1.623978	-1.372958
Mg18	4.543910	-1.233009	-0.607829
Mg19	1.274787	2.098020	-2.879090
Mg20	-0.134762	2.873715	-0.349953
Mg21	0.348593	-4.464614	0.724171
Mg22	-1.957870	0.273976	2.808593
Mg23	2.356696	2.792583	1.428562
Mg24	1.339443	0.406272	3.193168

@mg24-isomer13 bp86/6-31G(d) Etot=-4802.280521 Eb=-15.89

Mg1	-1.151074	-0.349037	-0.159291
Mg2	1.579143	-0.288487	-2.125608
Mg3	-0.044133	1.228800	3.607138
Mg4	-3.245077	3.004564	-1.095411
Mg5	1.017845	1.517975	0.726129
Mg6	3.572842	-2.563946	-1.309440
Mg7	1.567759	-1.605390	0.815591
Mg8	4.486544	0.347296	-1.874549
Mg9	4.089556	2.002601	0.561772
Mg10	-2.444426	-0.406924	2.643530

Mg11	-3.619686	0.018905	-1.983904
Mg12	-1.828630	2.388236	1.498733
Mg13	-1.033858	-1.168562	-3.307077
Mg14	-0.782792	1.671527	-2.420355
Mg15	-4.266221	-1.864496	0.475092
Mg16	2.329029	2.745372	-1.786806
Mg17	4.835047	-0.911431	0.884546
Mg18	-2.499127	-3.081442	-1.507459
Mg19	2.769601	0.207856	2.918852
Mg20	0.487197	-3.196240	-1.528033
Mg21	-4.544280	1.048633	0.761737
Mg22	-0.325413	3.993234	-0.586330
Mg23	0.203650	-1.679191	3.581780
Mg24	-1.153495	-3.059850	1.209363

@mg24-isomer14 bp86/6-31G(d) Etot=-4802.279897 Eb=-15.88

Mg1	-1.317840	0.023023	-3.112996
Mg2	-4.147430	0.473883	1.011782
Mg3	-1.908439	1.422848	3.112609
Mg4	0.815254	3.996221	-0.288403
Mg5	-1.105628	3.061202	-2.473806
Mg6	0.278790	-0.658595	3.364231
Mg7	-3.600270	-2.508132	0.494487
Mg8	-1.978659	2.908975	0.486414
Mg9	1.101563	1.242025	-1.545406
Mg10	5.318876	-0.018269	0.666393
Mg11	3.534969	2.395257	0.238784
Mg12	-1.317993	-2.714500	-1.696384
Mg13	-3.934635	-1.050083	-2.013029
Mg14	4.080963	0.348472	-2.048324
Mg15	-3.735499	1.812192	-1.718759
Mg16	4.084610	-2.419444	-0.784911
Mg17	-0.638169	-2.865981	1.332968
Mg18	3.281588	0.400436	2.895651
Mg19	-1.233249	-0.079525	0.091893
Mg20	1.331396	-3.785173	-0.744453
Mg21	0.725026	1.845474	1.722332
Mg22	1.382598	-1.486925	-2.682988
Mg23	1.688478	-0.977538	0.579354
Mg24	-2.706298	-1.365843	3.112559

@mg24-isomer15 bp86/6-31G(d) Etot=-4802.279562 Eb=-15.87

Mg1	4.203287	-0.455085	1.756246
Mg2	-3.117574	2.652339	0.994030
Mg3	-4.241399	-2.064308	-0.207570
Mg4	1.004367	2.148281	-2.161002
Mg5	-0.276359	-2.670049	1.079721
Mg6	2.589052	3.982363	-0.248475
Mg7	-1.633337	-2.847218	-1.694428
Mg8	2.665452	-0.228528	-2.914353
Mg9	-0.213677	3.104598	0.428796
Mg10	-3.393272	-0.552600	-2.741468
Mg11	4.107085	1.414603	-0.690850
Mg12	1.378507	-0.938279	3.058253
Mg13	-0.330076	-0.427727	-2.999301
Mg14	-1.531580	-1.471755	3.541948
Mg15	4.415539	-1.658585	-0.986948
Mg16	-1.601722	-0.184735	0.028408
Mg17	2.159378	1.988371	1.976369
Mg18	-0.736847	1.268078	2.731037
Mg19	1.362639	-0.121755	-0.007321
Mg20	-2.058629	2.049529	-1.951829
Mg21	-3.913887	-0.095144	2.181089
Mg22	1.367116	-2.772016	-1.670957

Mg23	2.698993	-3.008440	1.078678
Mg24	-4.903055	0.888062	-0.580073

@mg24-isomer16 bp86/6-31G(d) Etot=-4802.279188 Eb=-15.86

Mg1	2.490318	2.460427	-2.396894
Mg2	-0.530327	2.905377	-2.015532
Mg3	-4.936001	-0.303307	-1.272043
Mg4	-1.701174	-1.166630	1.093108
Mg5	0.908313	0.107892	-0.149513
Mg6	2.956480	-0.644931	-2.360538
Mg7	0.481269	0.587501	-3.652246
Mg8	2.478457	-2.791060	-0.098079
Mg9	-1.868272	0.115218	-1.801303
Mg10	-1.379615	1.981274	0.749837
Mg11	3.873725	1.197177	0.023632
Mg12	0.986418	-1.867285	2.451066
Mg13	-0.324476	-3.807319	0.410756
Mg14	-0.881604	0.431881	3.449137
Mg15	1.444171	3.141822	0.333832
Mg16	2.071736	1.006476	2.630958
Mg17	-4.187084	0.756353	1.491473
Mg18	0.226647	-2.119610	-2.132218
Mg19	-4.841900	-2.362982	0.956381
Mg20	0.065916	3.258573	3.116908
Mg21	4.040769	-1.190757	2.098051
Mg22	5.184318	-1.506354	-0.568815
Mg23	-2.725476	-2.767306	-1.278084
Mg24	-3.832610	2.577569	-1.079876

@mg24-isomer17 bp86/6-31G(d) Etot=-4802.278859 Eb=-15.85

Mg1	2.389359	-3.166207	1.116592
Mg2	-0.212484	-2.978908	-0.413967
Mg3	2.979148	-0.772585	2.939588
Mg4	4.792698	-1.423072	0.654599
Mg5	0.045134	-1.802161	2.322020
Mg6	-2.832850	-2.351179	1.119146
Mg7	2.462417	-1.965883	-1.769750
Mg8	-2.881063	-2.629723	-1.982819
Mg9	-0.510598	-0.965925	-2.761635
Mg10	-2.206571	0.050777	3.073621
Mg11	3.811180	1.607230	1.191414
Mg12	-5.222844	-1.487030	-0.557873
Mg13	0.659971	1.199328	2.744583
Mg14	-1.359722	0.224169	0.152801
Mg15	4.490807	0.491858	-1.583766
Mg16	1.488365	0.134736	-0.035802
Mg17	-4.346302	0.919294	0.977117
Mg18	-3.409027	0.409481	-2.116929
Mg19	1.928566	0.553147	-3.449676
Mg20	-1.847871	2.918822	2.423118
Mg21	-2.731907	3.008265	-0.583524
Mg22	2.590454	2.844338	-1.484751
Mg23	0.285208	3.112532	0.367603
Mg24	-0.362066	2.068697	-2.341710

@mg24-isomer18 bp86/6-31G(d) Etot=-4802.277616 Eb=-15.82

Mg1	3.490134	2.978742	1.646018
Mg2	-0.726059	2.970086	-0.765935
Mg3	-2.535293	1.596936	-2.909856
Mg4	-1.882381	-1.359078	-2.562909
Mg5	1.527848	-0.386012	-0.211153
Mg6	4.810923	-1.719957	-0.222623
Mg7	4.938529	1.288996	-0.350828
Mg8	2.396204	-3.340589	0.270143

Mg9	0.351299	0.754893	-2.772778
Mg10	-1.418806	0.020126	0.167256
Mg11	3.569862	-0.067442	2.103981
Mg12	-0.561260	-3.033786	-0.111930
Mg13	0.988801	-2.292568	-2.647285
Mg14	-3.639633	-2.448684	-0.061499
Mg15	0.807091	1.595272	2.022911
Mg16	0.666325	-1.595205	2.378856
Mg17	-3.895827	2.574537	-0.445640
Mg18	3.388718	-0.172381	-2.527819
Mg19	-2.144325	-2.557188	2.476383
Mg20	2.224893	2.596186	-1.072834
Mg21	-1.424854	0.121965	3.632085
Mg22	-4.154342	0.095932	1.588889
Mg23	-4.637126	-0.082248	-1.561869
Mg24	-2.140722	2.461465	1.938436

@mg24-isomer19 bp86/6-31G(d) Etot=-4802.276849 Eb=-15.80

Mg1	-4.668290	-0.902702	-1.538334
Mg2	0.697015	0.837155	3.572337
Mg3	2.377768	-3.269413	0.601325
Mg4	-0.522755	-2.818454	0.452041
Mg5	4.664741	0.922531	-0.308378
Mg6	3.389405	-1.485358	-1.642660
Mg7	0.352533	2.402048	-2.103477
Mg8	-3.524220	-2.706819	0.593884
Mg9	1.067472	-2.073322	3.085132
Mg10	-2.093024	3.570263	-0.948704
Mg11	1.227903	-0.121625	0.167752
Mg12	3.823651	-1.026313	1.880434
Mg13	-1.940433	-2.297749	-2.274243
Mg14	0.201547	2.631513	1.033207
Mg15	-4.679284	-0.111753	1.422196
Mg16	-1.629698	-0.659136	2.243182
Mg17	2.750959	3.286392	-0.628101
Mg18	0.511761	-0.536562	-2.885139
Mg19	-1.653660	0.375587	-0.759947
Mg20	2.989476	1.859042	2.015097
Mg21	-2.681520	2.151466	1.775931
Mg22	0.931295	-3.358955	-2.142620
Mg23	-4.692275	2.067853	-0.752546
Mg24	3.099632	1.264312	-2.858369

@mg24-isomer20 bp86/6-31G(d) Etot=-4802.276634 Eb=-15.79

Mg1	-2.320577	0.877694	-1.413724
Mg2	0.229029	0.241430	-3.082650
Mg3	0.427287	-2.618308	-2.148055
Mg4	2.559105	3.497104	0.059307
Mg5	-1.164773	-1.849025	2.671498
Mg6	1.941524	-1.868148	2.458209
Mg7	-2.219899	-1.501118	-3.313197
Mg8	0.397543	-0.117238	0.149001
Mg9	0.253034	-3.574960	0.674552
Mg10	-2.634322	3.539543	0.341838
Mg11	-2.102752	-2.003733	-0.273570
Mg12	2.746260	1.017237	1.769465
Mg13	-0.007412	2.765480	-1.249405
Mg14	4.661673	1.461427	-0.572015
Mg15	-4.462095	-1.197306	1.562748
Mg16	2.588494	2.092096	-2.670004
Mg17	0.152100	2.819155	1.754257
Mg18	-4.814373	-1.026828	-1.438019
Mg19	2.820965	-0.736368	-1.694936
Mg20	-4.888927	1.517282	0.349138

Mg21	0.338465	0.490543	3.655086
Mg22	3.050097	-3.444276	-0.224867
Mg23	-2.192405	0.842183	1.833823
Mg24	4.641960	-1.223868	0.801521

@mg24-isomer21 bp86/6-31G(d) Etot=-4802.276193 Eb=-15.78

Mg1	2.264656	-1.164780	-2.798007
Mg2	-0.467211	0.418446	3.536956
Mg3	-1.368456	2.910508	2.324300
Mg4	1.581106	2.078156	2.131763
Mg5	-3.180803	-0.966338	-2.380099
Mg6	-1.963919	1.820397	-2.447705
Mg7	-0.476823	-2.128458	-1.345708
Mg8	4.628791	0.272467	-1.543573
Mg9	1.176242	1.753092	-2.861471
Mg10	1.475728	-0.026600	-0.153020
Mg11	2.186957	-0.885347	2.732507
Mg12	3.105396	2.684273	-0.561313
Mg13	1.605272	-3.241549	0.566224
Mg14	4.458212	0.861383	1.443800
Mg15	-1.296350	-4.405237	0.416052
Mg16	-1.395531	0.379469	0.183673
Mg17	-3.526509	-2.293901	0.419398
Mg18	-0.529103	-0.456215	-3.801357
Mg19	-4.918499	0.271114	-0.350027
Mg20	-0.797948	-1.998751	2.002275
Mg21	-3.421061	2.761762	0.055762
Mg22	-3.412759	0.256130	2.337776
Mg23	-0.038205	3.103281	-0.425521
Mg24	4.310818	-2.003299	0.517314

@mg24-isomer22 bp86/6-31G(d) Etot=-4802.274714 Eb=-15.74

Mg1	1.038316	-0.190974	0.091472
Mg2	2.513900	-3.067382	0.658166
Mg3	0.772704	2.925995	-1.545734
Mg4	-1.702544	-0.891799	1.171121
Mg5	-1.471606	-1.988137	-2.108122
Mg6	-0.007090	2.470756	1.359851
Mg7	3.937221	-0.586158	1.600972
Mg8	-0.441810	-3.492990	0.406629
Mg9	1.956426	0.973629	3.206488
Mg10	-3.588783	-3.069207	0.046301
Mg11	0.880648	-0.131228	-3.017057
Mg12	-1.562335	0.903768	-1.382200
Mg13	-1.990376	3.802178	-0.768268
Mg14	3.544188	-1.134416	-1.559859
Mg15	-0.866033	0.565177	3.695932
Mg16	5.364118	1.004302	-0.485109
Mg17	0.776778	-1.899591	2.949450
Mg18	-4.845479	-0.394537	1.002092
Mg19	-2.879212	1.826385	1.601940
Mg20	2.901103	2.301996	0.614571
Mg21	3.320114	1.741825	-2.509649
Mg22	-4.297939	-0.728994	-1.932152
Mg23	-4.578573	2.124719	-0.970662
Mg24	1.226261	-3.065317	-2.126173

@mg24-isomer23 bp86/6-31G(d) Etot=-4802.273869 Eb=-15.72

Mg1	5.174929	-0.549688	0.481607
Mg2	-2.259947	-2.178604	1.677387
Mg3	1.444247	2.302400	0.149311
Mg4	-3.840017	1.046749	-0.158695
Mg5	-2.474794	0.746703	2.686807
Mg6	0.263609	1.395704	-2.628431

Mg7	-2.575579	2.800858	-2.222436
Mg8	4.318252	2.185760	1.531177
Mg9	-1.539042	2.965053	0.725501
Mg10	-4.308546	-1.928701	-0.831153
Mg11	2.083508	-0.596100	-1.049150
Mg12	1.478915	-3.625637	-1.697440
Mg13	0.728277	-2.552393	1.028525
Mg14	2.360990	-0.149890	2.067857
Mg15	-0.131338	-0.946426	3.537438
Mg16	4.115354	-3.261548	-0.031081
Mg17	4.229655	1.654052	-1.438882
Mg18	-5.002236	-0.875267	1.923451
Mg19	-0.736430	0.031130	0.088835
Mg20	-1.422470	-2.889250	-1.204217
Mg21	-2.440196	-0.248996	-2.570568
Mg22	0.371750	1.943718	2.952331
Mg23	-0.053938	4.237397	-1.641619
Mg24	0.215046	-1.507024	-3.376555

@mg24-isomer24 bp86/6-31G(d) Etot=-4802.271594 Eb=-15.66

Mg1	-4.359116	-0.519055	-1.486862
Mg2	4.392845	1.410466	-1.076204
Mg3	5.317779	-1.187888	0.233051
Mg4	-0.563418	2.824267	1.047054
Mg5	0.437700	-2.711346	-0.361565
Mg6	-2.020222	3.985581	-1.416459
Mg7	2.890023	-1.992345	1.834675
Mg8	-1.917645	0.826458	2.795972
Mg9	0.624491	2.588760	-1.722626
Mg10	4.203994	0.876597	2.049758
Mg11	-3.627420	2.037737	0.161013
Mg12	-1.854096	-1.902563	-2.504131
Mg13	1.227671	1.065874	2.944164
Mg14	0.807141	-3.105799	-3.279408
Mg15	-4.504121	-0.543487	1.491854
Mg16	1.615555	0.219038	0.024045
Mg17	-2.140705	1.337630	-2.788293
Mg18	0.554420	-0.157437	-2.921939
Mg19	-1.327254	-0.010900	-0.108267
Mg20	2.549079	3.079967	0.645799
Mg21	3.180536	-1.585007	-1.852134
Mg22	-0.084844	-1.693777	2.402474
Mg23	-2.536471	-2.751998	0.498947
Mg24	-2.865920	-2.090772	3.389081

@mg24-isomer25 bp86/6-31G(d) Etot=-4802.270582 Eb=-15.63

Mg1	4.787154	0.661186	1.573391
Mg2	-2.903459	2.690147	1.383502
Mg3	1.181425	1.842674	-1.469915
Mg4	-1.828893	2.612068	-1.417033
Mg5	-0.170785	-0.742025	-2.786870
Mg6	-4.796263	-2.146278	0.743029
Mg7	-2.970810	0.431338	-3.261946
Mg8	-3.259102	-0.131481	2.413574
Mg9	-0.515779	-0.972000	3.266587
Mg10	0.116665	3.294533	0.942920
Mg11	-2.736470	-2.034907	-1.583198
Mg12	-0.432488	1.996777	-4.039581
Mg13	3.068121	-3.793208	-0.629028
Mg14	0.060658	-3.276551	-1.093885
Mg15	1.616119	0.693892	1.842192
Mg16	-4.076313	0.546138	-0.503252
Mg17	5.232062	-1.734893	-0.299038
Mg18	3.226377	3.161354	0.636004

Mg19	1.302619	-2.492374	1.547133
Mg20	4.477140	1.197821	-1.324645
Mg21	-0.840973	1.948784	3.449669
Mg22	2.153608	-0.860477	-0.838502
Mg23	-0.851588	-0.037892	0.157503
Mg24	-1.839025	-2.854625	1.291391

@mg24-isomer26 bp86/6-31G(d) Etot=-4802.270201 Eb=-15.62

Mg1	0.188523	0.124704	-3.712213
Mg2	4.502609	-0.825509	-1.685105
Mg3	-0.038502	2.901422	-2.672649
Mg4	-2.456402	1.000006	-2.385264
Mg5	-1.532029	-1.910331	-2.222387
Mg6	-1.721951	2.919974	-0.083081
Mg7	1.563876	-1.995323	-1.980592
Mg8	-4.441801	1.715846	-0.133739
Mg9	1.308985	3.414090	0.011962
Mg10	2.007798	0.875493	-1.344285
Mg11	-4.509973	-0.997863	-1.516078
Mg12	-0.518560	0.004615	0.033449
Mg13	3.563905	-3.206187	0.038353
Mg14	4.700365	-0.581838	1.327579
Mg15	4.500679	2.133941	-0.156792
Mg16	-2.895449	-2.717454	0.325305
Mg17	-0.242390	2.849101	2.562325
Mg18	0.099960	-3.588643	0.103006
Mg19	-4.986301	-0.875146	1.473605
Mg20	2.464131	1.413626	2.001650
Mg21	-2.490472	0.639582	2.205969
Mg22	1.722768	-1.404641	1.525472
Mg23	-1.047984	-2.122079	2.538370
Mg24	0.258218	0.232613	3.745140

@mg24-isomer27 bp86/6-31G(d) Etot=-4802.269682 Eb=-15.61

Mg1	-4.695734	-0.666418	-0.361716
Mg2	1.116000	0.705299	2.734595
Mg3	-2.748909	0.523495	-2.550134
Mg4	3.529030	-1.156855	2.093386
Mg5	-1.518821	3.056233	-1.133841
Mg6	-1.531283	2.354811	2.130454
Mg7	-2.631510	-2.156773	1.460569
Mg8	1.034480	3.946332	-2.425415
Mg9	-3.949179	0.412043	2.440684
Mg10	3.356856	2.062319	-1.528673
Mg11	-0.937833	-3.606293	-0.525709
Mg12	1.847233	-0.493372	-0.504846
Mg13	4.465698	-2.663424	-0.551457
Mg14	-3.228294	-2.485869	-2.120476
Mg15	-0.361063	-1.750834	-2.816111
Mg16	0.991165	2.596419	0.428642
Mg17	-1.089106	0.032315	0.048873
Mg18	-1.362509	-0.423419	3.703620
Mg19	0.526592	-2.169517	1.821088
Mg20	0.336886	1.098453	-2.620741
Mg21	-4.017993	2.179327	0.074946
Mg22	1.809143	-3.523920	-1.405559
Mg23	5.263105	0.184091	-0.072274
Mg24	3.796047	1.945558	1.680093

@mg24-isomer28 bp86/6-31G(d) Etot=-4802.269638 Eb=-15.61

Mg1	1.625028	1.588948	1.095752
Mg2	-2.292528	-1.680630	2.145346
Mg3	-2.442190	-2.417521	-2.711731
Mg4	3.055739	-0.954328	1.952817

Mg5	0.530086	-2.552524	1.236321
Mg6	-0.250406	-0.316927	-3.004461
Mg7	1.728590	1.915561	-1.975415
Mg8	-2.660031	0.715223	4.004205
Mg9	-1.198678	2.419051	1.962189
Mg10	0.210115	3.912753	-0.358495
Mg11	5.435700	-1.750554	-0.134514
Mg12	-3.777596	0.873855	1.077561
Mg13	-0.838045	-0.021028	-0.056643
Mg14	3.230523	-3.729601	-0.014419
Mg15	4.579801	1.173101	0.092998
Mg16	-1.050532	2.647533	-2.920823
Mg17	2.172036	-0.805701	-0.882830
Mg18	-2.709510	3.191020	-0.526845
Mg19	0.410976	-3.107467	-1.706280
Mg20	3.364972	3.970507	-0.070139
Mg21	-3.123234	0.541449	-1.999792
Mg22	-2.001135	-3.724607	-0.051746
Mg23	0.184898	-0.131559	3.188295
Mg24	-4.184579	-1.756554	-0.341352

@mg24-isomer29 bp86/6-31G(d) Etot=-4802.269554 Eb=-15.60

Mg1	4.091042	-2.677498	-1.124856
Mg2	5.389115	-0.035712	-0.483956
Mg3	2.884309	-0.035621	-2.279505
Mg4	-0.293311	-0.057837	-2.747444
Mg5	3.952675	2.636912	-0.941430
Mg6	0.966139	-2.311273	-1.091276
Mg7	1.052770	2.697605	-2.004460
Mg8	3.619908	-1.464587	1.603502
Mg9	-1.862703	-2.677884	-2.336045
Mg10	4.468149	1.608950	1.828203
Mg11	-1.909203	2.515217	-2.509184
Mg12	1.508072	0.771616	0.372641
Mg13	-3.646464	-0.103506	-2.029690
Mg14	-1.229329	-3.860447	0.343113
Mg15	-1.387253	-0.424807	0.001275
Mg16	0.534148	-1.939873	2.000052
Mg17	-0.942057	2.929099	0.348427
Mg18	1.980214	0.620677	3.304794
Mg19	-3.976308	-2.611620	-0.222184
Mg20	-4.130868	2.608201	-0.556939
Mg21	-1.057425	0.859438	2.666330
Mg22	-4.250394	0.145413	1.174433
Mg23	-2.484644	-2.043762	2.400324
Mg24	-3.276584	2.851300	2.283877

@mg24-isomer30 bp86/6-31G(d) Etot=-4802.269243 Eb=-15.60

Mg1	-1.152085	2.842016	1.830910
Mg2	2.184263	-1.996419	1.574151
Mg3	4.312165	-0.253683	-2.203504
Mg4	-3.855782	0.696724	-1.802472
Mg5	-2.683013	3.233527	-0.866120
Mg6	-0.724248	1.512557	-2.612299
Mg7	5.020632	-1.262372	0.580674
Mg8	-2.455540	0.183802	3.047711
Mg9	3.327794	-2.930236	-1.284655
Mg10	-2.489423	-3.487340	-0.154763
Mg11	-4.140949	1.811585	1.212980
Mg12	-0.888975	-2.335004	2.097671
Mg13	3.712540	0.485890	2.582303
Mg14	0.533682	0.231914	2.940022
Mg15	-1.309220	0.256272	0.176602
Mg16	-1.404773	-1.562339	-2.300420

Mg17	0.149892	3.784180	-0.963089
Mg18	1.381022	-0.456751	-1.133105
Mg19	-4.150929	-1.274892	1.054018
Mg20	2.403257	2.210359	-2.204113
Mg21	4.608159	1.784029	-0.034689
Mg22	1.710600	2.077720	0.892496
Mg23	0.391848	-3.387665	-0.549727
Mg24	-4.480915	-2.163872	-1.880583

@mg24-isomer31 bp86/6-31G(d) Etot=-4802.268708 Eb=-15.58

Mg1	-0.272493	2.592396	1.421000
Mg2	2.158053	3.370065	-0.516729
Mg3	1.690668	-1.777926	2.544892
Mg4	-0.108267	1.911906	-2.219589
Mg5	-2.219769	-2.231204	-1.800594
Mg6	-0.759244	4.432237	-0.858791
Mg7	-3.241817	-1.641275	0.975644
Mg8	2.488768	0.577975	-1.848758
Mg9	4.573689	-1.001075	1.504337
Mg10	-5.153563	0.716751	1.237254
Mg11	2.287014	0.995363	1.443725
Mg12	0.303638	0.659196	3.707037
Mg13	0.255499	-0.972964	-3.153205
Mg14	-2.497005	0.849986	2.612776
Mg15	4.862257	1.772198	-0.099529
Mg16	5.067001	-0.984732	-1.366288
Mg17	0.381405	-3.770526	-2.213761
Mg18	2.336291	-2.188904	-0.416895
Mg19	-4.791097	-0.398540	-1.435460
Mg20	-2.553209	0.430891	-3.142918
Mg21	-0.461744	-3.195914	0.638904
Mg22	-0.367703	-0.217801	0.133350
Mg23	-1.231518	-1.832066	3.285415
Mg24	-2.746856	1.903962	-0.431817

@mg24-isomer32 bp86/6-31G(d) Etot=-4802.267399 Eb=-15.55

Mg1	0.624058	0.244069	-0.009962
Mg2	-1.778213	2.168068	-0.039734
Mg3	-2.577978	0.838159	2.559290
Mg4	0.727685	3.953273	-0.075208
Mg5	0.400819	0.002654	3.202336
Mg6	3.067582	-0.858836	1.774452
Mg7	2.517221	2.034919	1.595452
Mg8	-2.564146	0.735214	-2.586364
Mg9	0.413893	-0.123328	-3.206061
Mg10	4.933899	1.155081	-0.018279
Mg11	-1.969021	-1.285746	0.025454
Mg12	-4.639656	1.225116	-0.029940
Mg13	-0.261560	2.739972	-2.693289
Mg14	3.073970	-0.926165	-1.735076
Mg15	5.588128	-1.623097	0.038373
Mg16	-4.735141	-1.219177	1.607323
Mg17	0.429172	-2.572347	1.566246
Mg18	-0.265838	2.843999	2.587880
Mg19	2.944897	-3.318731	0.067721
Mg20	-2.083167	-1.975580	3.089174
Mg21	2.522987	1.974548	-1.669425
Mg22	-4.728725	-1.285790	-1.567706
Mg23	0.433660	-2.631486	-1.467924
Mg24	-2.074524	-2.094789	-3.014732

@mg24-isomer33 bp86/6-31G(d) Etot=-4802.266801 Eb=-15.53

Mg1	1.007442	-0.039742	-0.121503
Mg2	3.558148	-0.079086	1.814552

Mg3	4.153637	2.208290	-0.174018
Mg4	0.732805	0.659621	2.819646
Mg5	1.321809	3.186287	0.416956
Mg6	3.864734	-0.540520	-1.411765
Mg7	-1.406010	1.860050	0.658200
Mg8	-1.418048	-1.370330	1.653699
Mg9	-0.385579	-3.367439	-0.422375
Mg10	2.446700	-3.455203	-1.113712
Mg11	2.039321	1.683229	-2.410920
Mg12	3.090549	2.706173	2.760712
Mg13	-1.811616	-0.761576	-1.411663
Mg14	-2.538210	0.840340	3.281671
Mg15	-3.496630	-3.074729	-0.089020
Mg16	-4.955176	-0.577908	-1.022185
Mg17	1.584675	-2.409716	1.728622
Mg18	-0.510811	3.266450	-1.944775
Mg19	-3.295753	1.820841	-1.885049
Mg20	-4.448938	1.705540	0.912809
Mg21	0.947672	-1.428711	-2.835957
Mg22	-4.526622	-1.125150	1.963964
Mg23	-0.653154	0.921218	-3.815201
Mg24	4.699055	-2.627928	0.647310

@mg24-isomer34 bp86/6-31G(d) Etot=-4802.266094 Eb=-15.51

Mg1	-1.072604	0.076453	-0.070104
Mg2	1.306766	-0.944306	-1.742888
Mg3	0.616589	3.012154	1.654421
Mg4	-3.400890	-0.036773	-2.672767
Mg5	0.732340	2.122125	-1.518140
Mg6	3.429546	-2.152893	0.114705
Mg7	2.025443	0.472361	0.876220
Mg8	6.366785	-1.416466	0.090179
Mg9	4.380607	0.567862	-1.360970
Mg10	-2.293888	1.822551	2.528748
Mg11	-3.904192	-1.774436	-0.089768
Mg12	-1.711836	3.242477	-0.120990
Mg13	-1.778627	-3.677854	0.608343
Mg14	-1.441081	-2.284499	-2.090383
Mg15	-4.800403	-0.189266	2.511069
Mg16	-0.591040	0.190571	-3.733970
Mg17	5.083715	0.832257	1.530288
Mg18	-2.141686	-1.404888	2.589870
Mg19	3.433599	3.147429	0.054916
Mg20	0.605670	-2.105374	1.520717
Mg21	-3.942038	1.298989	-0.078110
Mg22	0.209551	0.422626	3.287330
Mg23	0.915739	-3.840275	-0.897493
Mg24	-2.028062	2.619173	-2.991223

@mg24-isomer35 bp86/6-31G(d) Etot=-4802.265600 Eb=-15.50

Mg1	4.459254	-2.228933	-0.245056
Mg2	5.326997	0.319893	1.229494
Mg3	1.864058	-3.865397	-0.243764
Mg4	1.785686	-0.813939	-1.078342
Mg5	-0.089941	-2.960523	-2.363488
Mg6	4.572467	0.513183	-1.634840
Mg7	2.396318	-0.227566	2.040262
Mg8	-0.501456	0.009731	-3.049135
Mg9	1.766786	1.943900	-2.374263
Mg10	0.135537	-2.024144	1.393701
Mg11	-2.289979	-1.298844	-1.051326
Mg12	-1.597508	-3.991515	0.081033
Mg13	-1.071042	2.929386	-2.746165
Mg14	3.001297	2.289446	0.417046

Mg15	-4.619848	-2.644146	0.333243
Mg16	-0.477700	0.708823	0.213539
Mg17	0.203124	3.572635	-0.007466
Mg18	-3.501178	1.060924	-2.412111
Mg19	-0.231502	-0.084849	3.770446
Mg20	0.851255	2.398969	2.701837
Mg21	-2.787730	3.008413	-0.187522
Mg22	-4.396981	0.607059	0.511647
Mg23	-2.583810	-1.120244	2.138497
Mg24	-2.214103	1.897738	2.562734

@mg24-isomer36 bp86/6-31G(d) Etot=-4802.263943 Eb=-15.46

Mg1	-1.248339	-0.324978	0.099013
Mg2	-3.884169	-1.753701	1.280456
Mg3	-5.533222	0.262283	-0.164564
Mg4	-1.829621	-0.233675	3.072559
Mg5	1.088667	-0.898760	2.108205
Mg6	0.679378	-3.093998	-0.190109
Mg7	3.714042	-2.027473	0.251694
Mg8	1.617596	0.199974	-0.950386
Mg9	-3.432915	1.673517	1.435001
Mg10	-3.419128	-0.781487	-2.049113
Mg11	-0.361543	2.193113	1.997176
Mg12	-1.000917	1.574265	-2.237677
Mg13	3.784900	2.597918	-1.388848
Mg14	2.668637	1.982975	1.674384
Mg15	5.172443	0.837646	0.536704
Mg16	2.469801	-2.512795	-2.520039
Mg17	0.960738	3.311417	-0.521665
Mg18	-2.299970	-3.364319	-0.772258
Mg19	-1.233787	-3.066713	2.082932
Mg20	4.013379	-0.530016	2.879541
Mg21	-0.483250	-1.758667	-2.592057
Mg22	-1.900921	3.725364	-0.154119
Mg23	-3.979977	2.243216	-1.696578
Mg24	4.438175	-0.255107	-2.180252

@mg24-isomer37 bp86/6-31G(d) Etot=-4802.262957 Eb=-15.43

Mg1	-1.585365	1.835461	2.550949
Mg2	-0.973330	0.415881	0.005970
Mg3	-1.915689	-1.738836	2.030286
Mg4	1.368153	2.102517	1.509049
Mg5	0.784557	-2.536077	-2.669555
Mg6	-4.498218	-2.319262	0.325298
Mg7	-2.159915	2.676606	-2.271988
Mg8	-0.799311	3.801746	0.296718
Mg9	0.999717	-0.775691	2.330625
Mg10	-4.214658	0.336204	1.731433
Mg11	-0.786785	0.002836	-2.979831
Mg12	-2.353623	-4.436035	0.701551
Mg13	-3.684213	2.861244	0.240311
Mg14	-1.970358	-2.311670	-1.505734
Mg15	2.192393	4.638865	-0.165273
Mg16	1.987191	-0.357339	-0.723101
Mg17	3.871467	2.105979	-0.378308
Mg18	3.810774	0.370217	2.142141
Mg19	5.224590	-0.784354	-0.228574
Mg20	0.947834	2.290903	-1.820562
Mg21	3.479159	-2.555780	1.460384
Mg22	3.606202	-2.916032	-1.566567
Mg23	0.480360	-2.978767	0.390316
Mg24	-3.810932	0.271385	-1.405540

@mg24-isomer38 bp86/6-31G(d) Etot=-4802.261883 Eb=-15.40

Mg1	4.486521	-0.987436	-1.451405
Mg2	5.237784	-0.920760	1.367343
Mg3	-1.191105	2.701580	-0.248591
Mg4	3.712087	1.599569	0.007579
Mg5	1.263882	2.767248	1.732913
Mg6	-0.590514	-0.517256	-3.074549
Mg7	2.245667	0.739282	-2.770649
Mg8	-4.073737	1.979643	0.694254
Mg9	1.578345	3.297620	-1.246474
Mg10	2.271348	-1.851445	1.435700
Mg11	-2.253234	-0.398030	-0.500896
Mg12	-3.856263	-3.288292	-0.087866
Mg13	-0.871569	-2.283682	1.421571
Mg14	-2.872758	-0.168441	2.546503
Mg15	0.186443	0.094381	3.028342
Mg16	-5.276935	-0.798827	0.644018
Mg17	-3.295589	1.753216	-2.346817
Mg18	3.139426	0.693707	2.902551
Mg19	0.698940	0.272925	-0.134471
Mg20	0.914831	-4.317928	0.150272
Mg21	1.680987	-2.173552	-1.779547
Mg22	-1.597838	2.552204	2.675659
Mg23	-0.340892	2.397571	-3.349730
Mg24	-1.195826	-3.143296	-1.615709

@mg24-isomer39 bp86/6-31G(d) Etot=-4802.260229 Eb=-15.36

Mg1	-0.779088	-0.183514	0.035196
Mg2	1.729585	-0.476934	1.813320
Mg3	-0.007817	0.985308	-2.910076
Mg4	-1.625985	2.324406	1.988015
Mg5	0.825944	2.408898	-0.042838
Mg6	4.422816	-1.499110	0.469465
Mg7	2.130036	-0.522052	-1.484271
Mg8	6.776015	0.420053	0.535098
Mg9	3.692671	1.541227	0.635524
Mg10	-2.744412	-0.265622	-2.477256
Mg11	-3.066936	-0.459566	2.062310
Mg12	-2.084428	2.460399	-1.065184
Mg13	-0.712342	-2.579420	2.224972
Mg14	-0.566751	0.024917	3.913389
Mg15	-5.256168	-0.611048	-0.278764
Mg16	1.209780	2.260573	2.971537
Mg17	5.157806	0.312783	-1.948594
Mg18	-2.850787	-2.405344	-0.355212
Mg19	2.735106	2.231253	-2.406644
Mg20	-0.831261	-4.567654	-0.291502
Mg21	-4.446026	2.015449	0.954492
Mg22	-0.315403	-2.229153	-2.386386
Mg23	1.532108	-2.950111	0.082307
Mg24	-4.924465	1.764263	-2.038897

@mg24-isomer40 bp86/6-31G(d) Etot=-4802.259879 Eb=-15.35

Mg1	-0.667130	3.921104	-0.843188
Mg2	-3.183413	2.141653	-0.540801
Mg3	1.229834	3.531951	1.438972
Mg4	-2.713522	-0.702931	-1.674347
Mg5	1.825496	2.263646	-1.377354
Mg6	1.753134	0.666136	-3.980851
Mg7	-2.710948	0.385670	2.099265
Mg8	2.241990	-1.083089	3.484720
Mg9	-3.183220	-2.410326	0.992628
Mg10	-0.893135	1.547177	-2.759424
Mg11	-5.066276	-0.118832	0.143506
Mg12	1.837062	-0.914374	-1.404121

Mg13	-0.562333	-2.679763	-0.677776
Mg14	2.118091	-2.729490	0.956188
Mg15	-0.408669	0.626492	0.085338
Mg16	-1.762360	3.275379	1.894249
Mg17	2.532302	0.790072	1.168903
Mg18	0.127135	1.171508	3.088237
Mg19	-6.139836	-3.132827	-0.360679
Mg20	4.693660	0.422264	-1.200130
Mg21	4.958504	-1.153109	1.642090
Mg22	4.789432	-2.615575	-0.937840
Mg23	-0.347170	-1.454949	-3.472624
Mg24	-0.468627	-1.747788	2.235037

@mg24-isomer41 bp86/6-31G(d) Etot=-4802.258771 Eb=-15.32

Mg1	1.558908	-0.542194	-3.653594
Mg2	1.107586	0.612402	2.953361
Mg3	-3.119860	3.019431	-2.266303
Mg4	-2.206077	-0.005215	-0.497423
Mg5	-0.450628	-2.915407	0.330952
Mg6	-2.770000	-4.065096	-1.547838
Mg7	-4.069129	0.122600	1.854350
Mg8	3.171023	1.736130	0.806580
Mg9	3.031312	-3.375615	0.670434
Mg10	3.626332	-0.787144	-1.050436
Mg11	2.298203	1.934853	-2.148806
Mg12	-4.380143	2.778938	0.393382
Mg13	-1.594968	1.916288	2.102557
Mg14	2.550525	4.370357	-0.391046
Mg15	-3.659128	-2.838182	1.029801
Mg16	3.644919	-0.938456	2.146522
Mg17	1.641802	-2.934211	-1.888962
Mg18	0.801485	-0.186238	-0.191567
Mg19	-1.436359	-1.097796	2.562346
Mg20	1.058771	3.557907	2.112023
Mg21	1.200774	-2.480142	2.884807
Mg22	-0.700818	1.177997	-2.983561
Mg23	-1.044398	-1.814809	-2.734152
Mg24	-0.260131	2.753603	-0.493428

@mg24-isomer42 bp86/6-31G(d) Etot=-4802.253673 Eb=-15.19

Mg1	0.792989	1.697718	2.133291
Mg2	2.641639	-3.350974	1.334706
Mg3	-0.844224	2.804060	-2.649634
Mg4	-3.038458	1.142454	-1.316406
Mg5	-3.897009	0.177385	1.593431
Mg6	4.389637	-0.286940	-1.676270
Mg7	-0.908261	-3.041104	-2.255769
Mg8	3.274375	2.995127	0.875284
Mg9	1.679368	-1.698840	-1.238753
Mg10	-3.125196	-1.228444	-3.260080
Mg11	5.781163	1.906546	-0.269855
Mg12	-1.684789	0.550500	3.718715
Mg13	-0.778740	-0.229192	0.256549
Mg14	3.015465	-0.246233	1.160293
Mg15	-0.381405	-0.134686	-2.986451
Mg16	-2.472052	-2.124103	2.754101
Mg17	0.611896	-1.337945	2.903193
Mg18	-2.566156	4.452633	-0.933612
Mg19	0.283781	4.091509	0.190311
Mg20	-0.472437	-3.253887	0.737022
Mg21	-3.222193	-2.044874	-0.344955
Mg22	1.483402	-4.808992	-0.994948
Mg23	-1.999967	2.532630	1.342753
Mg24	1.437174	1.435649	-1.072915

@mg24-isomer43 bp86/6-31G(d) Etot=-4802.251951 Eb=-15.14

Mg1	-3.795918	-1.393353	-1.899469
Mg2	-0.017326	0.350056	2.522554
Mg3	1.259861	-0.013476	-0.348305
Mg4	1.247014	-3.046629	-1.084661
Mg5	4.062816	-3.621244	-0.069493
Mg6	-1.774959	0.412865	0.135629
Mg7	0.295053	2.892428	0.803438
Mg8	-4.980848	0.057823	0.490382
Mg9	-0.516065	2.123701	-2.166455
Mg10	-3.700203	1.624859	-1.910933
Mg11	3.838070	-1.011616	-1.695368
Mg12	2.876767	1.217175	1.966614
Mg13	-3.446364	2.381617	1.846391
Mg14	2.505469	1.977909	-2.171756
Mg15	-3.117409	-0.595515	2.657483
Mg16	-0.841034	-2.352428	1.254562
Mg17	4.825895	1.559188	-0.360955
Mg18	4.918437	-0.991209	1.236737
Mg19	-0.789537	-1.028367	-2.361451
Mg20	3.083701	4.030077	0.208243
Mg21	2.168009	-2.006908	1.854175
Mg22	-2.324614	3.925730	-0.421826
Mg23	-3.907253	-2.831343	0.783976
Mg24	-1.869561	-3.661337	-1.269515

@mg24-isomer44 bp86/6-31G(d) Etot=-4802.249024 Eb=-15.07

Mg1	1.014017	-1.010027	-2.702728
Mg2	-2.164849	-0.372150	-1.738998
Mg3	0.948105	0.005881	0.121162
Mg4	-0.757519	0.682126	3.244374
Mg5	-3.906900	-2.987419	-0.577553
Mg6	1.098594	2.733995	1.734372
Mg7	2.057633	-3.059481	-0.468946
Mg8	3.938711	-0.756861	-1.645423
Mg9	2.522370	1.756784	-2.286637
Mg10	5.059685	-3.328597	-0.747470
Mg11	-1.566455	1.993169	0.271208
Mg12	-3.768216	1.340617	2.318843
Mg13	2.156648	0.198360	3.189456
Mg14	-5.173832	-0.769096	-2.137288
Mg15	-0.407206	1.716706	-3.060658
Mg16	0.526875	3.731653	-1.093178
Mg17	3.713750	-1.776847	1.630724
Mg18	-0.810881	-2.840249	-0.550233
Mg19	-4.453659	1.830339	-0.663607
Mg20	-5.430097	-0.749123	0.903540
Mg21	3.783565	1.124446	0.723069
Mg22	0.594542	-2.227659	2.247308
Mg23	-2.288536	-1.166285	1.461079
Mg24	3.313655	3.929719	-0.172415

@mg24-isomer45 bp86/6-31G(d) Etot=-4802.248624 Eb=-15.06

Mg1	-1.603984	-3.098654	1.626207
Mg2	-1.155405	1.562414	3.682410
Mg3	-2.771338	3.177232	-1.104192
Mg4	1.192365	-2.009388	1.259123
Mg5	-4.172222	-1.443639	0.640905
Mg6	4.614459	1.460767	1.876864
Mg7	1.541472	-1.982634	-2.350120
Mg8	-3.631838	1.938584	1.541014
Mg9	0.152939	2.875048	-2.231639
Mg10	0.512926	-4.345233	-0.578842

Mg11	1.542820	0.907984	2.282194
Mg12	2.444310	2.791633	-0.105516
Mg13	5.231349	1.772210	-1.120774
Mg14	-0.219463	-1.236168	3.833801
Mg15	3.507359	-3.718582	-0.344878
Mg16	-4.844027	1.040801	-1.011360
Mg17	-0.464560	2.840383	0.883791
Mg18	-1.388863	-2.170278	-1.325111
Mg19	-1.860724	0.584871	-2.469286
Mg20	2.629962	1.043822	-2.783864
Mg21	-4.147105	-1.510497	-2.403952
Mg22	3.722359	-0.678303	-0.175047
Mg23	-1.563704	-0.104622	1.034097
Mg24	0.730912	0.302247	-0.655824

@mg24-isomer46 bp86/6-31G(d) Etot=-4802.247209 Eb=-15.02

Mg1	-0.620467	0.899515	0.144285
Mg2	-3.810964	1.265887	-0.774059
Mg3	1.944895	-0.680773	-0.684284
Mg4	3.116860	-3.709699	-0.555619
Mg5	4.286416	1.174055	-1.748590
Mg6	0.360372	4.108468	-0.851714
Mg7	0.334684	-3.267351	-1.643978
Mg8	-0.073965	3.165123	2.097858
Mg9	-3.020692	1.698971	2.320964
Mg10	5.238315	-1.501221	-0.687694
Mg11	4.756276	0.766079	1.268228
Mg12	0.714914	-2.687157	1.394558
Mg13	-4.279339	-0.878927	1.329013
Mg14	-1.564422	2.426250	-2.480027
Mg15	2.433945	2.483199	0.435252
Mg16	1.319489	1.729824	-2.463487
Mg17	1.466849	0.268814	2.369823
Mg18	-1.976502	-2.411142	0.021417
Mg19	-4.113007	-1.426226	-1.941500
Mg20	-2.448447	3.809555	0.291362
Mg21	-1.508433	-0.976443	2.671031
Mg22	-5.085337	-3.717085	-0.038000
Mg23	-1.071349	-0.670829	-2.383085
Mg24	3.599908	-1.868885	1.908246

@mg24-isomer47 bp86/6-31G(d) Etot=-4802.246620 Eb=-15.01

Mg1	-0.890626	0.093593	-0.091374
Mg2	-0.133654	-3.177081	-1.511359
Mg3	-1.483839	-5.276436	0.327914
Mg4	-3.797007	0.332184	-1.040956
Mg5	-1.822386	-1.180545	-2.938943
Mg6	-1.868731	2.378465	1.760215
Mg7	-3.124763	-0.491294	1.953309
Mg8	-0.793545	-2.592945	1.677278
Mg9	0.326389	0.116932	2.812324
Mg10	1.198548	-0.739730	-2.657842
Mg11	1.635881	-1.479685	0.381403
Mg12	-2.992311	-2.554788	-0.376927
Mg13	1.754439	1.559271	-0.878177
Mg14	1.456709	-4.718775	0.720679
Mg15	-0.303015	3.885839	-0.528988
Mg16	-3.262387	3.352970	-0.768436
Mg17	1.184635	2.828531	1.880402
Mg18	2.702711	4.485972	-0.337289
Mg19	4.060534	-3.243316	0.189246
Mg20	4.942728	2.501589	-0.252961
Mg21	4.201825	-0.345801	-0.936263
Mg22	-1.321099	1.839047	-2.600773

Mg23	3.213316	0.584330	1.894100
Mg24	-4.884351	1.841671	1.323420

@mg24-isomer48 bp86/6-31G(d) Etot=-4802.243557 Eb=-14.92

Mg1	-2.693141	-1.613549	2.146255
Mg2	1.847080	-0.024001	1.909377
Mg3	3.076631	-2.879997	1.801086
Mg4	-1.968097	-3.386548	-0.371162
Mg5	4.570538	-0.511738	0.451990
Mg6	-2.551003	1.830883	1.791662
Mg7	0.114843	-2.614696	1.716078
Mg8	-5.155270	0.131280	2.102702
Mg9	-4.653549	-1.929046	-0.176993
Mg10	3.803950	2.366038	1.625208
Mg11	4.243209	-3.634063	-0.730089
Mg12	-0.819565	-0.170266	0.204903
Mg13	1.136995	-4.417095	-0.469215
Mg14	0.468887	2.550384	1.158765
Mg15	2.587610	4.734863	0.189590
Mg16	1.889113	-1.443372	-0.867343
Mg17	-4.402338	1.090787	-0.598269
Mg18	2.626180	1.538604	-0.900546
Mg19	-0.421853	5.224650	-0.021660
Mg20	-0.141761	-2.639614	-2.696694
Mg21	-2.625130	-0.786686	-2.231510
Mg22	-1.868067	2.517478	-1.153515
Mg23	0.191079	0.559518	-2.685222
Mg24	0.743659	3.506185	-2.195397

@mg24-isomer49 bp86/6-31G(d) Etot=-4802.229896 Eb=-14.57

Mg1	-2.823310	0.291591	0.359777
Mg2	0.148131	-0.008058	0.699101
Mg3	1.278871	2.272009	-1.037011
Mg4	-1.719490	-2.084212	2.230154
Mg5	2.991088	-0.075314	1.614332
Mg6	1.528249	-0.774425	-2.037376
Mg7	-5.830652	0.010902	-0.141625
Mg8	-3.911780	-0.968109	-2.268026
Mg9	-3.847600	2.178750	-1.704702
Mg10	1.150400	-3.795240	-1.622507
Mg11	-1.198057	3.669701	-2.440101
Mg12	1.039839	2.532510	2.202617
Mg13	6.065189	0.709378	1.091570
Mg14	1.145748	-2.729608	1.350129
Mg15	-4.426467	-0.732144	2.668749
Mg16	6.555069	-1.519725	-0.766727
Mg17	-1.672002	1.245138	2.958870
Mg18	-1.397642	3.035755	0.450712
Mg19	-1.132483	0.627727	-2.206096
Mg20	-1.392495	-2.329631	-0.886340
Mg21	3.670589	-2.365900	-0.448407
Mg22	4.175440	0.609968	-1.302690
Mg23	3.831606	2.834878	0.940457
Mg24	-4.228240	-2.635942	0.295142

@mg24-isomer50 bp86/6-31G(d) Etot=-4802.220612 Eb=-14.33

Mg1	1.752659	-0.051187	-0.794856
Mg2	-1.362141	0.998223	-1.160913
Mg3	-3.203639	-1.007085	-2.515543
Mg4	-0.547520	-3.859135	0.997733
Mg5	3.078645	1.126743	1.830090
Mg6	4.248288	-1.470842	0.821411
Mg7	-4.651542	-0.935897	1.953138
Mg8	-6.248405	1.452586	0.735658

Mg9	3.903029	1.586648	-2.428143
Mg10	-5.014866	4.102924	0.053575
Mg11	-4.308503	1.701962	-1.684365
Mg12	2.102752	2.989985	-0.426495
Mg13	6.088322	0.701113	2.065833
Mg14	-5.689344	-1.106999	-0.807275
Mg15	6.181108	0.221148	-0.872613
Mg16	-3.359650	-2.959252	-0.061684
Mg17	5.066045	2.838906	0.175005
Mg18	0.048919	1.420695	1.501532
Mg19	-1.719964	-0.974458	1.457072
Mg20	4.022892	-1.471157	-2.202805
Mg21	2.064174	-3.349512	-0.410471
Mg22	-0.581045	-2.109327	-1.413739
Mg23	-3.115319	1.730746	1.210161
Mg24	1.245102	-1.576828	1.977693

@mg24-isomer51 bp86/6-31G(d) Etot=-4802.220033 Eb=-14.31

Mg1	0.291081	0.762516	-2.126839
Mg2	-2.719651	0.032642	-2.168984
Mg3	1.937633	-1.675872	-1.084285
Mg4	-1.621067	2.176482	-0.004057
Mg5	-1.421527	0.503957	2.736790
Mg6	-0.200290	-4.005152	-0.349367
Mg7	-4.138501	1.412234	1.863487
Mg8	1.065882	3.567420	-0.570399
Mg9	-1.061329	-0.978899	0.158427
Mg10	3.328988	1.074629	-1.411795
Mg11	1.239177	-2.231352	1.900844
Mg12	4.958301	-1.598355	-1.709642
Mg13	3.389801	-0.194072	2.855416
Mg14	4.124266	-2.649163	1.043658
Mg15	-0.533631	-2.253502	-2.825811
Mg16	5.495358	0.108387	0.653867
Mg17	-7.021103	1.587390	0.447841
Mg18	3.977460	4.226724	-1.254690
Mg19	-3.136090	-3.007847	-0.876541
Mg20	-5.030907	-0.729945	-0.406034
Mg21	-4.447362	2.328639	-1.075952
Mg22	1.277283	0.754701	0.912145
Mg23	3.713270	2.480703	1.346165
Mg24	-3.467041	-1.692265	1.945755

@mg24-isomer52 bp86/6-31G(d) Etot=-4802.213658 Eb=-14.14

Mg1	-4.311766	-1.580517	0.958057
Mg2	0.961808	0.526417	0.630437
Mg3	5.508378	1.462799	1.213938
Mg4	-6.136204	2.692148	-1.164561
Mg5	-2.957283	-0.133872	3.287435
Mg6	-4.394178	0.084263	-1.546384
Mg7	-0.191542	-4.269980	0.007275
Mg8	1.918244	1.092318	-2.328360
Mg9	-2.690153	-2.581539	-1.461683
Mg10	-1.744059	1.704431	1.300626
Mg11	0.063169	3.185732	-0.985019
Mg12	4.948389	1.677608	-1.944285
Mg13	0.965084	-1.815368	-1.430317
Mg14	-0.532534	-3.997761	-3.070949
Mg15	7.021232	-0.243046	-0.710153
Mg16	3.757873	-0.710101	-0.247172
Mg17	-1.248976	-1.530104	1.026002
Mg18	0.230228	-0.565459	3.489997
Mg19	-3.020971	2.893154	-1.183268
Mg20	1.800139	-2.452057	1.586199

Mg21	-1.312335	0.333172	-1.506789
Mg22	2.918561	2.749526	0.086940
Mg23	-4.758820	1.409724	1.282526
Mg24	3.205717	0.068511	2.709508

@mg24-isomer53 bp86/6-31G(d) Etot=-4802.207816 Eb=-13.99

Mg1	-0.360060	-0.963826	1.121436
Mg2	1.574831	1.477866	0.720079
Mg3	-1.405962	1.993074	1.502789
Mg4	-5.572579	-0.724238	-1.240423
Mg5	-6.359043	0.846073	1.200615
Mg6	3.939627	-0.566285	-0.430398
Mg7	-3.030853	-2.063556	-0.092142
Mg8	-3.448527	-0.111810	2.187571
Mg9	-2.901713	-0.343987	-2.732888
Mg10	-4.284745	2.819927	2.092593
Mg11	4.318806	-3.715466	1.761757
Mg12	2.247869	-1.493880	-2.622765
Mg13	5.757267	-1.084715	1.997816
Mg14	1.873906	-2.988177	0.078018
Mg15	5.362161	2.101298	-1.080374
Mg16	2.714821	-0.894309	2.349666
Mg17	-0.581819	1.109320	-1.278418
Mg18	-0.502824	-2.199167	-1.699892
Mg19	-0.004930	-0.061351	-3.974793
Mg20	2.385529	1.551604	-2.224346
Mg21	3.235743	3.959134	-0.162927
Mg22	-5.749362	-2.111732	1.402241
Mg23	-3.666459	1.723298	-0.666739
Mg24	4.458314	1.740905	1.791522

@mg24-isomer54 bp86/6-31G(d) Etot=-4802.200064 Eb=-13.79

Mg1	1.096107	-0.383888	0.089294
Mg2	4.894174	-1.028573	0.900301
Mg3	-0.934636	-2.490519	0.984274
Mg4	-3.330810	-1.725825	-0.561079
Mg5	1.535212	-3.416982	-0.642143
Mg6	-1.398646	-0.050506	-2.306535
Mg7	0.655169	2.620403	0.816082
Mg8	3.564494	0.585162	-1.361006
Mg9	5.188725	2.063156	0.837414
Mg10	-1.719059	0.524640	1.041039
Mg11	-4.170614	1.360506	-0.811871
Mg12	1.393181	-1.204179	-2.875420
Mg13	4.285757	-3.940503	0.710340
Mg14	-4.535506	-0.391627	1.795993
Mg15	0.958922	1.907566	-2.332368
Mg16	2.135797	-2.362753	2.146959
Mg17	-6.466145	-0.986816	-1.111769
Mg18	-7.107492	1.558785	0.413981
Mg19	4.108667	-2.303866	-1.840299
Mg20	-7.500667	-1.189146	1.643487
Mg21	2.799367	0.683853	2.354905
Mg22	3.078108	3.592152	-0.871589
Mg23	3.187639	3.710794	2.213139
Mg24	-1.717744	2.868168	-1.233131

@mg25-isomer01 bp86/6-31G(d) Etot=-5002.399141 Eb=-16.48

Mg1	1.182678	-1.556087	3.210941
Mg2	4.384549	1.801954	0.848796
Mg3	-4.693539	1.377280	0.070109
Mg4	-0.415704	0.967189	2.937067
Mg5	-1.762626	-1.903237	2.579612
Mg6	0.245392	1.548714	-2.212923

Mg7	3.142744	-2.712633	-0.770680
Mg8	-3.472284	0.599501	2.652088
Mg9	-2.302778	-2.942305	-0.808095
Mg10	-1.995948	2.765381	0.936423
Mg11	0.443359	-3.193430	-2.234808
Mg12	-4.163407	-0.810143	-1.961678
Mg13	1.575248	-0.176409	0.142402
Mg14	-4.397214	-1.674459	0.950399
Mg15	0.367429	-2.965069	0.715489
Mg16	3.079118	2.187864	-1.757055
Mg17	-2.714161	1.893899	-2.109394
Mg18	-0.522645	4.186593	-1.323090
Mg19	1.089895	2.719403	0.807052
Mg20	4.125136	-1.191046	1.652285
Mg21	2.076433	-0.709948	-2.962175
Mg22	2.589934	1.058436	3.044356
Mg23	-1.400927	-0.097744	0.031257
Mg24	-1.188581	-0.871389	-3.019928
Mg25	4.727900	-0.302314	-1.418451

@mg25-isomer02 bp86/6-31G(d) Etot=-5002.398854 Eb=-16.48

Mg1	3.566654	2.623288	-0.772856
Mg2	0.161259	-0.224284	2.954353
Mg3	0.026414	-1.113872	-3.253182
Mg4	-4.196132	2.075520	1.296066
Mg5	1.306809	-2.696474	1.484921
Mg6	-2.398019	3.499486	-0.569994
Mg7	-4.181576	1.262722	-1.568397
Mg8	2.443264	-2.403352	-1.894883
Mg9	-2.869482	-1.367499	-2.221183
Mg10	0.461998	2.820705	-0.577850
Mg11	4.428250	-0.066193	-1.773332
Mg12	4.897128	0.896588	1.154225
Mg13	-1.228891	1.531253	-2.723242
Mg14	-3.440410	-3.707675	-0.322373
Mg15	-0.486943	-2.873872	-0.950988
Mg16	3.124892	-0.715572	2.893537
Mg17	-1.665030	-2.502306	1.857080
Mg18	-1.020084	2.515170	2.094452
Mg19	1.546819	-0.084508	-0.170427
Mg20	-1.424450	0.169328	0.035836
Mg21	-4.370492	-1.018373	0.585099
Mg22	-2.794786	0.090076	2.915071
Mg23	4.279467	-2.065499	0.483519
Mg24	1.775072	1.309705	-2.988139
Mg25	2.058269	2.045638	2.032688

@mg25-isomer03 bp86/6-31G(d) Etot=-5002.398561 Eb=-16.47

Mg1	-4.393318	-1.997196	-0.900571
Mg2	1.939464	-2.244301	-1.884834
Mg3	-4.064924	-0.373089	1.744661
Mg4	-2.887711	-0.539872	-3.009670
Mg5	-1.941605	2.252406	-1.872046
Mg6	2.061341	-1.614611	3.061766
Mg7	4.392630	1.998967	-0.889942
Mg8	-4.768603	0.948951	-1.224481
Mg9	-0.507578	2.954165	0.759399
Mg10	-2.463439	-2.993018	1.022239
Mg11	2.463629	2.988298	1.037144
Mg12	-2.061300	1.600143	3.065825
Mg13	1.488003	0.085287	0.041521
Mg14	-3.626694	2.652799	0.796652
Mg15	1.077480	2.696455	-1.797681
Mg16	3.624114	-2.653231	0.784406

Mg17	-0.878673	-1.210398	2.855955
Mg18	0.506675	-2.952505	0.746259
Mg19	-1.079773	-2.688361	-1.811330
Mg20	2.887880	0.554486	-3.007077
Mg21	4.066940	0.364762	1.748763
Mg22	-0.000491	0.007451	-2.933501
Mg23	-1.478504	-0.084528	0.044183
Mg24	0.875496	1.192262	2.853995
Mg25	4.768960	-0.945324	-1.231634

@mg25-isomer04 bp86/6-31G(d) Etot=-5002.398513 Eb=-16.47

Mg1	-4.196347	-0.830006	1.391637
Mg2	-4.016753	2.256368	0.314765
Mg3	-3.577100	-2.328174	-1.169348
Mg4	1.928360	3.092951	1.443857
Mg5	5.086911	-0.463088	-0.584474
Mg6	3.731444	-2.444544	1.078711
Mg7	-2.382795	-0.639462	-3.444577
Mg8	-0.991544	3.011256	0.770133
Mg9	-1.532271	0.009740	0.081625
Mg10	2.721054	-1.986415	-1.869595
Mg11	-2.819157	1.560056	2.885002
Mg12	-0.424813	-2.318735	-1.811129
Mg13	1.007339	2.931903	-1.514607
Mg14	-1.965066	2.157795	-2.117022
Mg15	1.222191	-3.843198	0.135598
Mg16	-4.631793	0.380375	-1.783817
Mg17	-1.571954	-2.932989	1.010793
Mg18	3.540740	0.412535	2.192272
Mg19	-1.789760	-1.156198	3.411959
Mg20	1.433116	0.125404	-0.018776
Mg21	4.348995	2.420108	-0.075609
Mg22	3.317685	1.019284	-2.488231
Mg23	0.968970	-1.826014	2.345205
Mg24	0.386399	0.342612	-2.971137
Mg25	0.206150	1.048437	2.786766

@mg25-isomer05 bp86/6-31G(d) Etot=-5002.396708 Eb=-16.42

Mg1	4.802621	-2.417486	0.360580
Mg2	-1.048128	-2.765163	1.786992
Mg3	-3.937267	1.482342	1.187163
Mg4	1.899339	-2.680940	1.208668
Mg5	-4.243631	-1.697855	1.627124
Mg6	-0.040680	-2.616535	-1.240087
Mg7	-1.586671	-0.108351	0.101959
Mg8	3.798899	-0.178348	2.021541
Mg9	4.855545	0.079523	-1.251195
Mg10	-2.077663	3.557721	-0.219864
Mg11	0.684834	-0.487434	2.945142
Mg12	0.880094	3.214740	-0.091894
Mg13	0.680799	-0.671385	-3.458924
Mg14	3.919725	2.430991	0.277803
Mg15	-2.243956	-0.302396	3.236345
Mg16	-0.836417	2.111815	2.137222
Mg17	2.085545	2.250429	2.624973
Mg18	-3.706086	1.837546	-1.946182
Mg19	-4.836959	-0.736541	-1.101174
Mg20	2.855429	-2.079134	-1.956515
Mg21	-0.581634	1.811495	-2.326556
Mg22	-2.938172	-3.020144	-0.676056
Mg23	1.327700	0.113189	-0.078452
Mg24	2.488675	1.663155	-2.385348
Mg25	-2.201943	-0.791235	-2.783263

@mg25-isomer06 bp86/6-31G(d) Etot=-5002.396669 Eb=-16.42

Mg1	4.556160	-0.772810	1.590759
Mg2	-1.226262	-0.001009	-0.002080
Mg3	4.519409	1.829209	-0.042765
Mg4	0.585498	-0.361611	2.871020
Mg5	2.238863	-2.669625	1.833001
Mg6	-3.869993	-2.130601	1.138399
Mg7	2.251011	2.731111	-1.769549
Mg8	0.631184	2.774956	0.789785
Mg9	-0.816550	2.593847	-1.807821
Mg10	-2.449632	-0.028577	2.870216
Mg11	3.654406	0.130670	-2.466667
Mg12	-4.803687	0.727080	1.062249
Mg13	-1.932499	-0.052073	-3.057889
Mg14	0.819064	1.033512	-3.760646
Mg15	0.714451	-1.567260	-2.349894
Mg16	2.862134	1.620004	2.527961
Mg17	0.796717	-3.878350	-0.497023
Mg18	-0.404524	2.317761	3.493546
Mg19	-2.418996	2.664002	1.078446
Mg20	-3.846586	1.893553	-1.536305
Mg21	3.619185	-2.367995	-0.859149
Mg22	-1.948178	-2.789703	-1.241880
Mg23	-4.428698	-1.022203	-1.564307
Mg24	-0.843085	-2.675976	1.685519
Mg25	1.740610	0.002086	0.015074

@mg25-isomer07 bp86/6-31G(d) Etot=-5002.396168 Eb=-16.41

Mg1	1.660967	-3.038985	0.297259
Mg2	4.424852	-1.935588	-0.263849
Mg3	3.130987	-1.555305	2.479532
Mg4	-1.090741	-3.587528	1.091309
Mg5	-0.451853	-2.235479	-1.693125
Mg6	2.412530	-1.479809	-2.599988
Mg7	0.094092	-1.258155	2.609766
Mg8	-3.327441	-3.124542	-0.806740
Mg9	4.792684	0.618346	1.440757
Mg10	4.434911	0.684384	-1.694402
Mg11	1.511704	0.019653	-0.094494
Mg12	-0.038976	-0.029475	-3.702829
Mg13	-2.976525	-1.503904	2.180583
Mg14	1.979268	1.359139	2.703803
Mg15	-1.474758	0.111400	0.118709
Mg16	1.726385	2.040703	-2.439748
Mg17	-2.916383	-0.530963	-2.496496
Mg18	-1.058696	1.583786	2.839352
Mg19	3.433347	2.805880	0.141296
Mg20	-4.900185	-0.801017	-0.088240
Mg21	-1.205069	2.231782	-2.040839
Mg22	0.420274	2.891169	0.429463
Mg23	-4.039849	1.306625	1.919321
Mg24	-2.382963	3.486376	0.765902
Mg25	-4.158562	1.941508	-1.096305

@mg25-isomer08 bp86/6-31G(d) Etot=-5002.392007 Eb=-16.30

Mg1	-1.127324	0.254573	-0.044860
Mg2	-0.066874	1.374770	-3.507790
Mg3	1.517657	-0.982769	2.927309
Mg4	-1.677747	-2.833042	-0.967068
Mg5	-1.060025	0.920921	2.954088
Mg6	0.420172	-1.451720	-2.583089
Mg7	0.968068	-3.077803	0.290181
Mg8	1.648028	2.087685	2.224776
Mg9	1.827042	-0.139032	0.016281

Mg10	-2.430030	-0.313033	-2.716052
Mg11	-2.047478	2.866188	-1.461657
Mg12	-3.720768	-0.334467	1.680898
Mg13	0.865137	2.569431	-0.929006
Mg14	-1.157028	-2.077986	2.166200
Mg15	3.863525	2.395900	-0.141786
Mg16	4.225536	0.500987	2.166216
Mg17	-4.531438	1.295860	-1.002349
Mg18	3.292271	-2.310804	-1.818103
Mg19	-3.575573	2.658087	1.462634
Mg20	2.824803	0.701725	-2.718932
Mg21	-4.551921	-1.700762	-1.041096
Mg22	3.882355	-2.294019	1.159236
Mg23	5.106163	-0.249974	-0.758511
Mg24	-0.785672	3.529788	1.383124
Mg25	-3.708879	-3.390505	1.259357

@mg25-isomer09 bp86/6-31G(d) Etot=-5002.391823 Eb=-16.30

Mg1	2.422203	-2.352567	1.946585
Mg2	-0.481607	-2.948751	2.766750
Mg3	0.316814	-0.147494	2.971732
Mg4	-2.904412	-0.655392	2.606494
Mg5	3.572758	0.372219	2.749109
Mg6	4.806052	-1.124778	0.478649
Mg7	0.153842	-2.813768	-0.267005
Mg8	2.936565	-2.182663	-1.681662
Mg9	-2.670777	-3.054014	0.769222
Mg10	-2.684905	-1.893760	-2.072379
Mg11	4.619189	0.343813	-2.191208
Mg12	1.639645	-0.046314	0.004093
Mg13	-1.330283	-0.018132	0.000312
Mg14	-1.534614	2.132420	2.195476
Mg15	1.840805	0.427482	-3.307274
Mg16	-4.284248	1.553384	0.880203
Mg17	0.165700	-2.008972	-3.177364
Mg18	-4.839370	-1.275962	0.087405
Mg19	1.498575	2.463984	1.892778
Mg20	3.998611	2.069728	0.164499
Mg21	-1.159240	0.700625	-3.090135
Mg22	-0.369507	4.447920	0.670730
Mg23	-4.167545	0.733269	-2.089147
Mg24	-2.291065	2.810313	-1.012227
Mg25	0.746814	2.467409	-1.295636

@mg25-isomer10 bp86/6-31G(d) Etot=-5002.390372 Eb=-16.26

Mg1	-0.675318	2.625527	-0.652886
Mg2	-1.842316	-0.083413	-0.092695
Mg3	1.160151	0.082203	0.115343
Mg4	-3.326095	-2.681061	0.843444
Mg5	3.854978	0.709991	-1.601725
Mg6	-3.347188	-0.297501	2.817113
Mg7	-3.790120	-1.409342	-1.991082
Mg8	1.428329	0.347067	3.362844
Mg9	-0.745405	-1.567795	-2.899613
Mg10	2.121364	3.300809	-1.508965
Mg11	3.958107	0.388564	1.608438
Mg12	1.653825	2.855995	1.629027
Mg13	-1.952137	1.167684	-3.166757
Mg14	4.431104	3.061586	0.316175
Mg15	-1.017679	1.683698	2.414261
Mg16	4.409781	-1.962665	-0.209008
Mg17	-3.800816	2.321609	1.323630
Mg18	-0.678263	-1.613168	2.532006
Mg19	0.959363	0.928660	-2.924731

Mg20	2.204570	-2.318835	1.951103
Mg21	2.553364	-4.252075	-0.383542
Mg22	-5.209231	-0.339663	0.474535
Mg23	-4.356469	1.748575	-1.506865
Mg24	-0.121299	-2.816515	-0.196004
Mg25	2.127401	-1.879934	-2.254049

@mg25-isomer11 bp86/6-31G(d) Etot=-5002.383646 Eb=-16.09

Mg1	-0.119043	-1.878703	-2.069197
Mg2	-1.792929	-0.035583	-0.036291
Mg3	1.212896	0.156512	0.195727
Mg4	-4.269008	1.016539	1.479950
Mg5	4.076122	0.256346	-1.295869
Mg6	-3.569413	-1.978180	2.162438
Mg7	-3.157701	2.952562	-0.622160
Mg8	1.285393	-2.066497	2.883775
Mg9	-0.139351	2.793765	-1.221341
Mg10	2.741254	-2.012907	-2.808532
Mg11	3.833574	-0.992142	1.639925
Mg12	1.927404	-2.994591	0.026334
Mg13	-1.771858	0.812512	-2.980869
Mg14	4.823423	-2.635164	-0.679074
Mg15	-0.873184	-2.769865	0.907256
Mg16	3.942408	1.993207	1.252330
Mg17	-3.171262	-2.013585	-1.976629
Mg18	-1.123342	-0.440890	3.113831
Mg19	1.317881	0.740049	-2.903338
Mg20	1.515393	1.099831	3.074469
Mg21	1.531224	3.701277	1.266424
Mg22	-5.415439	-1.634393	-0.022179
Mg23	-4.626347	0.689617	-1.730033
Mg24	2.822340	3.004028	-1.356249
Mg25	-1.000436	2.236255	1.699302

@mg25-isomer12 bp86/6-31G(d) Etot=-5002.373640 Eb=-15.84

Mg1	-0.474885	3.985561	-0.512355
Mg2	0.909020	1.990485	1.399541
Mg3	-0.736001	-3.021287	-2.384378
Mg4	1.932583	-1.352626	-2.446379
Mg5	2.227540	0.007067	3.348780
Mg6	-2.079266	2.057697	1.502406
Mg7	-2.194741	1.720987	-1.970672
Mg8	-2.143737	-3.288351	0.473457
Mg9	-3.258508	-1.296867	-1.941968
Mg10	-3.490099	3.903467	-0.426046
Mg11	0.898041	-3.421504	0.053676
Mg12	4.075838	1.697919	1.258692
Mg13	-0.683144	0.584697	3.718736
Mg14	0.930456	1.508715	-1.830185
Mg15	-0.717991	-0.340763	-3.536363
Mg16	-0.033134	-2.051999	2.609297
Mg17	3.939502	1.190812	-1.826516
Mg18	-0.846909	-0.405649	-0.069689
Mg19	-2.963991	-0.856675	2.361808
Mg20	3.856680	-3.483191	-0.035550
Mg21	-4.371547	0.767082	0.015040
Mg22	5.255349	-0.855699	-0.046392
Mg23	2.687522	3.788759	-0.594911
Mg24	-4.865777	-2.181422	0.441753
Mg25	2.147199	-0.647215	0.438216

@mg25-isomer13 bp86/6-31G(d) Etot=-5002.372332 Eb=-15.81

Mg1	-1.449415	-0.018841	0.201314
Mg2	1.418649	3.130896	0.648217

Mg3	-2.881289	-2.531341	-1.363598
Mg4	-4.070376	-1.374568	1.317774
Mg5	0.184642	2.081318	-2.086153
Mg6	3.139928	2.536393	-1.728234
Mg7	-0.288505	-0.962484	-2.454981
Mg8	1.518616	0.040433	0.023256
Mg9	2.508625	-2.297765	-1.865594
Mg10	-3.905635	1.687774	0.816646
Mg11	-0.065857	-3.681954	-1.164593
Mg12	0.169706	-0.777674	2.847775
Mg13	-0.844640	2.065564	2.354377
Mg14	4.580711	-0.026223	-1.810616
Mg15	-1.500645	3.555185	-0.088620
Mg16	-1.410407	-2.957633	1.421642
Mg17	3.222834	-1.040805	3.205010
Mg18	4.300206	-1.706361	0.572115
Mg19	-2.885277	1.750421	-2.165723
Mg20	2.020621	1.710637	3.287046
Mg21	1.620221	-2.913658	1.252497
Mg22	4.095337	1.381591	1.050943
Mg23	2.221393	0.389728	-3.663658
Mg24	-6.761650	0.267983	0.839900
Mg25	-4.937793	-0.308615	-1.446741

@mg25-isomer14 bp86/6-31G(d) Etot=-5002.372271 Eb=-15.81

Mg1	-0.422161	0.854158	3.204696
Mg2	-0.062197	4.501918	-1.727456
Mg3	-0.109465	2.894002	0.865106
Mg4	2.538526	3.172812	-1.208717
Mg5	-2.829233	2.468368	2.193789
Mg6	2.254612	1.214861	1.397290
Mg7	2.085269	-0.742649	3.718672
Mg8	-2.600582	2.953018	-0.892480
Mg9	4.834478	1.455948	-0.400452
Mg10	4.724882	-0.492407	1.904151
Mg11	-0.334840	-2.124872	2.527151
Mg12	-4.727599	1.285762	0.269670
Mg13	-0.264084	1.628772	-2.434437
Mg14	-0.545171	-0.157189	0.084071
Mg15	2.255221	-1.922372	0.806187
Mg16	2.320752	0.140243	-1.774294
Mg17	-3.118130	-0.544059	2.207616
Mg18	-2.600930	-3.210655	0.899799
Mg19	4.764389	-1.532765	-0.984594
Mg20	-2.971094	0.124395	-2.074025
Mg21	-0.026916	-3.261214	-0.624193
Mg22	-4.726963	-1.647568	-0.319258
Mg23	-0.250402	-1.359574	-3.017538
Mg24	2.486392	-2.799614	-2.467651
Mg25	-2.674755	-2.899317	-2.153103

@mg25-isomer15 bp86/6-31G(d) Etot=-5002.369873 Eb=-15.75

Mg1	0.117350	2.485191	-1.866933
Mg2	-1.316474	0.130482	0.024026
Mg3	2.466045	0.317619	1.797304
Mg4	3.044325	2.399655	-0.441880
Mg5	-2.890855	2.602195	-2.676452
Mg6	-1.172429	-0.010009	-3.068125
Mg7	1.526337	-0.099555	-1.284671
Mg8	-1.885112	-2.407566	2.723847
Mg9	4.227668	-2.215449	1.366449
Mg10	-2.839421	-2.554106	-2.413214
Mg11	-4.109063	1.550824	0.452995
Mg12	0.456744	2.421399	1.230763

Mg13	5.513011	0.683900	1.470974
Mg14	0.725189	-2.051436	1.063128
Mg15	0.105129	-2.598595	-2.042598
Mg16	-2.206172	2.450597	2.658895
Mg17	3.022667	-3.109014	-1.216490
Mg18	-4.136085	0.047392	-2.156040
Mg19	-0.368670	0.122036	3.125663
Mg20	-1.987591	3.590511	-0.066119
Mg21	5.953870	2.205341	-1.102094
Mg22	-3.560689	-0.059307	3.143186
Mg23	-3.813439	-1.570250	0.436895
Mg24	-1.650773	-3.707794	0.072149
Mg25	4.778441	-0.624061	-1.231658

@mg25-isomer16 bp86/6-31G(d) Etot=-5002.368247 Eb=-15.71

Mg1	-0.640737	0.776333	1.873332
Mg2	3.272730	0.298178	-2.748580
Mg3	-3.360398	-3.272647	-0.755084
Mg4	2.522518	-3.755148	0.259685
Mg5	4.326963	-2.018147	-1.214488
Mg6	-1.530511	-0.687535	-0.836898
Mg7	1.233473	-2.322472	-2.282114
Mg8	4.482468	0.824715	-0.014682
Mg9	-2.739669	1.211665	-2.938485
Mg10	3.711375	3.492734	1.200791
Mg11	2.465999	0.986225	2.407600
Mg12	1.497339	-0.346385	-0.113156
Mg13	-2.052297	-2.018235	2.151000
Mg14	-0.428430	-3.463729	0.041757
Mg15	-4.665771	-0.430375	-1.211142
Mg16	-0.944351	2.625660	-0.963572
Mg17	-2.408702	3.507061	1.566873
Mg18	0.739553	3.503231	1.356887
Mg19	-3.606920	0.698875	1.550738
Mg20	0.293446	0.753373	-2.898844
Mg21	-5.022805	-1.988822	1.370551
Mg22	0.945708	-2.053770	2.461252
Mg23	2.133212	2.682628	-1.322011
Mg24	3.951118	-1.638951	1.780120
Mg25	-4.175310	2.635537	-0.721530

@mg25-isomer17 bp86/6-31G(d) Etot=-5002.367965 Eb=-15.70

Mg1	2.339290	-0.870968	-2.899183
Mg2	0.625844	-2.948631	-0.935031
Mg3	-6.307006	0.087233	0.252065
Mg4	3.454597	1.861194	-2.031237
Mg5	-0.683148	-2.101499	1.872961
Mg6	1.007677	2.696226	2.630436
Mg7	1.772226	-0.259381	-0.067949
Mg8	-1.218107	0.741049	3.164514
Mg9	0.859001	1.780117	-3.471157
Mg10	-0.706829	-0.696863	-2.627998
Mg11	-1.697904	2.335902	-1.925619
Mg12	-1.455378	3.390125	1.115552
Mg13	3.556618	1.811317	1.138282
Mg14	5.351682	-0.010552	-0.732981
Mg15	-1.038803	0.375493	0.192968
Mg16	-5.367086	-2.512840	-0.596766
Mg17	-2.296589	-2.736119	-0.770077
Mg18	-3.728963	-0.106310	-1.676579
Mg19	2.107088	-3.011393	1.777620
Mg20	-4.003801	2.115382	0.437722
Mg21	4.446812	-1.049375	1.873807
Mg22	1.661514	-0.256362	3.017957

Mg23	3.824724	-2.619793	-0.713793
Mg24	1.034835	2.817204	-0.492905
Mg25	-3.538295	-0.831159	1.467393

@mg25-isomer18 bp86/6-31G(d) Etot=-5002.366426 Eb=-15.66

Mg1	-0.014977	0.020732	2.959018
Mg2	-0.441328	-0.663281	-0.221738
Mg3	2.454730	-1.796795	2.411689
Mg4	-0.665759	2.294770	-1.181988
Mg5	-4.860124	-0.192635	1.029618
Mg6	-2.811457	-1.300436	2.884119
Mg7	2.018524	0.811466	0.927746
Mg8	-0.258758	-3.670890	-0.932408
Mg9	-4.714931	2.804668	-0.041218
Mg10	0.214406	3.070993	1.700837
Mg11	-3.024418	-2.518813	0.122005
Mg12	1.725500	0.730274	-2.256997
Mg13	2.250145	3.372383	-0.682118
Mg14	4.737289	2.680382	1.169636
Mg15	-0.444534	-2.918604	2.034575
Mg16	-1.015414	0.421966	-3.614747
Mg17	0.683202	-1.956346	-3.324857
Mg18	-2.243142	1.363215	1.410329
Mg19	-3.082450	0.327251	-1.377211
Mg20	2.442260	-1.858281	-0.710943
Mg21	4.716243	1.537720	-1.571281
Mg22	4.830700	-0.417201	0.801951
Mg23	2.077321	-4.403230	0.942422
Mg24	-2.283724	4.508638	0.313575
Mg25	-2.289304	-2.247947	-2.792016

@mg25-isomer19 bp86/6-31G(d) Etot=-5002.363472 Eb=-15.59

Mg1	-2.453460	-3.588707	-1.415169
Mg2	-0.417304	-0.662338	0.420725
Mg3	2.653384	-2.475262	-2.177760
Mg4	0.294120	2.419228	0.892155
Mg5	-4.589682	1.095898	-1.000805
Mg6	-3.367697	-1.081855	-2.614796
Mg7	1.813034	0.425190	-1.404280
Mg8	-1.121657	-3.393144	1.378371
Mg9	-4.735887	3.907657	0.055265
Mg10	0.783494	3.238334	-2.011817
Mg11	-3.566356	-1.489338	0.466120
Mg12	2.319984	0.322870	1.787580
Mg13	3.154643	3.070708	-0.020016
Mg14	5.208204	1.589581	-1.703484
Mg15	-0.296291	-1.577427	-2.601781
Mg16	-0.298552	0.990734	3.516472
Mg17	0.592560	-1.787928	3.466622
Mg18	-1.460509	1.155117	-1.763856
Mg19	-2.554040	1.370086	1.348907
Mg20	1.994864	-2.627552	0.798560
Mg21	5.334518	1.496633	1.294212
Mg22	4.423049	-0.988703	-0.221833
Mg23	0.491523	-4.258209	-1.198026
Mg24	-1.850616	4.040276	-0.526219
Mg25	-2.351329	-1.191846	3.234851

@mg25-isomer20 bp86/6-31G(d) Etot=-5002.363319 Eb=-15.58

Mg1	3.121735	1.836357	-1.966740
Mg2	-4.872816	2.576756	-0.683607
Mg3	1.793301	-3.760443	1.233514
Mg4	0.117944	1.169578	-2.168169
Mg5	4.777120	1.279881	0.518628

Mg6	3.976725	-1.668856	1.071001
Mg7	-2.920609	0.575381	-2.393654
Mg8	1.558040	-1.626789	-0.996209
Mg9	-0.689585	0.165797	3.116262
Mg10	-3.463806	-2.454500	-1.860851
Mg11	-0.355593	2.961708	2.098311
Mg12	-1.851282	2.882659	-0.626549
Mg13	1.818152	-1.450567	3.152998
Mg14	1.045872	3.527551	-0.509415
Mg15	2.080441	-0.598541	-3.748079
Mg16	3.001748	3.252091	1.946981
Mg17	4.543529	-0.738746	-1.758073
Mg18	-0.797614	-2.762346	2.331113
Mg19	-0.748622	-1.612134	-3.102163
Mg20	-4.799317	-0.359406	-0.108603
Mg21	-3.290787	1.559688	1.801005
Mg22	1.550196	0.694146	0.864854
Mg23	-1.242879	-0.396157	0.130177
Mg24	-3.562971	-1.585823	2.242686
Mg25	-0.788923	-3.467285	-0.585416

@mg25-isomer21 bp86/6-31G(d) Etot=-5002.362508 Eb=-15.56

Mg1	1.016064	-0.197439	0.174886
Mg2	-2.620652	-1.714368	-0.869021
Mg3	0.136985	-3.174870	-0.051434
Mg4	-0.779141	-3.045967	-3.005615
Mg5	1.383771	-2.573060	2.715901
Mg6	2.143519	1.251790	-2.406615
Mg7	-0.382655	2.906608	-1.895200
Mg8	-4.943493	0.515226	-1.067176
Mg9	1.936573	-1.838234	-2.234712
Mg10	-1.992335	1.413091	3.034547
Mg11	0.200963	2.705370	1.265366
Mg12	1.010952	0.382102	3.251854
Mg13	4.829637	2.500010	-1.295448
Mg14	-2.532373	-4.843834	-1.026242
Mg15	-4.203694	-0.615745	1.683750
Mg16	4.213536	-0.435416	-0.636094
Mg17	-4.520820	2.361644	1.289970
Mg18	3.796925	-0.927655	2.429423
Mg19	-1.876896	1.020148	-0.038383
Mg20	3.224485	-3.064784	0.334035
Mg21	3.082874	1.766990	1.260332
Mg22	-0.577580	-0.092127	-2.672260
Mg23	-3.495488	3.243483	-1.520703
Mg24	2.233052	3.879488	-0.792229
Mg25	-1.284209	-1.422452	2.071069

@mg25-isomer22 bp86/6-31G(d) Etot=-5002.361793 Eb=-15.55

Mg1	-1.600248	2.390081	2.672928
Mg2	0.666383	0.434459	2.661981
Mg3	0.335084	-2.485778	1.727094
Mg4	3.010722	-3.511945	0.412451
Mg5	5.156426	-1.305219	0.430012
Mg6	-4.239036	-0.348975	-0.456512
Mg7	-3.089131	2.087586	-1.780400
Mg8	-4.318339	-2.975046	-1.917806
Mg9	-2.447982	-0.786255	2.187077
Mg10	-4.107440	2.069648	1.171652
Mg11	0.858989	2.934007	0.949618
Mg12	-4.662588	-2.850076	1.204330
Mg13	-2.141850	4.166748	0.242589
Mg14	-1.924463	-2.975141	-0.086537
Mg15	4.502824	0.948888	-1.514151

Mg16	0.568017	-2.411439	-1.595448
Mg17	3.549221	-1.838059	-2.094665
Mg18	-1.946525	-0.983215	-2.550487
Mg19	3.843295	1.502295	1.547489
Mg20	2.795085	3.337339	-1.280653
Mg21	-0.196892	3.203011	-1.908249
Mg22	3.195273	-1.439110	2.643543
Mg23	1.219820	0.584376	-2.626485
Mg24	1.993829	-0.285808	0.077993
Mg25	-1.020474	0.537629	-0.117364

@mg25-isomer23 bp86/6-31G(d) Etot=-5002.357405 Eb=-15.44

Mg1	-0.153782	0.046703	-0.018630
Mg2	-1.202976	-0.575534	-3.041140
Mg3	2.113522	-1.724891	1.444253
Mg4	-1.839255	-3.244731	-1.785954
Mg5	-3.957390	-3.050505	0.374803
Mg6	0.986304	-2.332429	-1.625831
Mg7	4.163044	0.840673	1.241825
Mg8	-0.529033	2.518849	-2.223683
Mg9	3.656250	-1.088638	-1.173333
Mg10	-3.659382	2.243429	1.529293
Mg11	-2.909543	0.956958	-1.095548
Mg12	6.582271	-0.119756	-0.447647
Mg13	-0.763700	-2.957289	1.007385
Mg14	-0.727553	2.919462	0.959559
Mg15	1.717140	0.505274	-2.890905
Mg16	-2.607676	-0.623445	1.673883
Mg17	1.970067	2.463618	-0.345499
Mg18	4.512784	1.808733	-1.716612
Mg19	1.384411	1.161511	2.501450
Mg20	-0.119915	-1.318192	3.570478
Mg21	-5.394796	-0.285447	0.309945
Mg22	-1.399630	1.433663	3.522925
Mg23	-2.821018	4.032487	-0.933595
Mg24	-4.206225	-1.492242	-2.221047
Mg25	5.206080	-2.118263	1.383626

@mg25-isomer24 bp86/6-31G(d) Etot=-5002.357306 Eb=-15.43

Mg1	0.626291	2.146643	1.846062
Mg2	0.115488	1.171364	-3.390796
Mg3	-2.314407	2.786568	1.471217
Mg4	1.742762	-0.378724	0.067735
Mg5	-0.634108	-2.366545	0.533581
Mg6	1.469833	-3.284021	-1.385014
Mg7	1.906298	-0.258328	3.162909
Mg8	2.437892	2.109513	-1.660264
Mg9	-0.610666	-1.670830	-2.772493
Mg10	-0.255132	3.297761	-1.002739
Mg11	-1.051529	0.507615	-0.456879
Mg12	2.187058	-2.988627	1.649607
Mg13	-1.233535	-0.044955	2.663485
Mg14	-4.330532	0.605254	1.400716
Mg15	2.282502	4.279293	0.420312
Mg16	2.401205	-0.866707	-2.938736
Mg17	-5.993655	0.242737	-1.304344
Mg18	4.724525	0.238032	-0.962663
Mg19	-3.282114	-2.175717	2.006533
Mg20	4.586895	-1.098107	1.861594
Mg21	-3.587167	2.054726	-1.234199
Mg22	-5.825324	-2.092882	0.494849
Mg23	3.604222	1.768453	1.472012
Mg24	4.297732	-2.630669	-0.805100
Mg25	-3.264535	-1.351846	-1.137387

@mg25-isomer25 bp86/6-31G(d) Etot=-5002.356121 Eb=-15.40

Mg1	0.945000	-1.005709	3.586746
Mg2	5.411968	0.934132	-1.482467
Mg3	-1.163009	-2.910548	2.629144
Mg4	0.469547	3.566360	-0.263524
Mg5	-1.304245	-1.247503	-2.905082
Mg6	4.567075	2.278174	1.157710
Mg7	1.620221	-0.483713	-3.480472
Mg8	1.385772	-2.907609	0.897711
Mg9	-4.948104	2.769770	0.398108
Mg10	-4.103055	-2.006956	-1.648083
Mg11	2.394844	1.415583	-0.997381
Mg12	0.149278	-0.321825	-0.044184
Mg13	-2.414703	3.502594	-1.361745
Mg14	0.969987	-3.067580	-2.149513
Mg15	1.006109	1.802554	2.160020
Mg16	3.352193	-1.552706	-1.172388
Mg17	3.086017	-0.410867	1.622090
Mg18	-0.323459	1.604895	-2.425775
Mg19	6.173799	-0.417234	1.001998
Mg20	-1.826768	2.839097	1.472011
Mg21	-3.766866	-1.937631	1.333474
Mg22	-1.455088	-3.034112	-0.392364
Mg23	-2.666556	0.499390	-0.552244
Mg24	-1.696435	0.065568	2.477165
Mg25	-5.863523	0.025875	0.139048

@mg25-isomer26 bp86/6-31G(d) Etot=-5002.354365 Eb=-15.36

Mg1	1.419668	1.106452	1.566980
Mg2	4.299515	-1.143211	-0.386364
Mg3	0.260975	-1.131715	-0.203813
Mg4	4.412899	0.724569	2.013758
Mg5	-0.086395	0.868518	-4.189878
Mg6	-1.978056	-3.610085	1.432764
Mg7	-2.302333	1.027506	-2.048043
Mg8	2.369535	-3.333845	-1.009897
Mg9	-4.104625	3.296783	-0.160125
Mg10	4.309742	3.736007	1.412873
Mg11	0.916825	-4.156441	1.444611
Mg12	2.172580	-0.523941	-2.543180
Mg13	-4.823612	0.378030	-0.158374
Mg14	1.691164	4.361889	0.139499
Mg15	-2.754859	-1.825588	-0.869272
Mg16	0.502520	1.872352	-1.320022
Mg17	-0.632591	-1.847086	-3.144729
Mg18	-3.460324	-1.124982	2.169133
Mg19	2.651022	-1.770751	2.028278
Mg20	-0.619653	-4.227021	-1.157513
Mg21	-1.637189	1.098898	0.889541
Mg22	-1.288550	4.077233	-0.263208
Mg23	3.417080	1.729012	-0.729014
Mg24	-4.372358	1.793738	2.406111
Mg25	-0.362979	-1.376321	2.679884

@mg25-isomer27 bp86/6-31G(d) Etot=-5002.353068 Eb=-15.33

Mg1	-0.914999	0.790564	-0.042415
Mg2	1.871088	-0.155721	-0.817955
Mg3	-3.009122	1.010450	-2.793703
Mg4	2.316157	-0.384837	2.312014
Mg5	-0.657777	-1.195663	-2.339186
Mg6	-3.794738	-1.566773	-1.491442
Mg7	4.844405	0.839962	-1.456156
Mg8	-0.073827	4.094655	-0.397328

Mg9	1.041398	2.425299	1.786885
Mg10	3.186966	-3.079846	1.099452
Mg11	-0.006385	2.063833	-2.653217
Mg12	5.198402	-0.874547	1.109009
Mg13	-4.471844	-4.198467	0.151404
Mg14	4.332462	-2.176448	-1.511098
Mg15	-2.816078	-1.663909	1.451766
Mg16	-4.116106	1.039687	0.073242
Mg17	-2.111031	2.920627	1.723492
Mg18	-0.751586	0.152028	2.924432
Mg19	0.167927	-2.228080	1.265468
Mg20	4.082959	1.893977	1.251313
Mg21	-2.821811	3.520541	-1.304339
Mg22	2.462501	2.877342	-1.138963
Mg23	1.421766	-3.208646	-1.439219
Mg24	-1.543166	-3.589957	-0.744684
Mg25	-3.837558	0.693931	2.981228

@mg25-isomer28 bp86/6-31G(d) Etot=-5002.352515 Eb=-15.31

Mg1	-0.341560	-0.352593	-3.340403
Mg2	2.793485	-3.293172	-0.574441
Mg3	4.751571	-2.314638	1.585025
Mg4	-2.813916	1.538622	-2.252348
Mg5	-4.050442	-0.089651	0.106894
Mg6	-0.852994	0.450941	-0.109770
Mg7	5.286862	-1.817987	-1.390851
Mg8	-2.398214	0.659090	2.704914
Mg9	-0.613352	-1.636977	3.898888
Mg10	-0.000049	-2.521726	-1.214029
Mg11	0.548652	2.250540	-2.200792
Mg12	-2.782120	-1.544695	-2.151639
Mg13	1.330381	-1.362695	1.470112
Mg14	-2.341367	-4.467526	-0.843212
Mg15	-0.742902	3.080073	1.818602
Mg16	-4.848476	-3.019458	-0.261458
Mg17	4.643315	0.468546	0.447557
Mg18	1.830468	1.623440	0.974629
Mg19	-1.592926	4.002459	-1.073543
Mg20	2.181806	-0.305352	-1.549227
Mg21	-3.560755	2.712726	0.699238
Mg22	3.507230	2.603544	-1.363603
Mg23	-1.862489	-2.082769	1.172390
Mg24	0.561959	0.961779	3.613044
Mg25	1.365832	4.457477	-0.165979

@mg25-isomer29 bp86/6-31G(d) Etot=-5002.351545 Eb=-15.29

Mg1	-1.171522	0.139622	-0.160909
Mg2	-3.525563	1.259263	-2.025075
Mg3	2.044039	1.261976	2.024391
Mg4	1.425359	-1.381018	0.430079
Mg5	-0.867860	0.913971	-3.397014
Mg6	1.387164	1.214900	-1.351664
Mg7	-1.021921	3.079440	-1.154309
Mg8	-5.318008	0.528874	0.390667
Mg9	-2.211458	-1.590681	-2.658039
Mg10	-0.166126	-0.411035	2.993865
Mg11	-3.026321	0.546581	2.358664
Mg12	-2.543967	-2.118217	3.613279
Mg13	-3.000919	-2.045049	0.472639
Mg14	-0.744361	2.516338	1.917265
Mg15	4.189038	1.989368	0.059829
Mg16	6.309344	-2.190117	-0.740187
Mg17	-0.372218	-3.301995	1.975997
Mg18	-5.189508	-1.422384	-1.759156

Mg19	0.881723	-1.460954	-2.806651
Mg20	-3.480705	2.932702	0.543364
Mg21	1.581330	3.727758	0.390107
Mg22	4.578749	-0.761589	1.436471
Mg23	6.979072	0.612532	0.050207
Mg24	3.784027	-0.682225	-1.618360
Mg25	-0.519389	-3.358063	-0.985457

@mg25-isomer30 bp86/6-31G(d) Etot=-5002.279388 Eb=-13.48

Mg1	1.698086	-1.712780	0.512165
Mg2	3.083935	0.882345	-0.426556
Mg3	-1.138132	-0.890642	-1.655032
Mg4	-0.254123	-3.677538	-0.778975
Mg5	-4.129471	-0.312554	-1.395214
Mg6	0.786197	1.504069	-2.321425
Mg7	-1.115201	-1.340590	1.633120
Mg8	-6.130782	0.463571	1.654895
Mg9	1.809061	0.205416	2.728078
Mg10	4.536857	-1.748806	-1.119510
Mg11	4.507467	-0.814748	1.828739
Mg12	0.019556	1.259516	0.627650
Mg13	-3.145621	-2.957681	-0.365586
Mg14	1.833767	3.666436	-0.376608
Mg15	-7.168081	0.274760	-1.133053
Mg16	1.929883	6.773631	0.380796
Mg17	-6.116153	-2.228325	0.104949
Mg18	-2.215919	2.013213	-1.314787
Mg19	7.634936	-1.773442	-1.118380
Mg20	1.833810	-1.395107	-2.404711
Mg21	-4.039019	-1.590332	2.287470
Mg22	-3.070863	1.158243	1.582932
Mg23	6.354997	0.840157	-0.270728
Mg24	7.576081	-1.024054	1.759655
Mg25	-5.081271	2.425242	-0.419884

@mg26-isomer01 bp86/6-31G(d) Etot=-5202.496575 Eb=-16.52

Mg1	3.352760	-2.210627	2.349690
Mg2	-4.662709	-1.277923	0.956439
Mg3	-1.774373	0.050986	0.225600
Mg4	3.071933	2.231725	-1.247086
Mg5	1.510654	1.125752	-3.702151
Mg6	-3.389122	0.614340	2.909705
Mg7	4.297314	2.783013	1.514763
Mg8	-4.749904	1.721139	0.484689
Mg9	3.954724	-0.364189	-2.551517
Mg10	-0.392791	1.524258	2.996606
Mg11	2.909999	-2.542532	-0.655741
Mg12	4.439847	-0.088409	0.438451
Mg13	1.409316	-1.784845	-3.312977
Mg14	-3.216609	-2.640624	-1.372743
Mg15	0.229253	-1.281321	2.467444
Mg16	-3.099320	2.400748	-1.942747
Mg17	2.524969	0.705539	2.780147
Mg18	1.220822	0.060397	-0.164557
Mg19	-1.913446	3.083646	0.928577
Mg20	-1.140987	-0.195106	-2.766079
Mg21	-0.156329	-2.574509	-0.941665
Mg22	-4.547511	-0.088862	-1.923658
Mg23	1.223092	3.125458	1.132775
Mg24	-0.033080	2.487343	-1.523954
Mg25	-2.057119	-2.933333	1.464479
Mg26	0.988616	-3.932064	1.455508

@mg26-isomer02 bp86/6-31G(d) Etot=-5202.496422 Eb=-16.52

Mg1	-3.479475	1.878797	-2.122967
Mg2	3.680297	3.014423	-0.212565
Mg3	0.508980	-1.492855	-2.661939
Mg4	-4.196685	2.185052	0.848157
Mg5	3.657396	0.712514	2.012237
Mg6	4.193427	-2.179805	0.869352
Mg7	-0.890567	-2.558329	1.105354
Mg8	-1.463108	0.251707	0.034157
Mg9	1.170838	3.764018	-1.652700
Mg10	-0.499145	1.473527	-2.663543
Mg11	1.675623	-3.480970	-0.297251
Mg12	-2.508981	-1.087542	-2.543784
Mg13	-3.678197	-3.013522	-0.202959
Mg14	4.881231	0.361123	-0.747356
Mg15	0.887903	2.559333	1.094348
Mg16	1.741464	-1.850182	2.628968
Mg17	-1.750178	1.869641	2.618123
Mg18	-1.165593	-3.773267	-1.634598
Mg19	-1.052721	-1.006682	3.607079
Mg20	1.461316	-0.253435	0.030900
Mg21	-3.669743	-0.700841	2.011382
Mg22	-1.673398	3.479194	-0.317067
Mg23	3.487596	-1.889944	-2.107537
Mg24	1.042245	1.029029	3.608739
Mg25	-4.879833	-0.364979	-0.757630
Mg26	2.519309	1.073996	-2.546900

@mg26-isomer03 bp86/6-31G(d) Etot=-5202.495232 Eb=-16.49

Mg1	2.171712	-2.011975	-2.166936
Mg2	3.217954	-3.344225	0.574360
Mg3	-2.897272	2.997315	1.794195
Mg4	0.006341	3.034124	1.008366
Mg5	-2.588272	-3.646444	-0.398834
Mg6	2.689258	3.610527	-0.253935
Mg7	3.259106	1.102057	-2.233400
Mg8	-2.174883	0.975060	-2.854777
Mg9	-2.329607	3.440077	-1.025425
Mg10	-0.673331	0.853988	2.956630
Mg11	0.728145	0.134463	-3.903707
Mg12	1.491408	-0.013588	0.078633
Mg13	-3.874564	-1.381242	-2.003579
Mg14	-1.497816	0.099233	0.015257
Mg15	-0.870035	-1.861485	-2.350068
Mg16	2.309622	1.513807	2.615430
Mg17	1.232246	-1.628957	2.786739
Mg18	0.278243	-3.049844	0.214349
Mg19	-4.399461	1.271823	-0.441522
Mg20	-3.619743	0.283260	2.443090
Mg21	4.111714	-0.924488	2.137888
Mg22	-4.603702	-1.896751	0.838250
Mg23	0.370702	2.210600	-1.839727
Mg24	4.631353	1.542493	0.534012
Mg25	4.780901	-1.200497	-0.836404
Mg26	-1.750020	-2.109328	2.311114

@mg26-isomer04 bp86/6-31G(d) Etot=-5202.495114 Eb=-16.48

Mg1	2.290557	-3.586263	-0.648899
Mg2	0.705785	1.591100	-3.389471
Mg3	1.699927	-1.240126	-2.913806
Mg4	1.456743	-0.150604	0.036642
Mg5	-4.974481	-0.373134	0.681758
Mg6	3.450680	1.326165	-1.858904
Mg7	0.419290	-2.398115	1.822538
Mg8	-0.461389	0.467754	2.891504

Mg9	-4.164864	0.495426	-2.067785
Mg10	1.641118	2.531062	2.215301
Mg11	-3.364937	1.236618	2.568720
Mg12	-3.418738	-2.297062	-1.019322
Mg13	0.911665	2.842456	-0.695271
Mg14	-4.100126	2.667817	0.043245
Mg15	-1.310277	3.048614	1.332143
Mg16	2.407053	-0.232353	3.104096
Mg17	-1.856510	2.536409	-1.995276
Mg18	3.839537	3.631528	0.329359
Mg19	-1.527294	0.152880	-0.042974
Mg20	-0.397440	-2.581346	-1.233750
Mg21	-1.821858	-4.351779	0.658943
Mg22	-1.374777	-0.507774	-3.076546
Mg23	3.791830	-2.271697	1.513450
Mg24	4.397435	0.735541	0.999587
Mg25	-2.600225	-1.770832	2.123936
Mg26	4.361295	-1.502284	-1.379219

@mg26-isomer05 bp86/6-31G(d) Etot=-5202.494940 Eb=-16.48

Mg1	-4.811457	0.765655	-0.467637
Mg2	-3.273044	3.262944	-0.629577
Mg3	1.293310	-0.534045	3.087147
Mg4	-0.339110	3.143683	0.531079
Mg5	-1.761845	-0.601455	3.391683
Mg6	-1.473484	0.300326	0.127724
Mg7	-3.921953	-1.816184	-1.693222
Mg8	-2.489386	-3.963888	-0.152756
Mg9	-0.420289	-2.321642	1.348595
Mg10	-3.360505	1.706654	2.050160
Mg11	0.699575	-4.312398	-0.576978
Mg12	-3.813760	-1.545555	1.391295
Mg13	4.630978	1.912472	-0.050225
Mg14	-0.384894	1.972140	3.255603
Mg15	2.343601	2.313573	1.925841
Mg16	2.206674	-2.143918	-2.181684
Mg17	4.136421	-0.187534	2.077653
Mg18	-0.822025	3.182097	-2.431317
Mg19	2.682830	-2.754115	1.069146
Mg20	-0.867550	-1.975999	-1.998753
Mg21	1.509650	0.001378	0.010034
Mg22	4.729364	-1.285363	-0.637669
Mg23	3.522563	0.623159	-2.536555
Mg24	0.521164	0.590950	-2.896560
Mg25	2.072288	2.950705	-1.334613
Mg26	-2.609115	0.716360	-2.678411

@mg26-isomer06 bp86/6-31G(d) Etot=-5202.494594 Eb=-16.47

Mg1	2.339874	-1.854911	2.290188
Mg2	-4.139238	-1.393552	-0.734581
Mg3	-4.643024	1.373865	0.629602
Mg4	-0.288957	3.650361	1.960942
Mg5	3.883242	-0.862490	-2.441471
Mg6	-0.721049	-2.554812	-1.006997
Mg7	0.864320	1.020412	2.756169
Mg8	4.643362	-1.483354	0.346794
Mg9	-4.113803	-0.996613	2.275426
Mg10	2.277303	1.555262	-3.011360
Mg11	0.738743	-1.078824	-3.139144
Mg12	-0.757861	-1.355221	2.309539
Mg13	4.218458	1.458233	-0.592482
Mg14	0.635822	2.722643	-0.687639
Mg15	1.482973	-0.113244	-0.114798
Mg16	-2.313899	-1.058796	-3.224013

Mg17	4.150450	0.629628	2.326141
Mg18	2.760098	3.085222	1.537063
Mg19	-1.455181	0.232782	-0.215345
Mg20	-2.380330	3.075771	-0.290928
Mg21	0.318305	-3.966605	1.389456
Mg22	-0.806018	1.596432	-3.043042
Mg23	-2.267192	1.444495	2.546390
Mg24	-2.770144	-3.373651	1.188900
Mg25	2.294232	-2.951772	-0.802593
Mg26	-3.950487	1.198739	-2.252217

@mg26-isomer07 bp86/6-31G(d) Etot=-5202.494297 Eb=-16.46

Mg1	-3.224490	2.025895	-2.291001
Mg2	-1.396561	-0.989842	3.296132
Mg3	1.338756	-1.737006	2.431989
Mg4	1.088195	2.544068	1.386654
Mg5	-3.780638	-2.644336	-0.134124
Mg6	3.534691	-2.000932	-2.038689
Mg7	4.953708	0.119460	-0.507758
Mg8	3.502973	0.514178	2.233262
Mg9	3.975983	-2.321173	1.036288
Mg10	-1.760117	1.939297	2.457803
Mg11	1.471086	3.648671	-1.515564
Mg12	-2.466264	-0.925651	-2.643955
Mg13	-1.361148	-3.609112	-1.643756
Mg14	-1.179250	-3.191801	1.287024
Mg15	0.545473	-1.514858	-2.702803
Mg16	1.622815	-0.032784	-0.165036
Mg17	-1.302931	3.257019	-0.359626
Mg18	1.414725	-3.292148	-0.305405
Mg19	2.845619	1.031358	-2.650422
Mg20	-4.096191	2.494366	0.592462
Mg21	3.877073	2.786962	-0.036608
Mg22	-1.317947	-0.167198	0.137544
Mg23	0.836326	0.938683	3.850995
Mg24	-4.879129	-0.050991	-1.008426
Mg25	-0.222413	1.433476	-2.619350
Mg26	-4.020345	-0.255603	1.912370

@mg26-isomer08 bp86/6-31G(d) Etot=-5202.493628 Eb=-16.45

Mg1	2.466187	-3.305995	-1.393309
Mg2	4.633271	0.395213	1.351910
Mg3	2.179276	-0.739298	2.873891
Mg4	0.774661	-2.942279	1.134326
Mg5	1.086589	-1.126288	-2.859299
Mg6	0.129984	1.361392	3.636916
Mg7	-2.371122	3.697833	-1.349764
Mg8	-4.212283	2.394694	0.723920
Mg9	3.872063	-2.508219	1.025581
Mg10	1.184934	3.637666	-1.049284
Mg11	-0.698113	-3.175835	-1.496883
Mg12	-3.793628	0.830686	-1.776612
Mg13	-0.593875	1.422386	-2.263831
Mg14	-1.498579	-0.516550	0.104640
Mg15	2.313227	2.387594	1.821374
Mg16	-2.735718	0.963038	2.823298
Mg17	-2.585084	-3.249236	1.210472
Mg18	4.075932	2.491439	-0.677314
Mg19	-0.733190	2.386827	0.955761
Mg20	4.033669	-0.653231	-1.527091
Mg21	1.403110	0.115061	-0.018941
Mg22	-0.843387	-1.348517	3.058608
Mg23	-4.576293	-0.696073	1.066690
Mg24	2.363961	1.583772	-2.878591

Mg25	-1.950993	-1.080652	-3.181944
Mg26	-3.924599	-2.325430	-1.314525

@mg26-isomer09 bp86/6-31G(d) Etot=-5202.493421 Eb=-16.44

Mg1	5.234660	-0.132366	0.211470
Mg2	-4.177522	-1.114491	-1.140073
Mg3	3.914395	0.071809	2.814268
Mg4	3.543519	2.302951	0.484446
Mg5	3.201020	-2.298840	0.925034
Mg6	-1.205007	-2.136431	-2.214174
Mg7	-2.671919	-3.564191	0.034885
Mg8	1.768468	-2.208859	-2.162585
Mg9	-2.714515	3.301454	0.876959
Mg10	0.273806	2.847500	0.665015
Mg11	-1.161960	1.244886	2.816860
Mg12	1.703270	1.989163	3.166443
Mg13	1.754484	2.820880	-2.012289
Mg14	-4.249607	1.931708	-1.243215
Mg15	-1.467194	0.167423	-0.119705
Mg16	3.578833	0.508425	-2.269485
Mg17	0.141028	-2.753253	0.511605
Mg18	-4.027687	0.647449	1.593214
Mg19	4.733189	-2.306739	-1.763517
Mg20	-4.858099	-2.254424	1.604317
Mg21	1.451276	0.043500	0.016439
Mg22	-2.744415	0.432301	-3.274303
Mg23	-1.949716	-1.690778	2.492541
Mg24	0.316077	0.371694	-3.036756
Mg25	-1.310136	2.812606	-1.928911
Mg26	0.923752	-1.033380	2.951518

@mg26-isomer10 bp86/6-31G(d) Etot=-5202.492291 Eb=-16.42

Mg1	-3.871707	-1.593410	-1.549102
Mg2	4.406424	-0.098258	1.752753
Mg3	1.614798	-0.861720	2.964147
Mg4	-4.871513	1.122345	-0.269263
Mg5	1.415294	0.200952	-0.011127
Mg6	-0.431585	2.670240	0.935099
Mg7	-2.994590	1.462126	2.120214
Mg8	-3.055414	1.201233	-2.642356
Mg9	-0.219385	1.405665	3.636122
Mg10	-3.071112	3.498015	-0.544618
Mg11	-0.974756	-2.709358	-1.864889
Mg12	-4.329813	-1.250595	1.573113
Mg13	4.488534	2.184420	-0.244103
Mg14	1.953711	-1.871456	-2.256665
Mg15	-1.529819	-1.199886	2.907077
Mg16	2.402663	2.162705	2.162786
Mg17	-0.295380	-0.028792	-3.073408
Mg18	-2.670004	-3.505639	0.570881
Mg19	-1.561225	-0.068340	-0.139182
Mg20	1.513583	-4.544815	-0.847798
Mg21	4.491550	-0.615771	-1.306035
Mg22	2.505442	1.349487	-2.653432
Mg23	0.213687	-2.563901	0.944188
Mg24	2.018207	3.594784	-0.634155
Mg25	-0.456093	2.726102	-2.148210
Mg26	3.308502	-2.666133	0.617964

@mg26-isomer11 bp86/6-31G(d) Etot=-5202.492036 Eb=-16.41

Mg1	-1.061603	3.581705	-0.180260
Mg2	-2.424092	-2.541949	2.262999
Mg3	3.952404	1.624833	1.754892
Mg4	-2.244784	-1.626945	-2.443540

Mg5	3.953894	-1.644843	1.744183
Mg6	2.436817	-3.695666	0.026038
Mg7	-1.115615	-0.015381	3.154763
Mg8	-1.213935	-0.001662	0.030550
Mg9	-4.018773	-0.008299	1.631858
Mg10	2.707972	0.015584	-3.153956
Mg11	1.978586	-0.015304	3.358173
Mg12	0.581035	-2.255597	1.981356
Mg13	2.436591	3.700230	0.059850
Mg14	0.777594	1.973936	-1.925059
Mg15	-4.650037	0.005453	-1.406393
Mg16	-2.421845	2.520949	2.283435
Mg17	0.778743	-1.958270	-1.952266
Mg18	4.327589	1.610219	-1.209552
Mg19	4.331466	-1.592751	-1.220016
Mg20	-1.059212	-3.573302	-0.211396
Mg21	-2.244567	1.649967	-2.426297
Mg22	-0.184254	0.019995	-3.966798
Mg23	-4.013875	-2.637403	-0.177228
Mg24	-4.014649	2.638627	-0.153547
Mg25	1.823244	-0.006173	0.146724
Mg26	0.581304	2.232050	1.991488

@mg26-isomer12 bp86/6-31G(d) Etot=-5202.490941 Eb=-16.38

Mg1	-1.490169	-0.471073	-0.106063
Mg2	-0.489209	2.268484	-0.766239
Mg3	-0.967156	-1.551949	2.768693
Mg4	4.214595	-1.807398	1.247254
Mg5	-3.995952	-1.915696	-1.224789
Mg6	4.595990	2.565387	-0.452793
Mg7	-0.417200	1.427429	-3.610992
Mg8	-4.934702	0.650779	0.205581
Mg9	-1.055211	3.877594	1.728463
Mg10	1.180753	-3.361610	1.354733
Mg11	-2.147461	-3.588015	0.631204
Mg12	0.364315	1.325316	2.475634
Mg13	4.277780	-0.265537	-1.428300
Mg14	-3.926820	-1.605841	1.887797
Mg15	1.472708	-0.286249	0.035192
Mg16	1.455295	-0.906096	-2.977472
Mg17	-3.226724	1.131559	-2.198952
Mg18	2.246479	1.978012	-2.234529
Mg19	0.017110	-3.004377	-1.351639
Mg20	-3.490180	3.279827	0.133787
Mg21	-1.596264	-1.275287	-3.165031
Mg22	3.038109	-3.057221	-1.092818
Mg23	3.612075	1.119435	1.954994
Mg24	1.976226	-1.119236	3.159803
Mg25	-2.644415	1.181836	2.273455
Mg26	1.930028	3.409927	0.753027

@mg26-isomer13 bp86/6-31G(d) Etot=-5202.490324 Eb=-16.37

Mg1	-3.094159	-1.223184	-2.259427
Mg2	-4.500120	1.235642	-1.152777
Mg3	-2.377873	1.592255	-3.235379
Mg4	-0.268814	2.834821	1.112714
Mg5	-1.408179	0.118026	-0.063118
Mg6	1.431722	-1.560260	2.705382
Mg7	4.859814	-0.920191	-1.032730
Mg8	2.516359	3.631867	-0.095219
Mg9	2.202276	1.624374	2.565722
Mg10	4.276313	-0.642635	2.057551
Mg11	3.295212	-2.992324	0.571511
Mg12	-1.614966	-2.145312	2.338697

Mg13	-2.665869	-3.478342	-0.327547
Mg14	0.009292	-0.267325	-2.755829
Mg15	-2.506071	3.453279	-0.832634
Mg16	1.556079	0.154981	-0.010834
Mg17	-0.645721	-3.138282	-2.698753
Mg18	4.716881	1.795534	0.363251
Mg19	-0.701720	0.671175	3.087324
Mg20	0.306033	-2.783572	0.077631
Mg21	-3.332161	1.845127	1.639921
Mg22	-4.271190	-1.153836	0.740959
Mg23	-3.628683	-0.328744	3.631793
Mg24	2.377459	-2.124927	-2.272268
Mg25	0.250599	2.548172	-1.860172
Mg26	3.217485	1.253681	-2.295768

@mg26-isomer14 bp86/6-31G(d) Etot=-5202.489687 Eb=-16.35

Mg1	2.673479	2.378308	1.604198
Mg2	0.180968	3.346681	-0.103213
Mg3	1.878539	-2.750107	-1.648340
Mg4	0.368210	-0.993083	-3.661243
Mg5	-1.133843	-2.106229	-1.370443
Mg6	-0.903437	-1.863905	1.919437
Mg7	4.837464	1.222855	-0.283353
Mg8	-0.213330	2.733105	2.715724
Mg9	-4.627792	1.291031	-0.843117
Mg10	4.041691	-0.280239	2.201764
Mg11	-4.162461	-1.655311	-1.337791
Mg12	-1.449608	0.591825	0.109276
Mg13	1.393128	-0.090543	-0.011139
Mg14	4.426015	-1.817327	-0.420375
Mg15	-2.476051	3.127557	-1.595709
Mg16	-3.051859	-3.638472	0.679427
Mg17	-2.432166	0.297734	-2.908223
Mg18	2.879808	2.958511	-1.547493
Mg19	1.154567	0.022427	3.099454
Mg20	-1.937811	0.484098	3.362489
Mg21	-3.195418	2.648231	1.450103
Mg22	0.288373	1.691180	-2.578560
Mg23	3.074571	0.025400	-2.552562
Mg24	-4.063279	-0.702507	1.566301
Mg25	0.144735	-4.240678	0.445166
Mg26	2.305508	-2.680541	1.708222

@mg26-isomer15 bp86/6-31G(d) Etot=-5202.489446 Eb=-16.35

Mg1	0.732066	0.193927	2.923163
Mg2	2.373157	-2.355171	-2.374218
Mg3	-3.878512	-2.026514	-1.520508
Mg4	-0.808153	-2.470442	-2.474359
Mg5	4.710624	1.711655	0.000032
Mg6	-0.597037	2.915632	2.898961
Mg7	-0.807862	-2.471133	2.473739
Mg8	-1.222561	-0.693555	-0.000057
Mg9	4.359487	-1.724418	-0.000461
Mg10	3.858206	0.195076	-2.356686
Mg11	-3.878377	-2.026927	1.520298
Mg12	-4.354691	0.587554	0.000266
Mg13	-3.335727	3.032767	1.524444
Mg14	2.249130	2.676058	-1.678656
Mg15	-2.322692	0.369626	2.619162
Mg16	0.852413	-3.257363	-0.000481
Mg17	2.249340	2.675440	1.679269
Mg18	-0.597424	2.916597	-2.898138
Mg19	2.373553	-2.356025	2.373369
Mg20	-3.336101	3.033258	-1.523576

Mg21	-0.490470	2.233881	0.000289
Mg22	0.731661	0.194882	-2.922996
Mg23	3.858570	0.194282	2.356444
Mg24	-2.134815	-3.855448	-0.000423
Mg25	1.739245	-0.064027	-0.000014
Mg26	-2.323031	0.370391	-2.618865

@mg26-isomer16 bp86/6-31G(d) Etot=-5202.488516 Eb=-16.32

Mg1	1.310099	-0.051112	-0.064627
Mg2	2.196898	2.291346	-2.008129
Mg3	-1.666909	0.056092	0.073090
Mg4	2.452445	-3.494391	1.134568
Mg5	4.345604	-2.306209	-0.821535
Mg6	-2.173817	3.089806	0.996016
Mg7	0.847695	3.290472	0.640743
Mg8	-1.691248	-1.329660	3.230262
Mg9	-3.629546	0.934119	2.444919
Mg10	3.838077	3.686271	0.232888
Mg11	0.285845	-0.101326	-3.251865
Mg12	-3.471967	-2.208068	0.854062
Mg13	2.828478	1.512474	2.238312
Mg14	1.278259	-1.255181	2.933310
Mg15	4.195528	-1.183951	1.958788
Mg16	-0.376806	-2.715719	0.766051
Mg17	1.334066	-2.690405	-1.796360
Mg18	-4.498140	-1.157496	-1.772009
Mg19	-1.625396	-2.197570	-2.126121
Mg20	-0.252830	1.328661	2.668782
Mg21	-0.760636	2.286830	-1.740529
Mg22	3.286854	-0.495310	-2.858460
Mg23	-4.062296	1.699172	-0.838606
Mg24	4.390767	0.784865	-0.357345
Mg25	-5.703893	-0.280306	0.844297
Mg26	-2.677129	0.506598	-3.380502

@mg26-isomer17 bp86/6-31G(d) Etot=-5202.488305 Eb=-16.32

Mg1	-0.692496	-1.045133	3.643102
Mg2	1.537959	0.139384	-0.032528
Mg3	1.499834	3.311938	0.159150
Mg4	-1.309993	-1.969854	-1.975089
Mg5	-4.501803	1.008725	0.490882
Mg6	-1.451263	0.180901	0.170469
Mg7	-1.659824	3.292170	0.957647
Mg8	-3.751405	3.447554	-1.132434
Mg9	-3.319583	-1.756215	1.973536
Mg10	2.239804	1.715707	-2.586202
Mg11	-2.435711	-3.958513	0.088424
Mg12	1.643710	-1.692598	-2.496333
Mg13	-0.301189	0.315981	-3.588499
Mg14	0.018085	-2.307090	1.064561
Mg15	-3.178778	0.687535	-2.378091
Mg16	-4.225206	-1.752966	-0.936851
Mg17	4.333398	-0.501533	-1.752570
Mg18	-0.744724	2.577305	-1.846945
Mg19	3.320745	1.888792	2.215199
Mg20	0.730805	-4.285377	-0.988642
Mg21	2.225588	-0.955099	2.791708
Mg22	-2.646837	1.101462	2.854156
Mg23	4.805400	-0.488929	1.178651
Mg24	0.334664	1.617832	2.565678
Mg25	4.366631	2.248967	-0.512750
Mg26	3.162189	-2.820947	0.073771

@mg26-isomer18 bp86/6-31G(d) Etot=-5202.487735 Eb=-16.31

Mg1	-0.469559	2.773683	-2.552147
Mg2	-2.455551	0.591633	-2.799444
Mg3	-4.744884	1.233719	-0.751764
Mg4	-3.831550	2.134624	1.977414
Mg5	4.462912	-1.773022	-0.165262
Mg6	0.965185	-0.980014	3.575495
Mg7	3.154802	2.898521	1.255560
Mg8	-2.985501	-3.795328	-0.023556
Mg9	-4.186121	-1.578302	-1.613622
Mg10	4.939704	1.246011	-0.319495
Mg11	0.714707	0.078969	-3.086089
Mg12	2.105331	-2.741731	1.366426
Mg13	-3.905435	-1.051818	1.429096
Mg14	0.803798	1.856531	2.873014
Mg15	1.390757	0.017588	0.054057
Mg16	0.101889	-4.345384	-0.221211
Mg17	1.977110	-2.620763	-1.809171
Mg18	-1.750509	0.386701	3.274272
Mg19	0.257939	3.250349	0.294125
Mg20	-1.048231	-1.912231	-1.716759
Mg21	3.549691	0.016539	2.203102
Mg22	-0.886988	-1.995934	1.498174
Mg23	-1.509008	0.693195	0.146583
Mg24	-2.770043	3.502813	-0.544342
Mg25	3.659983	-0.266192	-2.578957
Mg26	2.459569	2.379842	-1.765499

@mg26-isomer19 bp86/6-31G(d) Etot=-5202.487656 Eb=-16.30

Mg1	-0.000969	3.521279	-1.695686
Mg2	2.117188	3.253643	0.840192
Mg3	0.436626	0.703137	-2.700184
Mg4	4.607829	-1.395247	0.617123
Mg5	-2.211360	0.429809	2.856354
Mg6	1.469756	0.306497	0.112884
Mg7	0.587840	1.672347	3.083481
Mg8	-3.229095	-3.300852	-0.531279
Mg9	-3.151748	4.228968	-0.511612
Mg10	-1.510432	-2.610458	2.029516
Mg11	-1.028227	2.455757	0.835413
Mg12	1.635924	-2.303653	1.559658
Mg13	0.293877	-1.069221	3.928496
Mg14	-4.315074	-1.339361	1.498064
Mg15	-4.161012	1.542207	0.586075
Mg16	1.204495	-2.153044	-3.094049
Mg17	3.589822	-0.424460	-2.073842
Mg18	3.023366	-3.302435	-1.009605
Mg19	2.884281	2.489865	-1.977330
Mg20	-1.353664	-0.449247	-0.057750
Mg21	-0.098926	-3.389688	-0.710840
Mg22	3.214356	0.329329	2.622055
Mg23	4.644648	1.611656	0.241512
Mg24	-2.472059	1.593295	-2.115971
Mg25	-4.388728	-0.693996	-1.513094
Mg26	-1.788713	-1.706126	-2.819581

@mg26-isomer20 bp86/6-31G(d) Etot=-5202.487270 Eb=-16.29

Mg1	-4.317546	-0.287405	0.090884
Mg2	-2.711895	-2.322598	1.929467
Mg3	-1.272629	2.048319	-0.218708
Mg4	1.820281	-2.782356	-0.489331
Mg5	-1.071642	-0.847738	-0.165645
Mg6	0.334959	0.502305	-2.680192
Mg7	-0.344948	-2.414839	-2.686294
Mg8	-1.109537	0.571150	2.691118

Mg9	4.918159	0.581907	1.401294
Mg10	-3.582220	2.307479	1.590072
Mg11	-4.090114	2.327917	-1.515533
Mg12	-1.516389	2.794280	-3.130249
Mg13	0.386749	-2.037497	2.227975
Mg14	3.447686	2.997845	0.900736
Mg15	4.646865	-1.590683	-0.702377
Mg16	4.006435	1.255020	-1.573502
Mg17	2.819300	-1.244939	-3.023171
Mg18	-3.417384	-2.841940	-1.192537
Mg19	3.478210	-1.896258	2.049667
Mg20	1.635866	0.296384	0.176564
Mg21	1.235851	3.070219	-1.299105
Mg22	-0.871659	-3.941875	0.028681
Mg23	-4.184480	-0.081706	3.204833
Mg24	2.039228	0.676364	3.128062
Mg25	-2.736227	-0.151579	-2.664340
Mg26	0.457080	3.012226	1.921633

@mg26-isomer21 bp86/6-31G(d) Etot=-5202.486776 Eb=-16.28

Mg1	4.073943	0.199000	1.607468
Mg2	-0.680995	-2.265364	-1.820777
Mg3	-0.948970	2.606694	2.495986
Mg4	-2.214541	-0.120896	-3.331160
Mg5	-4.174164	1.383965	-1.517472
Mg6	2.398770	2.706478	2.477851
Mg7	0.819834	0.247005	2.896839
Mg8	2.354037	-2.419313	-2.333725
Mg9	3.954352	2.763421	-0.069421
Mg10	0.703704	2.625240	-0.032634
Mg11	-0.676732	-2.199301	1.935686
Mg12	0.846110	0.137159	-2.911921
Mg13	-4.047465	-1.565302	1.479337
Mg14	1.406505	-0.539466	0.006050
Mg15	-2.258104	0.035322	3.269021
Mg16	2.380524	-2.304793	2.416577
Mg17	-3.984940	-1.671828	-1.494501
Mg18	1.166311	-3.868807	0.089308
Mg19	-1.503792	0.316355	0.023393
Mg20	-4.247167	1.479449	1.447838
Mg21	4.160867	-2.470387	0.042502
Mg22	-2.465372	-3.792879	0.102144
Mg23	-0.980809	2.473823	-2.531066
Mg24	4.038160	0.136435	-1.638237
Mg25	2.362982	2.645339	-2.563485
Mg26	-2.483048	3.462651	-0.045601

@mg26-isomer22 bp86/6-31G(d) Etot=-5202.486704 Eb=-16.28

Mg1	-1.779578	3.526066	1.423030
Mg2	1.189801	0.872037	-0.429493
Mg3	1.530856	-1.005419	3.699955
Mg4	1.187840	3.613450	0.870929
Mg5	4.346051	0.076016	-0.567370
Mg6	2.178821	-1.195000	-2.407376
Mg7	2.968071	1.291517	2.094082
Mg8	-0.857080	2.920697	-1.508119
Mg9	3.994226	3.093952	-0.174701
Mg10	-0.148531	1.247889	2.524186
Mg11	-3.664803	-2.265498	-1.498001
Mg12	3.921664	-3.032515	-0.560276
Mg13	-1.505950	-3.421141	0.235839
Mg14	-3.820441	2.728187	-0.524943
Mg15	-3.286611	0.910333	2.199016
Mg16	-5.010473	0.056417	-0.274033

Mg17	2.882602	1.997024	-2.719094
Mg18	0.104033	0.836489	-3.434921
Mg19	-2.866813	0.612900	-2.589289
Mg20	-1.354424	-1.552781	2.891509
Mg21	-1.556683	-0.097995	0.031004
Mg22	1.166692	-3.963480	-1.343295
Mg23	-4.000903	-2.106231	1.566377
Mg24	4.088694	-1.525938	2.037044
Mg25	1.077848	-1.800834	0.839490
Mg26	-0.784906	-1.816142	-2.381551

@mg26-isomer23 bp86/6-31G(d) Etot=-5202.486638 Eb=-16.28

Mg1	2.606068	3.375105	1.512345
Mg2	-1.570106	-2.143436	2.406427
Mg3	1.554981	-2.142132	2.405100
Mg4	-1.573121	-0.182022	0.000030
Mg5	0.005318	1.543754	-2.143165
Mg6	-2.934704	0.694233	2.634167
Mg7	2.940942	0.683412	2.635194
Mg8	-4.527604	-1.573945	1.510702
Mg9	-2.931301	0.692500	-2.634867
Mg10	1.576066	-0.181194	-0.000101
Mg11	4.443756	1.263192	0.000848
Mg12	-2.591093	3.381981	1.507939
Mg13	-4.526618	-1.572425	-1.509412
Mg14	-0.007853	-3.172981	-0.000615
Mg15	4.518779	-1.594985	1.510070
Mg16	-1.572544	-2.147902	-2.406338
Mg17	0.008848	3.769892	0.000700
Mg18	-2.996733	-3.610370	0.001038
Mg19	0.002876	1.543847	2.143415
Mg20	-4.434169	1.281241	-0.000739
Mg21	4.519535	-1.595091	-1.510972
Mg22	2.975874	-3.619406	-0.001453
Mg23	2.943466	0.685942	-2.634728
Mg24	2.606568	3.375494	-1.507953
Mg25	1.553401	-2.137656	-2.405308
Mg26	-2.590633	3.382953	-1.512324

@mg26-isomer24 bp86/6-31G(d) Etot=-5202.485284 Eb=-16.25

Mg1	-4.309812	2.435367	0.521778
Mg2	-1.153702	0.102806	-3.560814
Mg3	-0.308861	-0.043276	2.504857
Mg4	2.126973	-3.793576	-0.385087
Mg5	1.901948	0.495139	-3.121217
Mg6	4.131224	-2.065639	0.968717
Mg7	-0.169949	2.637377	-2.457837
Mg8	-2.717783	-2.071960	-2.139947
Mg9	-1.567742	0.364909	-0.417730
Mg10	0.527548	-2.185377	-2.494476
Mg11	-3.253818	2.151205	-2.335953
Mg12	-3.516364	-0.086242	2.138428
Mg13	2.835895	0.234353	2.423235
Mg14	1.426729	-2.580092	2.346017
Mg15	-1.949221	2.543132	2.427692
Mg16	1.381133	-0.221903	-0.196847
Mg17	3.605962	-1.733036	-1.988037
Mg18	2.841026	2.987072	-1.637214
Mg19	4.480138	0.694542	-0.410202
Mg20	-1.868534	-2.575498	2.910481
Mg21	1.079115	2.581388	3.273440
Mg22	-4.739647	-0.192586	-0.861840
Mg23	-3.898756	-2.668614	0.586755
Mg24	3.457174	3.006965	1.304660

Mg25	0.392840	2.760201	0.440253
Mg26	-0.733516	-2.776658	0.160884

@mg26-isomer25 bp86/6-31G(d) Etot=-5202.485247 Eb=-16.25

Mg1	3.612027	-3.078419	0.540396
Mg2	0.395098	-2.662068	-0.419889
Mg3	-2.119383	-4.473064	-0.114859
Mg4	-3.765036	2.724327	1.040493
Mg5	-1.643122	2.391366	3.225512
Mg6	0.442236	-0.765383	-2.842916
Mg7	-0.052675	-0.015528	2.617711
Mg8	-3.425053	0.023684	2.266355
Mg9	-2.215733	0.482279	-3.490527
Mg10	-2.790624	2.814554	-1.709215
Mg11	-2.276567	-2.217235	-2.163396
Mg12	-4.451935	0.363734	-1.049638
Mg13	1.712856	2.397342	2.290615
Mg14	1.499770	0.302308	-0.054633
Mg15	-4.170762	-2.250340	0.333262
Mg16	3.100422	-2.017021	-2.192802
Mg17	0.182047	2.191121	-2.412120
Mg18	-1.594246	-2.461510	2.087828
Mg19	3.492501	-0.386809	2.195480
Mg20	3.220843	1.136463	-2.338850
Mg21	4.348003	2.068435	0.570564
Mg22	-0.657001	2.946010	0.453269
Mg23	5.079643	-0.574356	-0.503092
Mg24	1.390579	-2.640619	2.479670
Mg25	-1.449869	-0.026031	-0.244399
Mg26	2.135982	3.726761	-0.564818

@mg26-isomer26 bp86/6-31G(d) Etot=-5202.484290 Eb=-16.22

Mg1	-1.815111	-1.225713	-2.827287
Mg2	-2.507204	1.728770	-2.321131
Mg3	-2.507162	1.728450	2.321340
Mg4	1.710186	0.125802	0.000029
Mg5	1.251358	-1.544924	2.539413
Mg6	-1.214135	-0.143603	-0.000045
Mg7	4.873348	0.977962	0.000052
Mg8	-4.450664	-0.545769	-1.528471
Mg9	-3.246215	-2.891671	-0.000083
Mg10	-0.681075	-3.611901	1.427339
Mg11	-4.450692	-0.545916	1.528459
Mg12	-2.021610	3.650553	0.000246
Mg13	-1.815092	-1.226138	2.827035
Mg14	0.472452	2.679901	-1.483911
Mg15	3.011741	1.149954	2.550693
Mg16	-0.681151	-3.611575	-1.427773
Mg17	0.472483	2.679794	1.484302
Mg18	4.129830	-1.572318	1.540636
Mg19	3.164678	3.348759	0.000209
Mg20	0.151753	0.992483	3.805213
Mg21	0.151730	0.993033	-3.805163
Mg22	1.251321	-1.544527	-2.539611
Mg23	2.105933	-3.254271	-0.000219
Mg24	-4.498238	2.084701	0.000135
Mg25	4.129810	-1.572118	-1.540853
Mg26	3.011724	1.150282	-2.550554

@mg26-isomer27 bp86/6-31G(d) Etot=-5202.483726 Eb=-16.21

Mg1	-4.147405	0.675736	-1.846253
Mg2	-2.192359	-0.875172	3.227159
Mg3	3.630671	1.164317	2.334438
Mg4	0.667124	0.249989	2.933970

Mg5	-1.873747	1.839650	2.126083
Mg6	-2.479020	-3.060103	1.086164
Mg7	-1.227384	4.283240	0.537004
Mg8	3.583477	-2.671155	-0.898586
Mg9	5.073040	-0.338578	0.263086
Mg10	2.972687	-1.843578	2.073690
Mg11	1.616611	0.049347	-0.104964
Mg12	3.785590	2.313543	-0.613971
Mg13	0.668265	-3.011404	0.109578
Mg14	-4.286664	-0.103710	1.176078
Mg15	-1.293128	-0.469007	0.116687
Mg16	-4.174207	-2.173668	-1.168800
Mg17	0.080746	-2.692002	2.963742
Mg18	-1.516570	-3.274285	-1.857326
Mg19	1.198191	2.809143	1.463894
Mg20	1.157586	3.621207	-1.340988
Mg21	1.038674	1.128024	-2.904871
Mg22	3.723116	-0.153599	-2.451564
Mg23	1.073397	-1.883733	-2.738395
Mg24	-3.932726	2.838015	0.237358
Mg25	-1.642175	-0.564204	-3.127015
Mg26	-1.503791	2.141988	-1.596198

@mg26-isomer28 bp86/6-31G(d) Etot=-5202.483432 Eb=-16.20

Mg1	-3.733513	-2.612772	-0.435566
Mg2	-2.623931	1.589551	2.384906
Mg3	0.515421	2.745827	-1.863721
Mg4	-1.619373	1.043282	-3.236202
Mg5	1.574757	-3.186363	-2.233358
Mg6	-2.560789	3.082921	-0.947571
Mg7	1.112561	-0.223767	-2.800926
Mg8	0.201080	0.326776	2.798445
Mg9	-4.669132	-0.440790	1.418992
Mg10	0.849941	-2.686059	2.887525
Mg11	-1.408376	-1.874042	-2.299774
Mg12	-0.081779	3.014607	1.234839
Mg13	0.525741	-1.783515	0.145752
Mg14	-2.007582	-1.708471	2.138879
Mg15	-4.951347	2.384683	0.513003
Mg16	3.533545	1.695755	-2.235304
Mg17	2.969234	-3.628944	0.470537
Mg18	-1.180588	-4.175628	-0.168043
Mg19	-1.383299	0.411125	-0.169871
Mg20	3.794014	-1.214330	-1.223982
Mg21	1.686356	0.816484	0.056080
Mg22	2.913820	3.745588	0.079736
Mg23	3.263623	-0.957786	1.934243
Mg24	-4.169033	0.242412	-1.560977
Mg25	4.767831	1.298954	0.482574
Mg26	2.680816	2.094502	2.629782

@mg26-isomer29 bp86/6-31G(d) Etot=-5202.482986 Eb=-16.19

Mg1	3.156316	-0.509444	-2.722699
Mg2	0.026963	3.616013	2.305285
Mg3	-4.060092	-0.674942	1.949152
Mg4	4.853500	0.814300	-0.512311
Mg5	-2.700800	3.624799	0.647612
Mg6	4.236297	-2.182014	0.240473
Mg7	2.161840	-2.180697	2.804821
Mg8	2.112585	-3.233693	-1.597430
Mg9	-4.387680	-1.769440	-0.848271
Mg10	2.903552	2.497307	-2.017408
Mg11	0.122976	2.519147	-0.394312
Mg12	-1.988356	1.396583	2.514695

Mg13	-2.891093	-3.319280	1.251475
Mg14	-1.730102	-3.058686	-1.588151
Mg15	-2.465969	2.766274	-2.284132
Mg16	-1.365390	-0.236300	-0.026902
Mg17	3.975718	0.066147	2.246785
Mg18	2.875853	2.679322	1.154807
Mg19	1.635197	-0.212888	-0.170627
Mg20	0.171352	-2.981489	0.747750
Mg21	-4.334886	1.274647	-0.468050
Mg22	0.231285	-1.384458	-2.989322
Mg23	0.972919	0.719354	2.707598
Mg24	0.189403	1.492132	-3.149766
Mg25	-1.122574	-1.530250	3.017144
Mg26	-2.578816	-0.192444	-2.818216

@mg26-isomer30 bp86/6-31G(d) Etot=-5202.482442 Eb=-16.18

Mg1	-1.600922	-1.042757	3.010236
Mg2	-4.322069	-1.915776	-1.133260
Mg3	1.277339	1.177347	-0.604346
Mg4	-2.752614	1.844945	1.942194
Mg5	-0.045230	-3.337736	1.570749
Mg6	-3.338094	4.022727	-0.016578
Mg7	4.444844	1.376807	-0.563499
Mg8	2.790167	4.068069	-0.348579
Mg9	-1.237943	-0.304618	0.103550
Mg10	4.616930	-1.843764	-0.856153
Mg11	1.478902	-0.786336	2.209136
Mg12	-1.439073	2.331949	-1.649496
Mg13	0.324891	-1.824529	-3.549301
Mg14	-0.154135	3.583511	0.799729
Mg15	1.439806	-1.972679	-0.763634
Mg16	2.984466	-0.202243	-2.750487
Mg17	-4.212721	1.173523	-0.874234
Mg18	4.447609	-0.535566	1.857419
Mg19	-1.424485	-3.024409	-1.343153
Mg20	0.358579	1.102230	-3.637450
Mg21	-4.364722	-0.646684	1.596946
Mg22	-2.260298	-0.371070	-2.824597
Mg23	0.006093	1.652728	3.055065
Mg24	3.156787	-3.279855	1.468317
Mg25	2.877709	2.053770	2.025681
Mg26	-3.051817	-3.299583	1.275745

@mg26-isomer31 bp86/6-31G(d) Etot=-5202.478205 Eb=-16.08

Mg1	3.883995	1.208981	-1.922105
Mg2	-1.125380	0.128973	0.108240
Mg3	1.530097	0.770720	2.968304
Mg4	5.136336	-1.083730	-0.506182
Mg5	1.014727	-2.266660	2.217636
Mg6	-2.318220	0.442903	-2.703214
Mg7	-1.202087	3.267476	-1.666245
Mg8	-0.119657	-1.588171	-3.284790
Mg9	1.819960	-0.250178	0.047825
Mg10	-4.553582	-3.635771	0.190671
Mg11	-4.532278	-0.717074	-0.741618
Mg12	2.281468	3.758640	-1.427386
Mg13	2.798902	-1.694362	-2.433519
Mg14	-1.003152	-0.735897	3.679772
Mg15	-2.569501	-2.593282	-1.933531
Mg16	3.857224	1.924522	1.013452
Mg17	-1.197620	2.109547	3.063405
Mg18	0.169320	-2.902306	-0.589542
Mg19	0.544977	2.658688	0.735765
Mg20	-2.577577	3.657718	0.967357

Mg21	3.257307	-3.274824	0.329778
Mg22	0.793712	1.173201	-2.479021
Mg23	-4.081891	2.220333	-1.058105
Mg24	-3.643958	0.731128	1.746780
Mg25	4.019814	-0.946945	2.234474
Mg26	-2.182937	-2.363630	1.441798

@mg26-isomer32 bp86/6-31G(d) Etot=-5202.476831 Eb=-16.04

Mg1	1.722634	-2.604673	2.085335
Mg2	0.888750	0.825646	-3.805916
Mg3	-1.028155	-1.811699	3.185647
Mg4	-2.243571	-2.661745	-1.457269
Mg5	1.202394	4.144029	-0.102747
Mg6	-2.227877	0.012776	-3.007696
Mg7	3.891783	-2.530350	-0.038215
Mg8	-4.589686	-0.788786	-1.197282
Mg9	-4.464950	1.150541	1.221574
Mg10	0.865578	-2.877909	-0.779006
Mg11	2.826197	2.164840	-1.812046
Mg12	4.841105	0.369239	-0.528738
Mg13	-2.020333	1.040857	2.941713
Mg14	0.311279	2.972932	2.465621
Mg15	1.210888	0.246702	2.948171
Mg16	-1.290190	-3.907778	1.140768
Mg17	3.251617	2.261923	1.313467
Mg18	-2.168602	3.213400	0.745645
Mg19	-0.562749	2.183674	-1.652521
Mg20	0.017303	-1.969294	-3.430256
Mg21	4.029968	-0.592201	2.241243
Mg22	1.438778	0.073641	-0.114120
Mg23	2.970340	-1.026797	-2.561267
Mg24	-1.431241	-0.169689	0.231546
Mg25	-3.780533	2.146342	-1.528568
Mg26	-3.660727	-1.865621	1.494917

@mg26-isomer33 bp86/6-31G(d) Etot=-5202.472172 Eb=-15.93

Mg1	-1.559091	-4.181156	1.091576
Mg2	4.900047	0.254161	0.683289
Mg3	0.302772	-2.627171	-0.734459
Mg4	-2.740634	0.890348	-2.976250
Mg5	-1.320632	0.090478	-0.032808
Mg6	5.077825	-0.815860	-2.100464
Mg7	-3.970098	1.372293	1.191019
Mg8	0.497389	1.096361	3.029336
Mg9	1.669034	-0.169720	0.429716
Mg10	0.270666	1.456790	-2.430362
Mg11	-0.283577	-1.728455	2.309027
Mg12	1.660211	-4.235819	1.633529
Mg13	-2.307872	0.242322	3.455406
Mg14	3.649079	-2.600551	-0.002674
Mg15	-3.483953	-1.749984	1.505012
Mg16	0.938651	2.772743	0.340120
Mg17	3.298647	1.949167	2.603933
Mg18	2.137013	-1.063073	-2.622232
Mg19	-1.920954	3.047061	-0.873157
Mg20	-2.691072	-2.717227	-1.312958
Mg21	-4.819952	2.534299	-1.538738
Mg22	-0.782853	-1.304841	-3.209910
Mg23	-1.578743	2.974850	2.146155
Mg24	4.510539	3.312578	0.285579
Mg25	-4.656047	-0.496620	-1.046233
Mg26	3.203609	1.697025	-1.823454

@mg26-isomer34 bp86/6-31G(d) Etot=-5202.468864 Eb=-15.85

Mg1	-0.127641	0.796202	-0.316502
Mg2	-1.887186	0.494959	-2.811971
Mg3	0.733442	2.352860	-2.735647
Mg4	0.335198	3.764706	0.111127
Mg5	1.026544	-0.743306	-2.881585
Mg6	2.973529	2.369867	0.021680
Mg7	0.957933	1.829812	2.470927
Mg8	-4.226914	1.531481	-0.633294
Mg9	-1.225102	-2.398523	-1.917292
Mg10	3.956893	0.794738	2.612271
Mg11	3.539474	0.975694	-2.594830
Mg12	-2.456046	-0.574536	0.514788
Mg13	1.400170	-3.391443	-1.154615
Mg14	5.126601	0.273019	-0.101734
Mg15	-3.129921	-3.488745	0.168601
Mg16	-1.992193	2.498097	1.531500
Mg17	1.626911	-1.122578	3.312087
Mg18	-1.178548	-0.131040	3.248846
Mg19	-5.275220	-1.439899	0.888632
Mg20	4.049331	-1.963947	-1.809220
Mg21	-4.250942	0.856955	2.567535
Mg22	-0.233733	-2.444760	1.234102
Mg23	-2.080812	3.314345	-1.639061
Mg24	2.158930	-0.713076	0.259582
Mg25	-4.233804	-1.348987	-1.985094
Mg26	4.413107	-2.091895	1.639168

@mg26-isomer35 bp86/6-31G(d) Etot=-5202.468090 Eb=-15.83

Mg1	-1.189436	0.299864	0.111544
Mg2	-1.182551	-2.779236	-0.635447
Mg3	-0.018302	3.265049	1.892022
Mg4	1.088504	2.838469	-0.935637
Mg5	1.684881	-0.103396	-1.071854
Mg6	-0.999805	0.508383	3.204076
Mg7	-3.285985	-4.623445	0.792885
Mg8	-0.469611	1.261409	-2.991781
Mg9	-1.899990	3.224511	-0.946656
Mg10	-4.073431	0.017382	2.458443
Mg11	0.087332	-1.692739	-3.137832
Mg12	-3.359163	2.090896	-3.365558
Mg13	1.911237	-3.109951	-1.037651
Mg14	4.733038	-0.809902	-1.225930
Mg15	4.960450	1.125123	1.256388
Mg16	3.110802	3.594234	1.202284
Mg17	-2.172140	-2.219381	2.441958
Mg18	-2.790198	-0.793440	-2.574978
Mg19	-2.876500	2.608742	1.849279
Mg20	3.719759	-1.646664	1.550040
Mg21	-4.040041	-1.725759	0.016283
Mg22	-4.182189	1.195691	-0.556540
Mg23	4.050466	2.164968	-1.406447
Mg24	0.622683	-1.830227	1.579578
Mg25	4.795322	-3.781853	-0.315179
Mg26	1.774868	0.921272	1.846710

@mg26-isomer36 bp86/6-31G(d) Etot=-5202.465771 Eb=-15.78

Mg1	-4.653241	-1.792452	1.226159
Mg2	0.116647	3.307038	0.722049
Mg3	2.602388	-0.738698	-2.116040
Mg4	3.259633	4.241412	-0.194893
Mg5	0.465693	-2.836991	0.148150
Mg6	-2.206602	-0.452371	2.386024
Mg7	0.266017	1.229866	2.930890
Mg8	-2.463559	2.522243	2.395657

Mg9	3.150272	-3.655826	-1.307023
Mg10	4.469022	1.415156	-0.418417
Mg11	-2.480093	-0.149626	-2.839801
Mg12	0.479875	-1.870409	3.032552
Mg13	1.631706	2.027537	-1.543253
Mg14	-2.950608	4.114607	-0.010330
Mg15	-3.668158	1.074305	-0.011220
Mg16	-1.352479	2.527854	-1.968946
Mg17	-2.429573	-2.430142	-0.807791
Mg18	-0.577622	0.132700	-0.235040
Mg19	-2.056860	-3.443268	1.960117
Mg20	2.190111	-0.271766	1.015846
Mg21	0.269373	0.602528	-3.793717
Mg22	3.009636	2.454065	2.162242
Mg23	4.953594	-1.619357	-0.072929
Mg24	3.147711	-3.181660	1.720447
Mg25	-0.002340	-2.112165	-2.733594
Mg26	-5.170543	-1.094578	-1.647139

@mg26-isomer37 bp86/6-31G(d) Etot=-5202.404278 Eb=-14.29

Mg1	0.261827	0.434214	0.250097
Mg2	1.158058	2.360123	-1.799252
Mg3	6.141693	0.896625	-1.223671
Mg4	2.484674	2.443622	1.102471
Mg5	0.542895	-0.814584	-2.521041
Mg6	-1.905300	-1.715081	-0.854634
Mg7	0.882423	-2.668577	0.008614
Mg8	2.750873	-3.049992	-2.270246
Mg9	3.127854	0.043220	-0.928350
Mg10	4.074629	3.118380	-1.398873
Mg11	-2.595354	1.010621	1.200064
Mg12	-3.948572	-1.898639	1.387845
Mg13	3.709410	-3.584336	0.597188
Mg14	-1.797149	1.435103	-1.939196
Mg15	-4.363852	-0.158008	-1.480767
Mg16	5.526409	2.608582	1.214921
Mg17	-0.930152	-1.492227	2.240533
Mg18	-5.652807	0.721998	1.507215
Mg19	2.310257	-0.881232	2.077161
Mg20	-7.014246	1.376805	-1.171071
Mg21	-6.597823	-1.836573	-0.106242
Mg22	-8.718022	0.073932	1.020858
Mg23	-4.293420	2.797383	-0.532233
Mg24	4.030513	1.321836	3.477430
Mg25	5.476380	-2.021354	-1.239431
Mg26	5.338802	-0.521842	1.380610

@mg27-isomer01 bp86/6-31G(d) Etot=-5402.604423 Eb=-16.79

Mg1	0.791825	-3.416341	0.547699
Mg2	2.018044	1.742619	2.613760
Mg3	-4.649163	0.834430	-0.134105
Mg4	3.682768	-2.935885	1.024574
Mg5	-3.707290	-0.396947	2.650494
Mg6	1.493767	-1.512622	2.818836
Mg7	2.035648	3.822439	0.094991
Mg8	-3.187454	-1.430394	-2.233462
Mg9	1.973460	-0.224222	-3.134643
Mg10	-0.835895	0.490827	3.075284
Mg11	1.480781	0.021331	-0.001472
Mg12	-0.915465	0.067533	-3.984950
Mg13	4.417764	2.161482	0.618270
Mg14	4.213958	-0.311969	2.200539
Mg15	-0.165466	-1.970068	-1.960247
Mg16	-0.006493	2.171808	-1.831527

Mg17	3.169846	2.253432	-2.104773
Mg18	4.508513	-0.504096	-1.033757
Mg19	-1.569112	-2.419995	2.207021
Mg20	-3.045953	1.560792	-2.659051
Mg21	-2.778709	3.476507	-0.513610
Mg22	-3.223994	2.439993	2.213999
Mg23	-2.100132	-3.762383	-0.538671
Mg24	-1.586388	0.069385	0.029084
Mg25	-0.448569	2.914866	1.304530
Mg26	-4.331631	-2.256527	0.509535
Mg27	2.765340	-2.885995	-1.778348

@mg27-isomer02 bp86/6-31G(d) Etot=-5402.604262 Eb=-16.79

Mg1	2.970913	-3.931810	-1.304149
Mg2	3.989310	-1.031939	-1.439532
Mg3	3.687263	-2.763363	1.268501
Mg4	1.224637	-1.842309	-2.488100
Mg5	4.366109	1.912077	-1.067403
Mg6	1.955669	1.025145	-2.923901
Mg7	4.122509	0.276783	1.594897
Mg8	-0.988227	-0.191288	-3.437613
Mg9	0.444039	-2.783223	0.342275
Mg10	1.398732	0.363399	0.066110
Mg11	-1.631914	-2.874865	-2.079194
Mg12	1.934372	3.673840	-1.296896
Mg13	1.570261	-1.382184	2.853267
Mg14	1.738959	1.614788	3.124429
Mg15	-2.827307	-3.624176	0.531444
Mg16	-0.674214	2.390454	-1.992417
Mg17	-1.516085	-0.156448	-0.230078
Mg18	-1.273752	-2.623148	2.835984
Mg19	-3.435851	1.181394	-2.376737
Mg20	-0.290022	2.843846	1.092535
Mg21	-4.250207	-1.545740	-1.165289
Mg22	-3.047125	3.520280	-0.419184
Mg23	-0.922192	0.313542	2.863695
Mg24	3.251775	3.313701	1.306517
Mg25	-3.663795	-0.945269	1.973600
Mg26	-5.013423	1.097404	0.156098
Mg27	-3.120434	2.169110	2.211140

@mg27-isomer03 bp86/6-31G(d) Etot=-5402.603956 Eb=-16.78

Mg1	2.186029	-3.459105	1.273440
Mg2	-0.629891	-2.384314	0.483822
Mg3	4.365771	2.050695	1.193334
Mg4	-2.197774	-2.179539	3.007195
Mg5	-0.519467	-0.824170	-2.664041
Mg6	4.029039	-2.727188	-0.861490
Mg7	-1.616837	0.491619	-0.084386
Mg8	0.816621	-1.313177	2.987484
Mg9	2.525535	-0.423297	-2.728927
Mg10	-4.624949	1.608840	-0.933635
Mg11	2.183654	3.881276	0.346899
Mg12	-3.469281	2.599200	1.628546
Mg13	-2.465217	1.437862	-3.015894
Mg14	-1.863925	-3.539162	-2.056509
Mg15	-3.613067	-1.153396	-1.802484
Mg16	-4.132256	-0.418198	1.457055
Mg17	3.776303	-0.899064	1.865402
Mg18	0.335831	2.247185	-1.942155
Mg19	3.385792	2.394498	-1.862534
Mg20	-2.423084	3.700825	-1.068830
Mg21	-1.359907	0.712085	3.019757
Mg22	4.989686	0.057046	-0.898826

Mg23	1.404694	-0.026481	0.060495
Mg24	-3.563656	-3.300027	0.503548
Mg25	-0.505292	3.000860	1.221144
Mg26	1.252839	-3.095124	-1.812538
Mg27	1.732810	1.560253	2.684127

@mg27-isomer04 bp86/6-31G(d) Etot=-5402.602532 Eb=-16.75

Mg1	-3.046661	3.620346	-0.741040
Mg2	-0.441117	2.779792	0.748474
Mg3	-4.671907	1.155451	-1.045876
Mg4	-3.369274	2.002637	1.813452
Mg5	1.445464	-0.128940	-0.006513
Mg6	-2.119722	-1.161358	2.917547
Mg7	-0.797052	1.454016	3.438050
Mg8	-1.590729	-0.009402	0.168074
Mg9	-3.454534	-1.555119	-1.859780
Mg10	-0.257839	-2.733308	1.018403
Mg11	-3.258107	-3.282870	0.804711
Mg12	4.005356	-0.265677	1.830200
Mg13	4.606610	2.604568	0.992183
Mg14	-1.599882	-4.002629	-1.537412
Mg15	1.047085	-0.832126	3.077036
Mg16	-2.053677	1.205773	-2.639417
Mg17	-0.418235	3.698341	-2.170262
Mg18	2.638501	-1.298262	-2.867091
Mg19	4.099383	0.919472	-1.463358
Mg20	2.015117	2.032839	2.392126
Mg21	1.664017	-3.603188	-1.231277
Mg22	1.194486	1.305053	-2.778716
Mg23	2.285052	3.340007	-0.697515
Mg24	-0.352812	-1.393826	-2.372522
Mg25	-4.685346	-0.730191	1.224682
Mg26	4.384005	-2.120614	-0.629785
Mg27	2.731818	-3.000786	1.615625

@mg27-isomer05 bp86/6-31G(d) Etot=-5402.602454 Eb=-16.75

Mg1	-0.345428	-0.023395	4.010724
Mg2	-3.116995	-0.493607	2.462154
Mg3	2.313008	-1.495011	2.714309
Mg4	3.313984	3.313062	0.644003
Mg5	2.242875	-3.120346	-1.953798
Mg6	-1.468211	0.348840	-0.015233
Mg7	-2.423938	-0.546420	-2.778559
Mg8	5.054833	1.983784	-1.300884
Mg9	1.615964	-3.941789	0.859556
Mg10	3.742925	-0.543040	-2.072983
Mg11	-1.553193	2.335956	2.379552
Mg12	4.326398	0.450321	1.281780
Mg13	-3.150423	-3.244130	1.007276
Mg14	-4.348686	1.987626	1.147724
Mg15	2.145350	2.152631	-2.252630
Mg16	-0.968729	2.240196	-2.575521
Mg17	0.688887	-0.465839	-2.905217
Mg18	-2.493901	3.900577	-0.220193
Mg19	-3.940381	1.918800	-1.877456
Mg20	-0.533199	-2.072941	1.872982
Mg21	0.375814	2.987602	0.081613
Mg22	-0.648270	-2.658691	-1.122992
Mg23	-4.493544	-0.699415	-0.383255
Mg24	-3.542454	-3.252263	-1.925261
Mg25	1.610080	1.631543	2.501326
Mg26	1.465843	-0.241984	0.054044
Mg27	4.131388	-2.452067	0.366940

@mg27-isomer06 bp86/6-31G(d) Etot=-5402.602216 Eb=-16.74

Mg1	2.196991	0.416985	-3.131012
Mg2	2.778460	3.017533	-1.676438
Mg3	-0.916892	-0.240181	-3.853578
Mg4	-3.446551	-0.293079	2.263763
Mg5	3.038144	0.273867	2.629545
Mg6	1.490744	0.114318	-0.022579
Mg7	0.714768	-2.086099	-2.203272
Mg8	-0.177359	2.109746	-2.287058
Mg9	4.269735	-1.926337	1.045317
Mg10	-4.789953	-0.759192	-0.706634
Mg11	0.427540	3.278980	0.401286
Mg12	-0.335251	-0.003229	2.723515
Mg13	1.122206	2.548148	3.166392
Mg14	-4.462898	1.946427	0.482963
Mg15	-2.513577	-2.206822	-2.156364
Mg16	1.502536	-2.397384	2.296291
Mg17	3.736007	-1.864798	-1.948648
Mg18	-2.007638	2.514014	2.207176
Mg19	-1.673419	-2.655414	2.866604
Mg20	3.410819	2.944550	1.216945
Mg21	-3.201945	1.237387	-2.398580
Mg22	2.378609	-3.866178	-0.207577
Mg23	-3.593356	-3.086041	0.638455
Mg24	-0.648683	-3.383934	0.150952
Mg25	-1.459899	-0.007285	-0.194377
Mg26	-2.383673	3.621062	-0.699485
Mg27	4.544538	0.752957	-0.603603

@mg27-isomer07 bp86/6-31G(d) Etot=-5402.600918 Eb=-16.71

Mg1	2.044235	3.510349	-1.572518
Mg2	4.541640	2.194695	-0.699614
Mg3	3.850924	-2.881028	1.022829
Mg4	-0.677014	-2.688484	-1.410645
Mg5	2.158640	-1.594558	3.084796
Mg6	-2.360164	-0.623568	-3.003028
Mg7	-3.679063	-2.859805	-1.151631
Mg8	2.711746	0.683722	-2.648870
Mg9	-4.813893	-0.100024	-1.283216
Mg10	-4.563574	1.723796	1.015613
Mg11	2.415017	-2.684127	-1.698577
Mg12	-1.625937	0.003669	-0.055720
Mg13	2.697925	3.296560	1.394474
Mg14	-0.176452	1.510216	-2.414506
Mg15	1.372668	-0.237926	0.023244
Mg16	-3.843898	-1.206037	1.732585
Mg17	-3.004255	2.467214	-1.592448
Mg18	-2.779819	4.071653	1.054569
Mg19	-2.066184	1.454274	2.701975
Mg20	0.898651	-3.362062	1.074307
Mg21	0.542463	-1.124167	-3.691717
Mg22	0.992887	1.168029	2.816686
Mg23	-0.863731	-1.363125	2.709747
Mg24	-0.151229	2.723335	0.431349
Mg25	3.901585	0.454621	1.815004
Mg26	-2.200922	-3.714972	1.266782
Mg27	4.677756	-0.822249	-0.921469

@mg27-isomer08 bp86/6-31G(d) Etot=-5402.600376 Eb=-16.70

Mg1	-4.334970	1.769642	1.362452
Mg2	-1.626128	0.846232	2.935136
Mg3	-1.693681	3.279870	0.930577
Mg4	-3.901127	-1.070531	2.125399
Mg5	0.779089	2.731411	2.808945

Mg6	1.288712	-0.282278	2.882450
Mg7	-1.115192	-2.138818	2.266631
Mg8	-3.772649	2.810010	-1.298233
Mg9	-4.511461	-0.484298	-0.913664
Mg10	3.547955	1.607636	2.115502
Mg11	-1.682128	0.252490	-0.080854
Mg12	1.005339	1.702497	0.061327
Mg13	1.913031	-3.264445	2.125604
Mg14	3.202048	3.812403	0.055835
Mg15	0.928342	-1.237558	-0.024435
Mg16	4.012481	-1.203669	1.114309
Mg17	4.795092	1.327334	-0.615631
Mg18	-0.781491	2.900277	-2.124418
Mg19	-2.645133	0.697935	-3.058551
Mg20	-3.283828	-3.274253	0.265003
Mg21	-1.943042	-2.091676	-2.158833
Mg22	-0.378256	-3.932589	-0.161457
Mg23	3.259063	-0.775368	-2.048617
Mg24	0.301540	0.144917	-2.796583
Mg25	2.504630	2.266044	-2.536142
Mg26	3.071508	-3.605356	-0.562327
Mg27	1.060257	-2.787859	-2.669425

@mg27-isomer09 bp86/6-31G(d) Etot=-5402.600161 Eb=-16.69

Mg1	1.523056	-0.336580	0.076861
Mg2	-0.847408	1.547305	-2.518520
Mg3	4.046811	0.239657	2.264910
Mg4	-0.027557	-2.529701	-1.598510
Mg5	0.357485	-0.802800	-3.976274
Mg6	-0.535463	-3.029804	1.366810
Mg7	-1.491929	2.412490	2.149883
Mg8	2.943021	-1.901941	-2.135957
Mg9	2.142839	1.152691	-2.594674
Mg10	1.953650	-1.933732	2.664539
Mg11	3.396838	3.065865	1.503573
Mg12	-2.533577	-1.101469	-2.710071
Mg13	0.722783	2.688941	-0.075801
Mg14	3.492343	3.533288	-1.384920
Mg15	-4.736988	-1.233098	-0.533313
Mg16	-3.408052	-2.475756	1.960393
Mg17	-3.862130	1.501339	-1.545684
Mg18	-2.784701	-3.542035	-0.773290
Mg19	2.162441	-3.851407	0.127047
Mg20	4.447529	-2.131413	0.579514
Mg21	4.516850	0.620443	-0.756324
Mg22	-3.902548	0.477237	1.913005
Mg23	1.242353	1.265231	2.767557
Mg24	-1.998737	3.792203	-0.815680
Mg25	-1.466548	-0.090552	0.028659
Mg26	-4.233444	3.260530	0.967414
Mg27	-1.118916	-0.596933	3.048853

@mg27-isomer10 bp86/6-31G(d) Etot=-5402.598701 Eb=-16.66

Mg1	-1.690406	0.000745	-0.042293
Mg2	1.353623	-0.003811	0.220865
Mg3	1.397938	-2.702213	-1.542000
Mg4	-1.204773	-3.367823	-0.186095
Mg5	-1.186974	-1.581589	-2.831134
Mg6	-0.532761	1.554260	2.493093
Mg7	4.019824	1.470643	-2.175511
Mg8	-1.189865	1.583356	-2.829850
Mg9	-1.212793	3.374210	-0.183367
Mg10	3.836999	2.970649	0.363117
Mg11	1.229335	3.755234	1.479851

Mg12	2.571381	1.472530	2.773941
Mg13	-4.788483	-0.003696	0.333674
Mg14	-3.071455	-0.003317	3.046179
Mg15	3.840662	-2.965931	0.358764
Mg16	-0.528970	-1.557034	2.494399
Mg17	1.235005	-3.754646	1.477057
Mg18	2.576746	-1.475248	2.775491
Mg19	-3.692265	-0.001764	-2.661803
Mg20	1.391001	2.700465	-1.533500
Mg21	1.459755	0.002076	-3.098555
Mg22	4.022279	-1.460310	-2.176473
Mg23	-3.373687	-2.589232	1.680836
Mg24	-3.378096	2.582741	1.681152
Mg25	4.553970	0.002993	0.700666
Mg26	-3.821002	2.584985	-1.309096
Mg27	-3.816986	-2.588272	-1.309410

@mg27-isomer11 bp86/6-31G(d) Etot=-5402.597821 Eb=-16.64

Mg1	-3.314282	0.968781	-2.270488
Mg2	3.785516	-2.667913	1.583706
Mg3	-1.555065	-0.182021	0.083076
Mg4	2.430004	1.438549	-2.858560
Mg5	1.337812	0.404330	-0.290146
Mg6	2.595041	3.119468	1.776786
Mg7	1.763999	-1.564792	3.640942
Mg8	2.221798	-1.536771	-3.083140
Mg9	-0.397354	3.290709	0.980394
Mg10	-4.837213	1.261963	0.496469
Mg11	-4.851161	-1.505545	-0.668909
Mg12	-2.423499	-3.256282	0.438561
Mg13	0.514518	0.987149	2.663164
Mg14	-0.503317	-0.201026	-3.002369
Mg15	2.846669	-3.576168	-1.018986
Mg16	0.683188	-2.471194	1.004550
Mg17	1.937574	3.838766	-1.068246
Mg18	-3.043255	3.447542	-0.317598
Mg19	4.251451	-0.822209	-0.959145
Mg20	3.606849	0.323091	1.977281
Mg21	-4.007678	-1.118859	2.144532
Mg22	-1.264869	-1.412541	3.100398
Mg23	-0.104384	-3.031041	-1.803412
Mg24	-2.755700	-2.147572	-2.544132
Mg25	4.296048	2.181342	-0.477323
Mg26	-0.687650	2.580069	-2.006968
Mg27	-2.525040	1.652175	2.479565

@mg27-isomer12 bp86/6-31G(d) Etot=-5402.597032 Eb=-16.62

Mg1	3.584004	1.951382	1.252778
Mg2	2.798827	2.701615	-1.828847
Mg3	4.557565	0.232479	-1.253347
Mg4	4.713558	-0.910328	1.581772
Mg5	1.839547	4.351987	0.464624
Mg6	4.117776	-2.768874	-0.778444
Mg7	0.381689	2.047344	1.792814
Mg8	1.538431	0.141481	-0.502178
Mg9	1.881914	-0.462025	2.592517
Mg10	2.794677	-3.258083	1.868945
Mg11	2.377992	-1.549965	-2.915599
Mg12	-1.481111	4.318595	1.182302
Mg13	-0.927078	-0.017318	3.596568
Mg14	-0.323344	2.758144	-1.261213
Mg15	1.016884	-2.975867	-0.588030
Mg16	0.645613	0.910412	-3.406324
Mg17	-0.285866	-2.643171	2.231631

Mg18	-1.282189	-0.143213	0.221508
Mg19	-2.884318	1.805072	2.121846
Mg20	-3.374724	3.079706	-0.669843
Mg21	-0.761322	-1.668599	-2.735626
Mg22	-3.210759	-1.446007	2.205675
Mg23	-2.459851	0.936187	-2.644439
Mg24	-2.053426	-3.191644	-0.273434
Mg25	-4.456910	0.287437	-0.157373
Mg26	-3.772216	-1.746890	-2.324460
Mg27	-4.975365	-2.739857	0.226176

@mg27-isomer13 bp86/6-31G(d) Etot=-5402.596295 Eb=-16.61

Mg1	0.072760	-0.954671	-2.913780
Mg2	-2.981089	0.144410	-2.685051
Mg3	2.438119	1.138507	-2.760575
Mg4	2.838796	-4.127795	0.216022
Mg5	2.085635	3.224892	1.838897
Mg6	-1.604763	-0.296912	-0.060257
Mg7	-2.381470	0.984373	2.783126
Mg8	4.695492	-1.997593	0.930109
Mg9	1.466784	3.647547	-1.202547
Mg10	3.732386	0.693407	1.960093
Mg11	-2.107675	-2.885968	-2.345552
Mg12	4.807877	0.114770	-1.133957
Mg13	-3.047090	3.116362	-1.497596
Mg14	-4.514792	-1.912484	-0.963591
Mg15	2.000660	-1.927439	2.341559
Mg16	-0.971934	-1.850923	2.613163
Mg17	0.644212	0.722448	2.994026
Mg18	-2.557814	-3.720483	0.576314
Mg19	-3.931334	-1.458326	1.996065
Mg20	-0.531086	1.892088	-2.463160
Mg21	0.222790	-2.719464	-0.275486
Mg22	-0.705395	2.566870	0.753924
Mg23	-4.456771	0.949124	0.156428
Mg24	-3.498262	3.526699	1.475135
Mg25	2.804826	-1.990529	-1.945060
Mg26	1.361268	0.248797	-0.051087
Mg27	4.117872	2.872292	-0.337160

@mg27-isomer14 bp86/6-31G(d) Etot=-5402.594957 Eb=-16.57

Mg1	1.791341	-0.381613	-0.076868
Mg2	3.704579	1.637414	1.349935
Mg3	1.259805	-2.873349	1.690058
Mg4	-0.151673	1.986159	-0.033973
Mg5	-1.130655	-1.716659	3.173758
Mg6	3.953869	-1.400644	2.037651
Mg7	-1.228005	-0.690376	0.146582
Mg8	3.080269	1.421785	-2.118554
Mg9	-2.283199	1.020757	-2.385228
Mg10	0.639350	-3.015968	-1.403375
Mg11	0.348971	2.773347	-2.774785
Mg12	-3.891718	-1.156794	1.702188
Mg13	-3.764386	1.732693	0.555702
Mg14	-2.249179	-2.153377	-2.351813
Mg15	-4.629443	-0.483492	-1.281203
Mg16	1.318981	0.058010	2.859191
Mg17	4.972069	-0.529172	-0.613623
Mg18	-1.828193	-3.551132	0.804950
Mg19	0.355160	-0.306745	-2.845720
Mg20	-2.486592	3.826691	-1.339278
Mg21	-4.472405	-3.292700	-0.424206
Mg22	3.050296	-1.630180	-2.655041
Mg23	-1.515562	1.202969	2.657226

Mg24	2.370980	3.785952	-0.391218
Mg25	-1.981978	3.989468	1.599870
Mg26	1.194077	3.055887	2.376201
Mg27	3.573241	-3.308931	-0.258428

@mg27-isomer15 bp86/6-31G(d) Etot=-5402.594825 Eb=-16.57

Mg1	-1.971983	0.000133	-0.042618
Mg2	0.922299	-0.000969	0.054146
Mg3	1.686860	-1.631360	-2.621908
Mg4	-0.965925	-2.729279	-1.582700
Mg5	-0.900371	-0.001903	-3.039252
Mg6	-1.078098	0.001699	3.128463
Mg7	4.158093	2.614574	-1.057921
Mg8	-0.965140	2.726895	-1.585372
Mg9	-1.046214	2.652126	1.533005
Mg10	3.925869	2.985886	1.871994
Mg11	1.508115	-1.538796	2.784201
Mg12	1.510105	1.539115	2.780727
Mg13	-4.963684	0.000593	-0.128462
Mg14	-3.675697	-1.447754	2.440145
Mg15	4.157558	-2.617013	-1.055653
Mg16	-1.047823	-2.650001	1.535308
Mg17	1.497595	-3.359852	0.044857
Mg18	3.925833	-2.981625	1.875176
Mg19	-3.539580	1.493220	-2.578921
Mg20	1.498255	3.359932	0.040343
Mg21	1.687243	1.627786	-2.623398
Mg22	4.237242	-0.001853	-2.416254
Mg23	-3.629038	-3.056610	-0.082802
Mg24	-3.674769	1.452270	2.439012
Mg25	3.910528	0.000875	0.952048
Mg26	-3.627777	3.057941	-0.085554
Mg27	-3.539495	-1.496031	-2.578610

@mg27-isomer16 bp86/6-31G(d) Etot=-5402.592741 Eb=-16.52

Mg1	-2.635699	3.425769	0.982320
Mg2	-4.534034	-1.930592	-0.133349
Mg3	-2.833619	-1.553812	2.482216
Mg4	-2.685553	-2.675961	-2.392380
Mg5	1.461692	0.037091	-0.016362
Mg6	1.668942	3.482071	-0.927643
Mg7	0.169312	-2.801378	1.614523
Mg8	-1.100990	2.245708	-1.450367
Mg9	2.709370	-1.861546	2.888791
Mg10	-0.719773	-0.440928	-3.034097
Mg11	-3.642469	0.243743	-2.217062
Mg12	5.079340	-1.357842	-1.680118
Mg13	1.335104	1.661568	-3.252185
Mg14	-2.513887	1.407956	3.181934
Mg15	0.141341	2.363257	1.642536
Mg16	-1.449920	-0.392187	0.091059
Mg17	2.998059	-2.817928	0.091138
Mg18	-2.334123	-3.871062	0.361564
Mg19	2.532537	1.122761	3.063185
Mg20	3.955146	1.391221	-1.673909
Mg21	-4.321595	0.893770	0.846869
Mg22	3.777071	2.805274	1.017759
Mg23	-4.168863	3.041971	-1.536765
Mg24	4.551457	-0.211934	1.112324
Mg25	-0.035183	-0.317209	3.194692
Mg26	2.366346	-1.141901	-2.876317
Mg27	0.229991	-2.747880	-1.380356

@mg27-isomer17 bp86/6-31G(d) Etot=-5402.592332 Eb=-16.51

Mg1	1.947595	-1.308697	2.797225
Mg2	4.213168	0.276341	1.260061
Mg3	4.432709	-2.723557	1.819821
Mg4	-3.301056	-1.870975	2.594535
Mg5	-4.870465	-0.879061	0.117151
Mg6	-0.780599	-0.082621	3.087846
Mg7	-0.751675	0.591007	-2.575031
Mg8	2.032724	-3.028477	0.080977
Mg9	1.955875	-1.077998	-2.608881
Mg10	1.669908	2.507410	-2.086226
Mg11	-3.616653	3.536886	0.389999
Mg12	-0.573708	-2.835332	1.794453
Mg13	4.564554	-1.922831	-1.075604
Mg14	1.863061	1.902994	2.463720
Mg15	-1.833289	-0.226909	0.178211
Mg16	3.758017	3.103179	0.228251
Mg17	-3.695948	1.413459	-1.746151
Mg18	-3.167245	-1.597610	-2.288089
Mg19	-3.213851	-3.494962	0.106600
Mg20	1.144654	0.160407	0.063303
Mg21	-0.610740	-1.861497	-4.229823
Mg22	-0.529413	-2.635685	-1.321838
Mg23	-1.271000	3.271589	-1.412039
Mg24	1.136579	4.224685	0.399602
Mg25	-1.031817	2.517204	1.597406
Mg26	4.197998	0.944983	-1.848100
Mg27	-3.669382	1.096066	2.212621

@mg27-isomer18 bp86/6-31G(d) Etot=-5402.589285 Eb=-16.44

Mg1	2.840212	-0.002988	0.001280
Mg2	-0.001792	0.000536	-0.001592
Mg3	-1.325710	-0.995380	2.903949
Mg4	1.328102	-2.311055	2.012836
Mg5	1.325936	0.586515	2.999362
Mg6	1.326402	-0.585868	-3.004582
Mg7	-3.931560	2.907862	0.997183
Mg8	1.325996	2.898947	0.993519
Mg9	1.327367	2.311586	-2.012525
Mg10	-3.929555	2.320723	-2.020500
Mg11	-1.326999	-2.017197	-2.316490
Mg12	-1.326684	0.991870	-2.894322
Mg13	-3.932233	-0.589000	-3.014112
Mg14	3.931050	-2.017458	-2.317818
Mg15	-3.929082	-2.321092	2.019923
Mg16	1.327311	-2.896187	-0.994663
Mg17	-1.324760	-2.996783	0.585237
Mg18	-3.929738	-2.909420	-0.997695
Mg19	3.929347	2.019823	2.318014
Mg20	-1.326228	3.004679	-0.585556
Mg21	-1.328172	2.011537	2.311231
Mg22	-3.932272	0.587171	3.014637
Mg23	3.931761	-3.016587	0.589312
Mg24	3.930108	0.998648	-2.905952
Mg25	-2.841999	0.000172	0.000523
Mg26	3.931447	3.015863	-0.588339
Mg27	3.931745	-0.996919	2.907139

@mg27-isomer19 bp86/6-31G(d) Etot=-5402.588973 Eb=-16.43

Mg1	-4.128659	3.193579	-1.886240
Mg2	3.958266	-1.121787	-1.743628
Mg3	2.003787	0.435866	0.197532
Mg4	-2.004443	-1.052392	4.397203
Mg5	-1.581032	1.697308	-2.635913
Mg6	0.613671	2.609355	1.914252

Mg7	3.726620	1.906722	-2.121104
Mg8	-4.176434	0.158651	-2.643285
Mg9	3.457267	1.228507	2.768627
Mg10	0.892221	-2.391920	0.502747
Mg11	-4.137113	1.064869	0.267203
Mg12	-1.644858	-1.490370	-2.811919
Mg13	0.852435	2.905511	-1.196111
Mg14	-1.118914	0.009952	-0.026304
Mg15	-1.884102	3.219292	0.121589
Mg16	3.904741	-1.552033	1.468423
Mg17	-1.800106	-2.632045	1.827805
Mg18	3.398153	-3.900752	-0.576674
Mg19	-1.455007	-3.928004	-0.893162
Mg20	-4.237302	-0.945848	2.428017
Mg21	1.013446	0.067445	-2.605730
Mg22	1.153694	-2.914895	-2.429355
Mg23	0.442018	-0.379395	2.752236
Mg24	3.462953	3.414640	0.523117
Mg25	-3.734813	-1.971896	-0.488847
Mg26	-2.136908	1.422209	2.615007
Mg27	5.160419	0.947430	0.274514

@mg27-isomer20 bp86/6-31G(d) Etot=-5402.588131 Eb=-16.42

Mg1	-1.688876	-0.285282	0.122354
Mg2	2.343436	0.429334	-2.827339
Mg3	4.686205	-0.872249	-1.332596
Mg4	-0.906994	0.958532	-2.736490
Mg5	3.886596	-0.666797	1.713372
Mg6	-3.316784	-3.389737	0.175033
Mg7	4.510800	-3.344477	0.400990
Mg8	-1.943217	0.303564	3.208622
Mg9	-0.328043	2.238215	1.481197
Mg10	0.237639	-1.725601	-3.304694
Mg11	2.572853	1.996515	2.354973
Mg12	3.843414	1.847676	-0.357490
Mg13	0.918770	-0.450583	3.009493
Mg14	-4.161028	-1.369325	2.197987
Mg15	1.298727	-0.283566	-0.084991
Mg16	-0.291115	5.527122	-0.109760
Mg17	0.924448	2.734670	-1.253292
Mg18	-3.879424	1.234301	-2.031095
Mg19	2.490318	-2.971459	-1.737080
Mg20	-3.864085	1.602105	1.055838
Mg21	2.354904	4.457239	0.779113
Mg22	-1.181148	-2.591555	2.356771
Mg23	-0.382472	-3.058489	-0.629968
Mg24	-2.653514	-1.621880	-2.416671
Mg25	-2.150833	3.366695	-1.002324
Mg26	1.763923	-2.995398	1.567466
Mg27	-5.084501	-1.069570	-0.599421

@mg27-isomer21 bp86/6-31G(d) Etot=-5402.576842 Eb=-16.15

Mg1	2.347261	-2.134146	3.071690
Mg2	0.470242	2.535636	2.179305
Mg3	0.817932	4.697650	0.005273
Mg4	-2.780162	-1.698387	2.871931
Mg5	5.293220	0.875537	0.001072
Mg6	2.944077	0.661271	-2.006019
Mg7	4.951229	-1.631126	-1.530441
Mg8	4.951359	-1.631190	1.533440
Mg9	-0.278922	-2.563843	-1.474665
Mg10	-2.777941	-1.690968	-2.877423
Mg11	-3.892911	-2.836299	-0.004066
Mg12	2.383526	-2.197991	-0.000657

Mg13	2.942751	0.658151	2.005299
Mg14	-5.073077	-0.437804	-1.496930
Mg15	0.470791	2.539504	-2.172101
Mg16	-2.170008	-0.412343	-0.000331
Mg17	0.610768	0.297550	0.000090
Mg18	-0.049452	-0.214781	3.224711
Mg19	-0.279757	-2.573091	1.470317
Mg20	-0.046532	-0.207869	-3.232835
Mg21	2.349689	-2.129973	-3.074130
Mg22	-2.644412	1.358880	2.514839
Mg23	-4.442159	1.983821	0.001744
Mg24	3.182413	3.020013	0.001063
Mg25	-2.640959	1.364817	-2.510626
Mg26	-1.564593	2.807696	0.004208
Mg27	-5.074373	-0.440716	1.495241

@mg27-isomer22 bp86/6-31G(d) Etot=-5402.576343 Eb=-16.14

Mg1	0.002257	-1.000122	-2.433192
Mg2	2.423864	0.870543	-2.255516
Mg3	-1.694000	-0.670335	0.182993
Mg4	4.975376	-0.468463	-1.289328
Mg5	-0.223105	1.806430	-0.920507
Mg6	-0.248537	1.159975	2.349778
Mg7	2.629352	-2.352115	-1.871192
Mg8	3.838965	2.101859	0.118782
Mg9	-2.860819	3.181975	-1.683587
Mg10	1.474631	-0.482484	0.449299
Mg11	2.293000	-3.207506	1.578878
Mg12	1.269880	3.731653	1.306626
Mg13	0.069321	-3.478611	-0.577761
Mg14	-3.981788	-1.837406	1.968017
Mg15	-0.702798	-2.510521	2.224081
Mg16	4.335790	-0.759147	1.659849
Mg17	-2.304815	-2.892921	-2.388275
Mg18	1.986034	3.897598	-1.631201
Mg19	-4.712687	-1.914654	-0.956148
Mg20	-4.340725	1.069941	0.100530
Mg21	-2.913052	0.198479	-2.432289
Mg22	4.813595	-3.263186	0.001487
Mg23	-0.633586	5.216881	-0.703447
Mg24	-3.147032	0.892666	2.847547
Mg25	-2.182120	3.236487	1.238187
Mg26	-2.838100	-4.030075	0.364789
Mg27	2.671099	1.503057	2.751597

@mg27-isomer23 bp86/6-31G(d) Etot=-5402.575680 Eb=-16.13

Mg1	1.035998	2.709392	-0.516907
Mg2	-1.125126	2.060397	-2.593843
Mg3	-1.145306	0.347537	0.157027
Mg4	2.932738	1.759532	1.737354
Mg5	-3.834679	1.743910	-0.908792
Mg6	4.030042	1.663447	-1.148676
Mg7	3.515738	-0.981649	-2.796886
Mg8	-3.257435	-0.039567	-3.316275
Mg9	-4.088906	-0.242225	1.387739
Mg10	-2.627898	-2.096922	-1.241701
Mg11	-1.686203	3.669299	0.020545
Mg12	1.257887	-3.187861	2.056609
Mg13	0.696221	-0.318647	2.640817
Mg14	1.762625	-0.317104	-0.296006
Mg15	5.499465	-1.003049	-0.566869
Mg16	-4.852111	-3.035190	0.688080
Mg17	3.326068	-3.005765	-0.452935
Mg18	-3.403361	2.657591	2.175372

Mg19	1.748390	1.486398	-3.225525
Mg20	-2.005662	0.408253	3.479920
Mg21	5.888251	1.195059	1.306317
Mg22	0.139702	-2.907884	-0.657629
Mg23	-0.220405	-0.824751	-2.797431
Mg24	-5.521167	-0.894121	-1.278766
Mg25	-1.664608	-2.291321	1.742575
Mg26	3.807076	-1.165843	1.978172
Mg27	-0.207334	2.611081	2.427715

@mg27-isomer24 bp86/6-31G(d) Etot=-5402.573075 Eb=-16.07

Mg1	-0.715938	-0.960561	3.809749
Mg2	-0.764371	2.138017	-1.098975
Mg3	2.004191	0.550793	-1.086011
Mg4	1.725550	0.352883	2.002864
Mg5	1.425823	-2.657964	2.579705
Mg6	-3.135099	0.088826	-0.501201
Mg7	0.659900	3.266596	1.463459
Mg8	1.111423	-4.058462	0.003445
Mg9	-4.464221	1.867966	1.677397
Mg10	-4.243008	3.130338	-1.165862
Mg11	4.666794	-0.698481	-1.886184
Mg12	-0.389007	-0.344785	-2.883389
Mg13	2.129749	3.561705	-1.221597
Mg14	-0.833996	-3.315231	-2.242251
Mg15	-3.188716	-1.707080	-3.003096
Mg16	5.092285	0.245767	1.094124
Mg17	3.677410	2.859122	1.414141
Mg18	3.392532	-2.150422	0.466943
Mg19	-2.339436	4.002202	0.913979
Mg20	1.977711	-2.229151	-2.321441
Mg21	-3.373230	-1.104054	2.291209
Mg22	4.908348	2.223710	-1.242411
Mg23	-3.127002	-3.006079	-0.259502
Mg24	-1.430292	1.239904	1.979304
Mg25	-2.942232	1.344443	-3.162548
Mg26	-0.326329	-1.154347	0.209927
Mg27	-1.498839	-3.485656	2.168222

@mg27-isomer25 bp86/6-31G(d) Etot=-5402.572731 Eb=-16.06

Mg1	4.132270	2.951698	0.920367
Mg2	-3.413463	1.253238	1.802820
Mg3	-4.532190	2.301707	-0.844374
Mg4	-0.372876	-5.435173	-0.137785
Mg5	-1.517008	3.158242	-0.813480
Mg6	4.148886	-2.125029	-0.375143
Mg7	-2.900328	-3.686828	0.039061
Mg8	-3.203134	-1.674226	2.222816
Mg9	4.502202	0.037240	1.875629
Mg10	1.990719	1.617422	2.951373
Mg11	-3.432385	4.274576	1.267412
Mg12	-0.687486	-0.032810	3.057267
Mg13	-4.265079	-0.728866	-0.494525
Mg14	3.376831	2.909204	-2.046208
Mg15	1.693705	-0.955460	1.333524
Mg16	0.446152	-2.467206	-1.154812
Mg17	-2.360603	-2.126738	-2.373190
Mg18	1.238965	2.040531	0.039525
Mg19	5.164890	0.690910	-0.994871
Mg20	2.231455	-4.118003	0.949165
Mg21	-0.080714	-0.713177	-3.699621
Mg22	0.404474	2.047516	-2.890178
Mg23	-1.122182	-0.024452	-0.070070
Mg24	2.373812	-0.146599	-1.951514

Mg25	-0.828296	2.863979	2.189357
Mg26	-0.486762	-2.887017	1.893997
Mg27	-2.501855	0.975322	-2.696540

@mg27-isomer26 bp86/6-31G(d) Etot=-5402.571851 Eb=-16.04

Mg1	1.669617	0.069768	0.121605
Mg2	2.368461	-0.824381	3.060246
Mg3	2.929265	2.289157	1.808037
Mg4	-2.305574	1.763683	1.579480
Mg5	1.856179	2.801568	-1.160059
Mg6	0.543203	-2.944086	-0.250271
Mg7	-0.823797	-2.113233	-2.865436
Mg8	4.912474	0.007987	1.713104
Mg9	-1.163071	2.593224	-1.285751
Mg10	1.234903	-3.617142	2.562532
Mg11	-0.651017	-1.292855	2.256579
Mg12	-3.995466	-1.625734	-1.639717
Mg13	3.432812	-2.496284	0.688454
Mg14	0.127253	3.633945	1.204670
Mg15	2.282833	-1.766218	-2.353611
Mg16	-6.752581	-0.149336	0.264842
Mg17	-3.923543	-0.896281	1.433278
Mg18	-5.326279	1.912606	1.947295
Mg19	-1.258486	-0.269948	-0.462104
Mg20	4.978563	-0.798920	-1.191713
Mg21	3.490264	0.990905	-2.973807
Mg22	-4.166906	1.397976	-0.938966
Mg23	0.490582	0.651501	-3.078292
Mg24	-2.646117	0.435789	-3.311728
Mg25	0.300508	1.394441	3.063528
Mg26	4.840400	2.110490	-0.483208
Mg27	-2.444480	-3.258620	0.291011

@mg27-isomer27 bp86/6-31G(d) Etot=-5402.567754 Eb=-15.94

Mg1	0.579348	1.005746	-3.000799
Mg2	-2.876228	0.773734	-2.639192
Mg3	-1.375325	-4.227880	-0.709714
Mg4	4.637290	1.285517	-0.479044
Mg5	2.010299	2.823262	-0.983141
Mg6	1.613705	-0.138246	-0.241970
Mg7	2.127963	-1.734683	-3.212798
Mg8	-0.945305	3.390515	-1.558908
Mg9	0.153606	3.204444	1.440713
Mg10	4.159542	-1.752121	-0.945441
Mg11	-2.985409	3.425350	1.216059
Mg12	-4.122215	-4.276601	0.464196
Mg13	-4.557131	0.932013	0.348267
Mg14	0.442535	0.393149	2.763925
Mg15	-1.257359	0.777002	0.062021
Mg16	3.681450	0.725556	-3.141856
Mg17	-4.126899	-1.633330	2.007912
Mg18	2.875705	2.043452	1.882921
Mg19	-4.081456	3.254249	-1.519377
Mg20	4.835031	-0.500512	1.833548
Mg21	-0.825840	-1.998442	1.302457
Mg22	3.048593	-0.009135	4.130082
Mg23	2.280303	-2.078601	1.975866
Mg24	1.536963	-3.345403	-0.740674
Mg25	-0.640073	-1.554739	-2.043709
Mg26	-2.684261	0.832130	2.766617
Mg27	-3.504833	-1.616427	-0.977961

@mg27-isomer28 bp86/6-31G(d) Etot=-5402.564542 Eb=-15.87

Mg1	-0.992607	-0.717800	0.525783
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Mg2	1.902239	0.089285	-0.005533
Mg3	0.908491	-0.266479	3.225827
Mg4	-1.541175	-3.112282	-1.307634
Mg5	1.498056	-3.107153	-0.824438
Mg6	-2.344156	0.014095	3.100667
Mg7	-2.653279	-0.217982	-2.089804
Mg8	2.581930	-2.430317	1.929314
Mg9	2.549577	2.175964	2.431585
Mg10	-3.351342	2.201598	1.095788
Mg11	0.273168	-0.922649	-2.616721
Mg12	4.979558	0.205586	-1.594076
Mg13	-0.370482	2.236043	2.021609
Mg14	4.037392	2.626132	-0.185776
Mg15	-4.369392	-0.502588	1.011223
Mg16	-0.192101	-3.362884	1.836990
Mg17	-4.490336	-2.578239	-1.127541
Mg18	-1.717160	4.426260	0.034795
Mg19	4.426966	-0.025322	1.585818
Mg20	-0.520208	1.777713	-1.065265
Mg21	4.463568	-2.491544	-0.418366
Mg22	1.404279	3.824225	0.033534
Mg23	2.423987	1.533951	-2.619477
Mg24	-5.424898	0.497094	-1.734453
Mg25	3.107214	-1.597258	-2.968472
Mg26	-3.165599	-3.101414	1.640151
Mg27	-3.423691	2.825963	-1.915528

@mg27-isomer29 bp86/6-31G(d) Etot=-5402.552698 Eb=-15.59

Mg1	4.476478	1.267547	2.242259
Mg2	1.231230	-1.476267	-3.596794
Mg3	5.031218	-0.719684	0.130602
Mg4	-3.403988	-0.259715	2.688116
Mg5	-0.274434	-3.376314	-1.825236
Mg6	4.342469	2.078594	-0.774890
Mg7	1.608266	0.811938	-1.806191
Mg8	-1.562984	-0.542811	-2.516463
Mg9	-3.680385	1.972815	-2.080252
Mg10	1.715480	1.658082	0.996478
Mg11	-3.849030	-0.520231	-0.304987
Mg12	-0.956089	1.544577	2.388096
Mg13	-0.422314	-1.421643	3.312340
Mg14	2.521913	-2.280760	-0.936332
Mg15	-3.348361	-3.178603	-1.582929
Mg16	1.899428	3.901478	-1.109135
Mg17	1.590180	0.803219	3.916076
Mg18	-0.886040	5.013576	-0.483906
Mg19	-0.987472	1.992770	-0.681939
Mg20	0.523802	-3.634397	1.153746
Mg21	2.511050	-1.291415	1.832436
Mg22	-3.921847	4.812234	-0.771831
Mg23	-0.303901	-0.816736	0.237136
Mg24	-2.599042	-2.808834	1.333373
Mg25	-1.809783	-5.330037	-0.009548
Mg26	-3.664503	2.267743	0.967605
Mg27	4.218661	-0.467125	-2.717831

@mg27-isomer30 bp86/6-31G(d) Etot=-5402.551631 Eb=-15.57

Mg1	-0.354108	0.341075	-0.361918
Mg2	-0.654871	-2.683101	-1.473189
Mg3	0.329618	2.990371	1.625090
Mg4	-2.731552	-0.880301	-3.098034
Mg5	-0.211502	-5.911552	-0.173853
Mg6	0.108453	0.254348	3.054145
Mg7	2.641262	3.505611	-0.405723

Mg8	-2.386056	1.259826	1.810360
Mg9	2.371573	0.622935	1.190713
Mg10	-0.401044	3.386006	-1.211286
Mg11	-2.164354	-4.034366	0.960239
Mg12	2.126545	-1.287645	-1.344681
Mg13	-3.025425	-1.243318	-0.125210
Mg14	2.215555	-4.212926	-0.358610
Mg15	-1.268991	1.680773	-3.642088
Mg16	4.027789	-2.038941	0.827028
Mg17	1.645460	1.561446	-2.494722
Mg18	-5.175747	2.405926	1.068460
Mg19	5.753985	0.031831	1.956376
Mg20	-2.568677	4.097044	0.769759
Mg21	-5.037611	-0.475392	2.086522
Mg22	4.351402	0.936632	-1.047174
Mg23	-2.194785	-1.660744	2.783037
Mg24	-3.119399	1.657081	-1.270131
Mg25	4.953489	2.817135	1.330586
Mg26	0.200160	-0.934823	-3.792865
Mg27	0.568831	-2.184928	1.337169

@mg27-isomer31 bp86/6-31G(d) Etot=-5402.545637 Eb=-15.43

Mg1	-3.351113	-1.824506	-0.399036
Mg2	1.970866	-1.550462	-2.363950
Mg3	4.220225	-2.204510	-0.487173
Mg4	-1.657899	0.895414	3.385382
Mg5	1.986789	-1.983092	1.523019
Mg6	-0.267313	-1.760028	3.550429
Mg7	-0.912041	-3.390155	1.007737
Mg8	-3.498049	1.460575	1.103938
Mg9	6.658234	-0.141198	-0.276809
Mg10	4.049954	0.245489	1.602373
Mg11	-0.429070	-0.402154	-3.776249
Mg12	-0.572393	2.638460	1.142904
Mg13	1.293915	0.823460	2.696970
Mg14	-0.713746	-0.383027	0.428798
Mg15	2.477799	2.721728	0.537130
Mg16	-5.001142	0.684425	-1.434300
Mg17	-0.859582	-2.735835	-1.962902
Mg18	-5.682042	-0.528076	1.292363
Mg19	0.856308	1.335645	-1.658498
Mg20	-2.135784	1.334913	-1.736051
Mg21	1.695109	-4.110861	-0.625537
Mg22	-3.087311	4.145199	-0.485825
Mg23	-3.124440	-1.612153	2.546456
Mg24	5.598670	2.625762	0.349486
Mg25	-0.060716	4.210019	-1.260287
Mg26	3.847567	0.677434	-1.437461
Mg27	-3.302793	-1.172465	-3.262907

@mg27-isomer32 bp86/6-31G(d) Etot=-5402.534974 Eb=-15.18

Mg1	-0.167621	0.672811	0.230063
Mg2	1.762015	-3.172378	1.233455
Mg3	-2.417602	1.473156	-1.773082
Mg4	1.646621	2.770219	1.762973
Mg5	4.469375	-1.739906	1.342762
Mg6	-0.625856	-2.317217	-0.444532
Mg7	1.623397	1.755821	-2.267432
Mg8	-3.521864	-3.465298	0.623662
Mg9	2.169795	-0.157740	2.304373
Mg10	3.800405	1.342829	0.198645
Mg11	6.346189	-0.494826	-0.645420
Mg12	-0.293211	-0.492566	-2.884823
Mg13	-5.622300	-1.491262	-0.463617

Mg14	-0.720995	1.238033	3.281486
Mg15	-0.619261	-1.731328	2.735885
Mg16	-0.306028	3.603389	-0.686386
Mg17	-2.778254	2.565819	1.053195
Mg18	-2.910066	-0.456100	0.942934
Mg19	-0.908181	4.180701	2.637710
Mg20	-2.960632	-1.608541	-2.133762
Mg21	-5.348286	1.434015	-0.060461
Mg22	4.193689	0.099422	-2.721241
Mg23	-1.033441	-4.643045	1.727917
Mg24	2.670681	4.150040	-0.703354
Mg25	2.081165	-1.038344	-0.940480
Mg26	4.627005	-2.827315	-1.529444
Mg27	-5.156739	0.349611	-2.821028

@mg27-isomer33 bp86/6-31G(d) Etot=-5402.525785 Eb=-14.97

Mg1	1.500759	-0.449281	-2.030727
Mg2	2.211022	-2.219687	0.826045
Mg3	2.257813	-3.437524	-1.900685
Mg4	-2.881717	-0.129704	-1.264798
Mg5	2.335741	2.678119	2.285638
Mg6	4.507926	-1.520273	-1.264310
Mg7	3.874173	0.256987	1.228754
Mg8	-0.765760	2.254663	-1.759728
Mg9	-0.309808	0.154228	0.441647
Mg10	4.364269	1.321799	-2.592386
Mg11	-0.583600	-2.500018	2.112371
Mg12	1.187060	-5.176370	0.360829
Mg13	-0.575842	-2.622127	-1.046503
Mg14	-3.154765	-2.591435	0.564855
Mg15	-2.678212	3.002940	0.757371
Mg16	-3.173067	0.204432	1.906882
Mg17	6.476064	0.682837	-0.703486
Mg18	-3.672646	2.873895	-2.177708
Mg19	0.148323	4.065925	0.702392
Mg20	-5.632345	-1.104137	-0.075196
Mg21	-1.690900	-5.258743	0.510497
Mg22	-0.770833	1.961493	2.979153
Mg23	-5.752121	0.709040	-2.502914
Mg24	1.398163	-0.198074	2.961479
Mg25	-5.356262	1.876991	0.197561
Mg26	2.016807	2.132539	-0.660315
Mg27	4.719756	3.031486	0.143280

@mg27-isomer34 bp86/6-31G(d) Etot=-5402.524175 Eb=-14.93

Mg1	-0.382839	-0.560149	0.984729
Mg2	-0.852427	1.996090	-1.859929
Mg3	-2.979597	1.189874	1.409142
Mg4	1.844799	-3.241209	-1.209221
Mg5	-0.214635	2.489308	1.691236
Mg6	-1.938899	4.168311	-0.127294
Mg7	-2.697312	-0.507110	-1.220476
Mg8	-4.029313	2.244625	-1.386148
Mg9	4.674479	1.255605	1.099141
Mg10	6.371480	-1.503851	1.182509
Mg11	-3.148573	-2.098905	1.436508
Mg12	1.282992	4.183603	-0.917123
Mg13	-5.005715	-0.442719	3.147072
Mg14	1.944578	0.603351	2.733287
Mg15	-5.947536	1.060760	0.637439
Mg16	-1.155962	-3.228274	-0.836013
Mg17	4.057245	2.689141	-1.478766
Mg18	0.247478	-0.745440	-2.166038
Mg19	1.730299	1.190294	-0.325877

Mg20	5.030535	-2.814833	-1.139960
Mg21	-5.650316	-0.414158	-1.982190
Mg22	6.073885	0.227605	-1.372262
Mg23	-4.278601	-3.116233	-1.245038
Mg24	-6.165040	-1.945467	0.751906
Mg25	3.324572	-0.546324	-2.211257
Mg26	4.737769	-0.594732	3.480703
Mg27	3.126656	-1.539163	0.923921

@mg27-isomer35 bp86/6-31G(d) Etot=-5402.518881 Eb=-14.81

Mg1	-1.439725	0.344976	-0.441367
Mg2	0.873962	-0.078782	-2.753550
Mg3	-0.762574	5.102563	-0.051680
Mg4	-1.643829	-2.142152	-2.211107
Mg5	-0.531938	2.635351	1.698873
Mg6	-3.226009	0.856127	1.933298
Mg7	2.070284	3.797357	0.374684
Mg8	-0.322469	-0.448596	2.298412
Mg9	0.490545	-2.257070	-0.005515
Mg10	3.709455	1.914357	-1.499028
Mg11	1.564654	0.668341	0.201658
Mg12	1.329406	-3.055957	-2.826720
Mg13	-4.548497	-1.529121	-1.481677
Mg14	5.312745	-2.595973	0.782844
Mg15	5.903089	0.232284	-0.041755
Mg16	-2.933466	3.070019	-0.420059
Mg17	3.013467	-4.066056	-0.471755
Mg18	-5.277538	1.141109	-0.419662
Mg19	3.517915	-1.183017	-1.413617
Mg20	-5.511172	-1.131457	1.501206
Mg21	0.059494	2.731249	-1.883254
Mg22	2.708650	-1.429354	1.966642
Mg23	-3.134990	0.929424	-2.770734
Mg24	-2.621730	-2.143236	0.816452
Mg25	-8.065428	-2.659037	2.471510
Mg26	5.494682	-0.527285	2.954598
Mg27	3.971014	1.823935	1.691305

@mg28-isomer01 bp86/6-31G(d) Etot=-5602.717408 Eb=-17.16

Mg1	-2.054797	0.001783	0.001176
Mg2	0.804691	-0.008693	-0.008744
Mg3	1.391237	-1.572630	2.740203
Mg4	-1.164240	0.014378	3.131776
Mg5	-1.181219	-2.717740	1.589433
Mg6	-1.162501	2.698645	-1.572729
Mg7	3.915112	-2.675414	-1.525127
Mg8	-1.168511	-2.700904	-1.543062
Mg9	-1.171741	-0.009279	-3.125605
Mg10	3.931453	-0.018742	-3.069706
Mg11	1.401654	3.165320	-0.021013
Mg12	1.389639	1.582966	-2.779624
Mg13	3.945229	2.655615	-1.558259
Mg14	-5.015211	0.010982	0.008611
Mg15	-3.765688	2.978553	-0.004897
Mg16	3.946327	0.006604	3.078671
Mg17	-1.152428	2.700737	1.547428
Mg18	1.405161	1.607368	2.757942
Mg19	3.946867	2.678768	1.533453
Mg20	-3.776813	-2.955925	0.012665
Mg21	1.381926	-1.612931	-2.773445
Mg22	1.381390	-3.196958	0.015740
Mg23	3.938675	-2.670663	1.542944
Mg24	-3.767815	1.500868	2.557103
Mg25	-3.775340	1.473763	-2.559364

Mg26	3.931082	0.008328	0.008322
Mg27	-3.780813	-1.485135	-2.551078
Mg28	-3.773322	-1.459663	2.567187

@mg28-isomer02 bp86/6-31G(d) Etot=-5602.713802 Eb=-17.08

Mg1	1.591081	-0.084548	-0.199258
Mg2	-1.330338	0.455235	0.219716
Mg3	-1.294481	2.589742	-2.065195
Mg4	1.485320	1.439605	-3.036954
Mg5	1.120610	3.108763	-0.367420
Mg6	1.434112	-3.594244	0.241948
Mg7	-4.030297	1.560507	2.212343
Mg8	0.853192	1.962037	2.393347
Mg9	0.374409	-1.165961	2.393479
Mg10	-2.994136	-1.337723	2.428713
Mg11	-0.910157	-2.281527	-0.932325
Mg12	-1.209990	-3.698464	1.787666
Mg13	-3.684042	-3.245535	0.147006
Mg14	4.712153	0.097169	0.390494
Mg15	3.944020	-2.590688	-0.966711
Mg16	-3.769590	1.004271	-2.949226
Mg17	1.565922	-1.906297	-2.752865
Mg18	-0.980185	-0.238233	-3.123628
Mg19	-3.478394	-1.940193	-2.571432
Mg20	3.590882	2.784893	1.470666
Mg21	-1.573165	0.987502	3.673360
Mg22	-1.613404	3.318643	1.299743
Mg23	-3.946052	2.741092	-0.547968
Mg24	4.072380	-0.181862	-2.689532
Mg25	3.408381	-2.310324	2.009280
Mg26	-4.449552	-0.288562	-0.187755
Mg27	3.200655	0.338737	3.178769
Mg28	3.910668	2.475963	-1.456262

@mg28-isomer03 bp86/6-31G(d) Etot=-5602.712447 Eb=-17.05

Mg1	-1.408018	-0.536754	0.111844
Mg2	1.537598	-0.000259	-0.080036
Mg3	1.347666	0.226378	-3.341852
Mg4	-1.511506	-1.051431	-3.229424
Mg5	-0.878743	1.690208	-1.883487
Mg6	-4.249230	-2.236680	1.091773
Mg7	4.280438	2.354453	0.501057
Mg8	-0.696507	3.907399	0.243281
Mg9	-0.220317	1.545451	2.042998
Mg10	2.843346	0.852482	2.752476
Mg11	0.586178	-2.955475	0.998708
Mg12	0.371625	-1.030814	3.321896
Mg13	3.154627	-2.097422	2.523477
Mg14	-3.045079	2.792235	1.969507
Mg15	-4.406728	0.648648	0.191000
Mg16	3.686802	-1.662096	-2.637526
Mg17	-4.205987	-1.711254	-1.861544
Mg18	0.799262	-2.459704	-1.975742
Mg19	3.314401	-3.316589	-0.240769
Mg20	-3.383942	3.311781	-0.976952
Mg21	1.968522	3.601740	1.759254
Mg22	1.837502	2.930668	-1.315015
Mg23	4.106042	1.163074	-2.235206
Mg24	-3.716415	1.000617	-2.827808
Mg25	-2.839002	-0.072742	2.932515
Mg26	4.634758	-0.629798	0.239765
Mg27	-2.000623	-3.372543	-0.717955
Mg28	-1.906670	-2.891574	2.643765

@mg28-isomer04 bp86/6-31G(d) Etot=-5602.711481 Eb=-17.03

Mg1	-3.737854	0.439108	-2.972955
Mg2	-4.254458	-2.107582	-1.487133
Mg3	-1.556587	-1.629908	-2.923369
Mg4	-2.062079	-3.547233	-0.029334
Mg5	-4.259645	0.629326	0.040793
Mg6	-4.275338	-2.052846	1.510042
Mg7	-0.933377	1.303402	-1.969330
Mg8	-1.909045	-2.364423	3.139794
Mg9	0.740000	-2.815444	-1.448869
Mg10	-1.330370	-0.681383	0.269000
Mg11	1.267207	-0.331257	-3.287391
Mg12	-3.374753	3.114577	-1.611029
Mg13	1.827971	2.596424	-1.657173
Mg14	-0.178494	1.874147	1.413511
Mg15	-2.841088	0.469422	2.835525
Mg16	1.684317	-0.155322	-0.074786
Mg17	3.574236	-2.143625	-2.439009
Mg18	0.644922	-2.739386	1.616997
Mg19	2.037574	3.998808	1.024523
Mg20	4.073196	0.754291	-2.383039
Mg21	-0.710934	4.063440	-0.569354
Mg22	0.315251	-0.329892	3.388361
Mg23	4.098018	1.885322	0.477601
Mg24	3.310079	-3.229587	0.328610
Mg25	-3.006767	3.156941	1.390544
Mg26	5.058209	-0.896511	-0.079528
Mg27	2.460151	1.768566	3.003002
Mg28	3.339657	-1.029372	2.493994

@mg28-isomer05 bp86/6-31G(d) Etot=-5602.711432 Eb=-17.03

Mg1	1.424638	0.000034	-0.073616
Mg2	-0.718524	2.291305	-1.232903
Mg3	1.435666	-2.422776	2.125265
Mg4	2.148363	3.165271	-0.774739
Mg5	0.462042	-3.074247	-0.683448
Mg6	1.183575	1.351611	-3.368703
Mg7	-0.041319	2.274306	1.754743
Mg8	-0.581237	-0.445099	3.132587
Mg9	3.347148	-3.382565	-0.152016
Mg10	-0.536909	-1.022895	-2.587348
Mg11	2.274112	0.604390	3.087351
Mg12	-3.772846	2.326341	-1.861097
Mg13	3.926905	1.279416	-2.334053
Mg14	-3.715896	-0.685605	-2.247591
Mg15	-1.918780	1.249676	-3.893502
Mg16	-1.557383	-0.274898	0.214485
Mg17	4.983385	-1.070562	-0.912839
Mg18	-4.434434	-2.360348	0.258376
Mg19	4.241959	-1.359749	1.985629
Mg20	4.285684	1.411856	0.746912
Mg21	2.695665	3.498613	2.160596
Mg22	-2.811313	3.446596	0.754646
Mg23	-4.461025	0.742407	0.636303
Mg24	2.537985	-1.587446	-2.610811
Mg25	-1.642518	-3.140403	1.511836
Mg26	-3.566199	-1.178228	2.848357
Mg27	-2.421525	-3.331500	-1.589967
Mg28	-2.767219	1.694500	3.105548

@mg28-isomer06 bp86/6-31G(d) Etot=-5602.707398 Eb=-16.94

Mg1	2.528547	-2.935145	2.292035
Mg2	-2.464778	-3.435670	-1.193731
Mg3	1.836398	-3.619236	-0.574277

Mg4	-0.436367	-2.615377	1.358393
Mg5	-3.464087	-2.619525	1.442714
Mg6	4.427472	-2.339680	0.032177
Mg7	1.160812	-0.525632	3.454402
Mg8	-1.983084	-0.462221	3.197474
Mg9	4.211626	-0.472140	2.450263
Mg10	-4.392655	-1.003847	-1.187676
Mg11	-0.114038	-1.747899	-1.792877
Mg12	1.558308	-0.389663	0.394368
Mg13	2.895557	-1.409576	-2.479622
Mg14	-4.765575	-0.050341	1.821213
Mg15	-1.714355	0.027607	0.130971
Mg16	4.384510	0.643425	-0.506805
Mg17	-2.539260	-1.397360	-3.495425
Mg18	2.958895	2.151557	1.895951
Mg19	3.384792	3.429565	-0.899063
Mg20	-4.438668	1.974976	-0.388086
Mg21	2.951936	1.485147	-3.151976
Mg22	-2.467156	1.434509	-2.590702
Mg23	-3.146999	2.362866	2.363767
Mg24	0.188031	0.242932	-3.919358
Mg25	-0.179487	1.812991	2.104750
Mg26	-1.877023	3.455753	-0.149611
Mg27	0.489080	1.842569	-1.311303
Mg28	1.007569	4.159416	0.702035

@mg28-isomer07 bp86/6-31G(d) Etot=-5602.706535 Eb=-16.92

Mg1	1.347149	0.004284	-0.147886
Mg2	-1.531154	1.418385	3.104832
Mg3	-1.617531	-3.752094	1.947899
Mg4	-3.818133	-3.157501	0.035863
Mg5	-3.051098	0.878800	-3.211189
Mg6	-3.777086	2.762667	-1.118113
Mg7	4.522577	-1.108170	-2.837433
Mg8	1.706915	1.041436	3.149084
Mg9	1.890674	-2.365540	-2.142741
Mg10	-1.636001	0.419229	0.032169
Mg11	4.541284	0.313135	2.058477
Mg12	-4.583782	-0.266865	-0.641945
Mg13	2.192216	0.815483	-3.148622
Mg14	4.400290	1.110109	-0.899469
Mg15	-0.427080	-0.601771	-3.117292
Mg16	2.330561	3.285518	-1.410801
Mg17	1.495404	-3.512578	0.789020
Mg18	-0.854770	-2.450128	-0.730879
Mg19	-0.530134	2.319869	-2.030454
Mg20	3.367516	2.954836	1.384902
Mg21	0.372465	2.770506	0.992774
Mg22	-0.148773	-1.185491	2.332353
Mg23	-2.337481	3.788208	1.219989
Mg24	-3.126833	-2.047656	-2.687753
Mg25	-4.233669	1.594136	1.747714
Mg26	2.774405	-1.871829	2.892283
Mg27	4.038578	-1.973674	0.084567
Mg28	-3.306510	-1.183304	2.352651

@mg28-isomer08 bp86/6-31G(d) Etot=-5602.703993 Eb=-16.86

Mg1	-4.429176	-0.904800	0.215059
Mg2	-2.081042	2.489097	-2.238430
Mg3	-4.524124	2.264337	-0.485474
Mg4	-2.128923	3.236439	1.018233
Mg5	2.893320	-2.428608	1.806126
Mg6	-1.220711	-0.474134	-3.311487
Mg7	1.963107	-0.944952	-3.043605

Mg8	5.631846	1.783539	-0.372236
Mg9	-3.149653	-2.538221	-2.016788
Mg10	-1.450667	0.221223	-0.009521
Mg11	4.355929	-0.929816	-1.062794
Mg12	-2.401928	-3.454388	0.752109
Mg13	-1.272450	0.932977	3.276990
Mg14	-4.083835	0.246989	-2.667288
Mg15	0.659981	1.775842	-3.532633
Mg16	0.590653	3.046529	2.415429
Mg17	4.506532	0.054311	1.843715
Mg18	0.513243	2.787122	-0.641680
Mg19	2.702677	-3.394545	-1.187451
Mg20	-0.178598	-2.432067	-1.249665
Mg21	1.871694	0.398076	3.194380
Mg22	3.155536	2.643874	1.032161
Mg23	-0.153147	-1.745099	2.143832
Mg24	3.206261	1.806219	-2.042553
Mg25	-4.121321	1.347981	2.363658
Mg26	0.722481	-4.335489	0.882166
Mg27	1.552941	-0.015378	0.044232
Mg28	-3.130626	-1.437059	2.873514

@mg28-isomer09 bp86/6-31G(d) Etot=-5602.703374 Eb=-16.85

Mg1	-0.645200	1.890361	-3.657601
Mg2	-0.369637	-0.788694	-2.565932
Mg3	-2.822371	-2.597002	-2.497123
Mg4	-3.247595	0.459010	-2.699860
Mg5	-4.363572	-1.207854	-0.292446
Mg6	-4.599684	1.797435	-0.411369
Mg7	2.316993	0.624388	-3.129352
Mg8	-2.035229	3.107280	-1.165397
Mg9	-3.267224	-4.111748	0.057279
Mg10	-0.588707	-2.615954	-0.221053
Mg11	1.063060	2.892646	-1.392692
Mg12	2.095663	-2.485883	-1.886073
Mg13	-1.584568	0.284216	0.178193
Mg14	1.785467	-3.819483	1.143277
Mg15	-2.574313	-2.001558	2.176541
Mg16	-4.256337	0.446138	2.318604
Mg17	1.471716	0.088148	-0.010713
Mg18	-2.996912	3.076684	1.822214
Mg19	4.057642	2.424372	-1.427079
Mg20	2.814703	3.513074	1.125725
Mg21	4.387389	-3.362954	-0.157469
Mg22	0.398709	-1.442597	2.539458
Mg23	-0.060408	2.716200	1.433047
Mg24	-1.358936	0.819774	3.401191
Mg25	4.373416	-0.522340	-1.190032
Mg26	3.486958	-1.450170	2.074659
Mg27	4.558751	1.158962	1.367585
Mg28	1.960228	1.107551	3.066418

@mg28-isomer10 bp86/6-31G(d) Etot=-5602.701695 Eb=-16.81

Mg1	-1.937282	2.943260	2.173653
Mg2	-3.819129	0.573932	2.366105
Mg3	-4.045885	2.776181	0.108886
Mg4	-4.868982	0.045302	-0.464241
Mg5	-0.134327	0.676517	2.841436
Mg6	-3.554793	-2.241902	1.022280
Mg7	-2.035579	-1.566122	3.523569
Mg8	-1.142166	3.323534	-0.752045
Mg9	1.467935	-1.611544	3.895084
Mg10	1.147770	3.038529	1.594880
Mg11	-3.092901	1.410984	-2.526151

Mg12	-1.566921	0.243954	0.024875
Mg13	3.109154	0.707881	2.786959
Mg14	-3.183596	-1.804994	-2.080018
Mg15	1.560119	0.244051	0.044188
Mg16	1.928851	3.441196	-1.334404
Mg17	-0.034505	-2.204090	1.321251
Mg18	-1.719902	-3.978549	-0.550136
Mg19	3.204876	-2.284279	1.535384
Mg20	0.166264	1.373942	-2.547087
Mg21	-1.430361	-0.553044	-4.166488
Mg22	4.041720	2.709282	0.596552
Mg23	0.044914	-1.843810	-1.835219
Mg24	1.721148	-3.997328	-0.444215
Mg25	3.765273	1.169358	-2.155701
Mg26	2.012613	-0.633359	-3.841681
Mg27	3.522006	-1.885607	-1.571573
Mg28	4.873688	-0.073276	0.433856

@mg28-isomer11 bp86/6-31G(d) Etot=-5602.700023 Eb=-16.77

Mg1	-2.056121	-3.257389	-0.798154
Mg2	2.941175	2.014618	2.913647
Mg3	-1.700775	-0.140185	3.151765
Mg4	2.027741	4.206627	1.051204
Mg5	4.099554	-2.744405	-0.489793
Mg6	4.368749	2.439133	0.326931
Mg7	4.083252	0.144468	-1.658074
Mg8	-0.758808	1.497457	-2.509329
Mg9	0.218252	1.732764	1.534276
Mg10	-0.304181	-2.496590	1.823339
Mg11	-2.940596	2.476657	1.340354
Mg12	-4.996394	1.075776	-0.594218
Mg13	-4.515918	-0.027820	2.109699
Mg14	1.080036	-3.428391	-0.734178
Mg15	1.785391	0.431553	-3.702807
Mg16	2.733899	-2.235045	-3.023318
Mg17	-0.791244	3.888740	-0.408711
Mg18	2.662788	-3.087161	2.066081
Mg19	-3.293786	-2.733550	2.047401
Mg20	1.331427	-0.430665	-0.212621
Mg21	-3.212160	3.003225	-1.830995
Mg22	1.910778	2.411044	-1.371376
Mg23	1.448591	-0.539290	3.306151
Mg24	-3.285481	-0.279588	-2.699561
Mg25	-0.386215	-1.503584	-2.701703
Mg26	-4.649252	-1.853463	-0.448983
Mg27	-1.803994	-0.175730	0.009061
Mg28	4.003294	-0.389206	1.503914

@mg28-isomer12 bp86/6-31G(d) Etot=-5602.699789 Eb=-16.77

Mg1	-0.201377	1.891372	2.774327
Mg2	0.446724	-3.407032	-2.490428
Mg3	2.693573	3.415373	-1.551515
Mg4	-3.321212	-3.950971	-0.206070
Mg5	-2.708800	3.525866	-1.383217
Mg6	-0.588158	-0.982089	3.064500
Mg7	1.834085	-2.600192	2.270966
Mg8	0.059185	3.044154	-0.002991
Mg9	1.437035	0.009123	0.237626
Mg10	2.445368	1.074247	-3.306023
Mg11	2.298403	0.209507	3.295968
Mg12	4.365995	0.936816	-0.946781
Mg13	3.066986	-1.635065	-2.290273
Mg14	-3.179059	-2.354704	2.286616
Mg15	5.044322	0.798840	2.124671

Mg16	-3.358800	0.601435	2.689898
Mg17	-0.315239	2.406501	-2.935549
Mg18	4.197550	-1.631364	0.654622
Mg19	-0.537116	-2.557749	0.288216
Mg20	-4.655234	1.830003	0.161887
Mg21	2.781443	2.579502	1.353378
Mg22	-3.172036	0.754275	-2.501553
Mg23	0.014094	-0.475928	-2.451329
Mg24	-2.614992	3.374883	1.641335
Mg25	2.447017	-3.906997	-0.341306
Mg26	-4.396656	-1.111669	-0.199510
Mg27	-2.509149	-2.173165	-2.424438
Mg28	-1.573953	0.335028	0.186975

@mg28-isomer13 bp86/6-31G(d) Etot=-5602.698879 Eb=-16.75

Mg1	-0.858092	-1.556216	-0.221406
Mg2	-1.009465	1.360824	-0.127572
Mg3	1.667036	0.077063	0.100234
Mg4	-2.971508	-2.916459	-2.159218
Mg5	-1.465127	-2.401128	2.568423
Mg6	-0.801023	1.961198	-3.001523
Mg7	-0.868890	4.761338	-0.310258
Mg8	-3.208394	0.121277	2.679323
Mg9	-2.393602	-4.581993	0.316819
Mg10	-2.483627	3.060454	1.855438
Mg11	-0.797142	-1.070756	-3.300257
Mg12	1.679846	-1.869420	2.500576
Mg13	4.127238	-1.489921	-1.886828
Mg14	0.825738	3.181364	1.806036
Mg15	-3.984572	-1.825392	0.511500
Mg16	-0.296843	0.452916	2.725044
Mg17	-4.695080	1.256984	0.419920
Mg18	1.815135	0.329933	-2.972626
Mg19	1.380183	-2.694196	-1.919738
Mg20	2.590013	0.985489	3.019514
Mg21	-3.242739	3.246916	-1.267012
Mg22	3.784338	2.812305	1.033846
Mg23	4.560056	-0.372051	1.066470
Mg24	4.333756	1.457350	-1.500989
Mg25	0.540232	-4.201886	0.877208
Mg26	-3.220170	0.187213	-1.981177
Mg27	1.596323	2.964914	-1.250044
Mg28	3.396381	-3.238117	0.418299

@mg28-isomer14 bp86/6-31G(d) Etot=-5602.696783 Eb=-16.70

Mg1	3.522970	2.066222	-2.257520
Mg2	5.133392	0.497345	-0.403454
Mg3	3.889261	3.039820	0.551060
Mg4	0.987103	3.215472	-0.777440
Mg5	3.287901	-1.078746	-2.404415
Mg6	2.120428	2.541051	2.782004
Mg7	3.680259	-0.011643	2.300425
Mg8	0.986936	0.887365	-3.301016
Mg9	4.323491	-2.242790	0.322823
Mg10	1.665943	0.342755	-0.042866
Mg11	-0.671579	2.071584	1.731884
Mg12	-2.007274	4.044249	0.001699
Mg13	0.587303	-0.110479	3.268954
Mg14	-1.450465	1.329519	-1.494507
Mg15	0.195034	-1.753904	-2.031317
Mg16	1.673235	-2.471839	1.674244
Mg17	2.234835	-3.746269	-1.131746
Mg18	-1.674773	-0.574498	-3.965349
Mg19	-1.053876	-0.751113	0.617778

Mg20	-4.340676	2.561645	-1.019219
Mg21	-3.682778	2.443844	2.015067
Mg22	-2.808811	-0.238750	3.125514
Mg23	-4.273197	0.049875	-2.686236
Mg24	-0.737974	-3.783831	0.063361
Mg25	-2.940478	-2.438371	-1.653074
Mg26	-1.072056	-2.707036	3.069289
Mg27	-4.150740	-0.175310	0.361540
Mg28	-3.423415	-3.006168	1.282516

@mg28-isomer15 bp86/6-31G(d) Etot=-5602.695908 Eb=-16.68

Mg1	-1.763619	-0.140964	0.083765
Mg2	-3.194701	-3.615064	-0.218522
Mg3	-0.404535	0.430299	3.056564
Mg4	-2.787787	1.016213	-2.731319
Mg5	-0.387072	2.490895	-1.269319
Mg6	0.773408	2.835007	1.691312
Mg7	4.303533	0.335675	0.065184
Mg8	-0.338838	-2.833065	-0.006561
Mg9	-3.434459	0.461277	2.899017
Mg10	3.358699	-0.749383	-2.641744
Mg11	-1.957274	-2.277213	2.562022
Mg12	-4.713840	-1.658371	1.362410
Mg13	0.282979	0.180725	-3.053626
Mg14	-1.843973	-1.983525	-2.631220
Mg15	1.206562	0.011920	0.017866
Mg16	4.269025	-1.840701	2.213463
Mg17	2.739697	0.692598	2.806424
Mg18	1.177484	-2.071733	2.672569
Mg19	1.706798	4.635851	-0.675415
Mg20	2.697765	2.143072	-1.994839
Mg21	3.639639	3.101797	0.973310
Mg22	2.622643	-2.787781	-0.065262
Mg23	-2.216787	2.874406	1.451984
Mg24	-4.532060	-1.215929	-1.655729
Mg25	-4.454125	1.280843	0.071575
Mg26	-3.148075	3.719999	-1.310196
Mg27	5.329527	-2.330570	-0.947809
Mg28	1.069383	-2.706278	-2.725906

@mg28-isomer16 bp86/6-31G(d) Etot=-5602.694845 Eb=-16.66

Mg1	2.788547	2.023966	2.136041
Mg2	-2.628903	-2.306418	-2.750661
Mg3	1.006155	3.351950	-0.198245
Mg4	4.526080	0.345445	-2.283853
Mg5	-1.964565	0.062158	3.896088
Mg6	-0.398469	-0.272731	-3.228983
Mg7	-3.412439	2.277373	2.463303
Mg8	-1.609451	0.043942	-0.245637
Mg9	-0.770695	-4.530278	1.142051
Mg10	0.008144	-2.513592	-1.136454
Mg11	-3.005234	-2.969191	0.194814
Mg12	3.868740	2.813869	-0.733125
Mg13	-0.100143	-1.525478	1.954132
Mg14	1.865703	1.779927	-2.871232
Mg15	2.082073	-3.643183	1.014620
Mg16	-3.340447	0.569938	-3.234847
Mg17	3.156346	-1.239982	2.420374
Mg18	-2.001452	3.836095	0.390157
Mg19	-4.112216	1.978907	-0.565992
Mg20	2.345772	-1.531144	-2.920933
Mg21	1.253162	0.266811	4.107819
Mg22	4.929231	0.465316	0.703335
Mg23	-3.955464	-0.588339	1.793521

Mg24	-0.334718	1.836927	2.020315
Mg25	4.102530	-2.158512	-0.513486
Mg26	-4.734239	-0.929442	-1.140965
Mg27	1.571661	0.105604	-0.199812
Mg28	-1.135709	2.450061	-2.212347

@mg28-isomer17 bp86/6-31G(d) Etot=-5602.692613 Eb=-16.61

Mg1	-4.320614	-0.748297	1.305854
Mg2	2.237811	-2.573006	-2.164184
Mg3	-3.291774	-2.776298	-0.833521
Mg4	-5.454437	-0.880127	-1.622655
Mg5	3.266374	-2.683680	1.358307
Mg6	4.950973	-2.147614	-1.098329
Mg7	-2.243836	-3.061570	1.875301
Mg8	-0.355508	3.780075	2.174387
Mg9	-0.769473	-2.722220	-2.471611
Mg10	4.555306	0.286235	0.689519
Mg11	2.663123	2.514489	2.017440
Mg12	-2.856011	1.909275	2.113369
Mg13	-1.330140	-0.335351	0.067748
Mg14	0.178629	0.936789	2.759789
Mg15	-2.291028	-0.634322	3.533244
Mg16	0.502561	-2.005797	2.900518
Mg17	3.010766	-0.283028	3.225476
Mg18	0.485148	-0.072784	-2.818461
Mg19	-3.859403	1.506432	-0.865002
Mg20	3.589208	2.804199	-0.804896
Mg21	0.389387	-3.323845	0.210548
Mg22	1.632351	-0.373178	0.164385
Mg23	1.749450	2.597096	-3.167988
Mg24	-2.722620	-0.454893	-2.913366
Mg25	-1.514769	2.337312	-2.699426
Mg26	-2.297859	3.838911	-0.125892
Mg27	3.646076	0.225936	-2.477909
Mg28	0.450307	2.339261	-0.332644

@mg28-isomer18 bp86/6-31G(d) Etot=-5602.683786 Eb=-16.41

Mg1	-6.459777	1.235919	0.579418
Mg2	2.096316	-0.013731	0.062960
Mg3	-3.659678	-3.044826	1.387028
Mg4	-3.051263	-1.941074	-1.371076
Mg5	0.027459	0.370466	2.671890
Mg6	2.716639	-1.118089	-3.359533
Mg7	0.735807	1.096328	-2.838839
Mg8	1.528513	2.949240	2.493485
Mg9	-0.617983	-3.023525	0.306287
Mg10	-1.367245	-2.214173	3.109064
Mg11	-4.057862	2.996527	0.471919
Mg12	-4.180489	0.800718	-1.533895
Mg13	-3.308821	0.079781	1.527359
Mg14	3.993054	2.806440	0.816273
Mg15	3.431945	0.496322	2.791905
Mg16	4.456257	-2.010692	1.376643
Mg17	-1.234006	2.762402	1.333657
Mg18	-2.110664	0.147180	-3.530200
Mg19	4.947188	-1.495043	-1.469280
Mg20	-5.903511	-1.580859	0.128374
Mg21	-0.012174	-1.910650	-2.497654
Mg22	-0.850717	0.084172	-0.279921
Mg23	-1.729342	2.752855	-1.735205
Mg24	5.769440	0.558977	0.520899
Mg25	2.246914	-2.943669	-0.774407
Mg26	1.164864	2.945793	-0.554979
Mg27	3.887299	1.427392	-1.866978

Mg28	1.541835	-2.214181	2.234803
@mg28-isomer19 bp86/6-31G(d) Etot=-5602.680400 Eb=-16.33			
Mg1	-1.578503	3.659846	-1.743758
Mg2	-5.143087	-0.224946	-0.263867
Mg3	-3.409280	2.460111	0.503322
Mg4	-4.105300	0.165820	2.504441
Mg5	-3.182371	1.141393	-2.265335
Mg6	0.283018	5.578902	-0.397795
Mg7	-3.352705	-2.264131	-1.595586
Mg8	-1.048311	-3.125502	0.552103
Mg9	-3.976001	-2.539044	1.420065
Mg10	0.260184	1.270349	-2.196618
Mg11	0.268986	2.433442	0.629841
Mg12	-1.377762	-1.403141	3.047904
Mg13	-1.540084	1.612950	2.808973
Mg14	-1.272432	-0.918178	-3.368790
Mg15	2.785419	5.000810	1.139819
Mg16	2.423861	3.426428	-1.483518
Mg17	-1.704868	-0.132268	0.070253
Mg18	3.383947	2.088961	1.185882
Mg19	-0.712604	-3.599784	-2.382286
Mg20	1.253362	0.457043	2.864090
Mg21	1.415734	-2.585622	2.502590
Mg22	1.164605	-0.758281	-0.008722
Mg23	1.666542	-1.479455	-2.850895
Mg24	1.708720	-3.927618	-0.652350
Mg25	3.920041	-0.820059	1.488426
Mg26	3.934500	-3.821563	1.294478
Mg27	3.698179	0.619147	-1.534934
Mg28	4.236212	-2.315612	-1.267732
@mg28-isomer20 bp86/6-31G(d) Etot=-5602.679598 Eb=-16.32			
Mg1	0.538816	2.397874	0.511068
Mg2	2.698259	1.241365	2.432157
Mg3	4.200721	0.170765	-1.921217
Mg4	-1.301522	2.222649	-1.933464
Mg5	-4.126511	1.532038	-1.000186
Mg6	1.671828	1.850008	-2.278851
Mg7	1.578388	-0.473536	0.018410
Mg8	-3.062804	0.124032	-3.429145
Mg9	-2.937134	-2.980399	0.476446
Mg10	-0.315282	0.476104	2.733286
Mg11	4.754817	-2.466840	-0.289667
Mg12	-2.381085	2.480045	1.225805
Mg13	-3.155341	1.122479	3.816482
Mg14	-1.539034	-0.311171	-0.027155
Mg15	2.527461	-2.304016	-2.245253
Mg16	3.705371	2.742603	-0.234235
Mg17	-0.154929	-0.611142	-2.737469
Mg18	4.977596	0.226605	0.976753
Mg19	0.092194	-2.529274	1.989921
Mg20	3.227382	-1.806140	2.360925
Mg21	-1.047101	4.960186	-0.267798
Mg22	1.922128	5.246320	-0.327666
Mg23	-2.449247	-1.675025	3.257665
Mg24	-4.392880	-0.262304	1.437243
Mg25	-0.170743	-3.136046	-0.951160
Mg26	-4.723884	-1.394601	-1.362628
Mg27	-2.507101	-2.754020	-2.707888
Mg28	2.369639	-4.088558	0.477620
@mg28-isomer21 bp86/6-31G(d) Etot=-5602.678163 Eb=-16.28			
Mg1	0.077986	-0.003387	2.744462

Mg2	0.517073	-0.269793	-2.624293
Mg3	-1.967900	2.970736	2.408363
Mg4	3.694244	0.919662	-1.979077
Mg5	1.092721	3.005115	1.973314
Mg6	0.792874	-2.992903	1.760586
Mg7	0.811227	-3.337076	-1.322943
Mg8	-0.671468	1.252603	0.043684
Mg9	-1.553783	-1.760462	0.028067
Mg10	-3.490780	2.688229	-0.318631
Mg11	-2.068135	-2.428770	3.001700
Mg12	-5.149842	0.058716	-0.226270
Mg13	-2.810022	0.229088	-2.176313
Mg14	3.357076	-3.650215	0.289338
Mg15	-4.550820	-2.454093	1.384623
Mg16	3.211293	-1.297533	2.502599
Mg17	-1.114952	4.454612	-0.045402
Mg18	-4.302248	-2.486514	-1.577816
Mg19	3.238949	-2.068215	-2.376820
Mg20	3.719340	1.703869	1.048061
Mg21	-3.110715	0.273441	1.964585
Mg22	1.814744	3.031678	-0.955944
Mg23	-0.971517	2.682618	-2.569539
Mg24	2.685520	1.364129	3.844183
Mg25	-1.672397	-2.483884	-2.991051
Mg26	4.889548	-1.102550	-0.018997
Mg27	1.841362	2.215534	-3.874401
Mg28	1.690623	-0.514635	0.063932

@mg28-isomer22 bp86/6-31G(d) Etot=-5602.674344 Eb=-16.20

Mg1	2.203891	1.836506	2.557261
Mg2	1.231611	0.225904	-0.148009
Mg3	-1.873648	0.224066	0.077968
Mg4	2.771569	-1.100422	3.278287
Mg5	4.191764	0.178651	0.934676
Mg6	3.035972	2.786380	-0.375402
Mg7	-0.069482	-0.490798	2.631403
Mg8	-3.788237	1.419893	-2.057954
Mg9	-3.011667	0.321949	2.979052
Mg10	1.232276	-2.809836	1.222118
Mg11	-4.795306	-1.628379	1.687535
Mg12	1.313835	4.504886	1.357149
Mg13	3.052604	-2.162538	-1.092511
Mg14	-0.020952	-2.226392	-1.499245
Mg15	-0.679232	0.518141	-2.807279
Mg16	-2.882514	3.587131	0.063338
Mg17	-0.096001	2.919910	-0.983193
Mg18	6.347461	-1.642221	-0.422687
Mg19	1.821417	-0.882919	-3.589886
Mg20	-4.916420	1.304267	0.793948
Mg21	4.404621	-2.925036	1.524589
Mg22	-2.924415	-1.618883	-2.225798
Mg23	4.155211	0.446224	-2.131968
Mg24	-1.878572	-2.692760	0.996865
Mg25	-5.601118	-0.898626	-1.143032
Mg26	-4.361906	-3.667161	-0.508060
Mg27	-0.765471	2.377906	2.016988
Mg28	1.902709	2.094157	-3.136152

@mg28-isomer23 bp86/6-31G(d) Etot=-5602.670737 Eb=-16.12

Mg1	0.163389	2.553489	1.298179
Mg2	0.912497	-0.006377	-0.206160
Mg3	-3.672985	1.516316	-1.930034
Mg4	-0.727825	2.303698	-1.733105
Mg5	-1.643985	0.144446	-3.666112

Mg6	2.987453	1.383095	1.710668
Mg7	1.235864	0.279964	-3.190048
Mg8	-1.966050	-0.122150	0.161308
Mg9	4.027703	0.243775	-1.715231
Mg10	2.537447	-2.339486	-1.386011
Mg11	7.044328	0.297766	-0.644984
Mg12	-2.680498	2.968247	0.677715
Mg13	-1.836615	1.417743	3.202184
Mg14	5.392371	-2.150056	-0.148563
Mg15	-4.562753	-2.367388	0.910657
Mg16	0.211095	-2.712019	1.030708
Mg17	2.279066	2.619778	-1.172697
Mg18	-4.443075	0.457129	2.028107
Mg19	5.160540	2.490373	0.015640
Mg20	-5.614207	2.652264	0.225139
Mg21	-2.121099	-1.815284	2.683878
Mg22	-2.204499	-3.839160	-0.107368
Mg23	3.105792	-1.676481	1.716283
Mg24	5.794048	0.006422	2.047281
Mg25	-5.860206	-0.207155	-0.620484
Mg26	-0.514897	-2.107643	-2.034664
Mg27	0.519149	-0.302385	2.866820
Mg28	-3.522049	-1.688923	-2.019105

@mg28-isomer24 bp86/6-31G(d) Etot=-5602.669727 Eb=-16.10

Mg1	0.902779	-1.642370	0.242653
Mg2	1.341458	1.356953	-0.284790
Mg3	-1.298733	0.831595	0.753817
Mg4	3.579947	-2.635683	-1.270402
Mg5	-1.269414	-1.128255	-1.799290
Mg6	0.888455	-3.230178	-2.500107
Mg7	-3.666221	2.664141	-0.478621
Mg8	1.565136	-4.959166	-0.099647
Mg9	1.774658	-0.301554	-2.638578
Mg10	-2.931036	-1.991547	1.246061
Mg11	-3.995982	-2.432690	-1.527150
Mg12	3.758809	2.409639	1.551598
Mg13	-3.673197	0.838791	2.369183
Mg14	-0.465697	4.305184	-0.594231
Mg15	1.682680	3.143525	-2.613731
Mg16	1.768838	0.162300	2.494077
Mg17	2.682781	4.573672	-0.152007
Mg18	-1.131200	1.869595	-2.244205
Mg19	3.051361	-3.208954	1.788409
Mg20	-0.937416	-0.944727	3.165853
Mg21	-2.192319	3.580050	1.968337
Mg22	4.140344	-0.544823	0.821236
Mg23	-5.242495	-0.098758	0.081618
Mg24	-1.348670	-4.013335	-0.584619
Mg25	-3.767805	0.451765	-2.474273
Mg26	4.091295	1.546515	-1.450354
Mg27	-0.102651	-3.736236	2.199612
Mg28	0.794294	3.134549	2.029551

@mg28-isomer25 bp86/6-31G(d) Etot=-5602.669401 Eb=-16.09

Mg1	-2.308522	-0.394269	-0.013867
Mg2	-4.526736	-2.989327	-0.592913
Mg3	-1.563810	-3.657969	-0.181971
Mg4	-3.203998	2.971906	-1.598306
Mg5	0.230524	-1.661541	-1.633147
Mg6	1.593251	-3.524604	0.318210
Mg7	-1.444417	0.813450	-2.635312
Mg8	1.973604	0.850724	-2.605438
Mg9	-0.220832	3.445753	-1.627253

Mg10	2.547988	-0.828278	1.457865
Mg11	-1.804735	2.941486	1.204407
Mg12	-3.248864	-2.551085	2.115678
Mg13	-4.627622	2.036272	0.775608
Mg14	0.527196	0.995857	-0.001541
Mg15	6.381487	-1.480940	-0.915142
Mg16	-0.314190	-1.694313	1.898215
Mg17	-2.690604	0.524844	2.750450
Mg18	4.607277	1.022743	-1.046748
Mg19	-4.688903	0.145049	-1.715812
Mg20	3.307752	-1.790074	-1.675441
Mg21	3.334689	2.083927	1.627199
Mg22	-2.656292	-2.108219	-2.620477
Mg23	1.092936	4.019922	1.331421
Mg24	4.559374	-3.087686	0.812275
Mg25	0.369920	1.406856	2.949950
Mg26	-5.476136	-0.762228	1.169906
Mg27	5.532821	-0.207585	1.542674
Mg28	2.716842	3.479329	-1.090491

@mg28-isomer26 bp86/6-31G(d) Etot=-5602.669258 Eb=-16.09

Mg1	-0.911237	-0.807517	-0.182764
Mg2	-3.033565	1.101374	-1.642010
Mg3	-1.240665	-0.915834	-3.342347
Mg4	-2.081086	1.778820	1.412096
Mg5	-2.112134	-3.594596	0.812140
Mg6	-2.576876	-1.076593	2.581123
Mg7	1.962631	-0.044872	-0.014945
Mg8	4.609250	-0.195760	-2.031642
Mg9	1.765537	-0.641552	-3.047314
Mg10	-4.033875	-1.337331	-0.094654
Mg11	-2.732957	-3.204890	-2.113282
Mg12	0.280224	-3.186369	-2.093126
Mg13	-4.910996	0.840280	1.913594
Mg14	-0.040837	1.602153	-2.070124
Mg15	0.290640	0.271750	2.637127
Mg16	-1.768679	3.786667	-0.828954
Mg17	-4.575565	3.345868	0.217603
Mg18	5.298961	1.918931	0.000726
Mg19	-0.106533	-2.556575	3.497507
Mg20	0.910546	-3.302766	0.830152
Mg21	2.850911	2.387151	-1.788225
Mg22	3.137487	-2.783073	-1.107761
Mg23	3.420584	4.053968	0.778696
Mg24	4.996443	-0.904664	0.856696
Mg25	3.294991	1.388594	2.335234
Mg26	0.678045	2.747590	0.754369
Mg27	-6.082176	1.101702	-0.868446
Mg28	2.710929	-1.772457	2.598530

@mg28-isomer27 bp86/6-31G(d) Etot=-5602.668771 Eb=-16.07

Mg1	1.153438	0.149494	-0.027323
Mg2	3.246012	1.722183	-2.764519
Mg3	-1.164715	-1.442428	2.687504
Mg4	4.164721	-0.612299	-1.142187
Mg5	-0.446578	-2.592303	-0.033931
Mg6	-3.251966	1.639776	-2.135494
Mg7	-2.107761	0.024524	0.130486
Mg8	-4.273306	-1.177962	-1.712214
Mg9	1.784698	-2.250220	2.064143
Mg10	1.619370	2.569745	1.718449
Mg11	-0.774652	2.723509	-0.204492
Mg12	-1.314260	1.730311	2.648843
Mg13	-3.752461	2.714727	0.806511

Mg14	1.676867	-0.934183	-2.903420
Mg15	-4.340805	0.132644	2.221018
Mg16	-3.585189	-2.517119	0.989114
Mg17	6.395275	0.149964	0.767625
Mg18	0.216134	-3.569319	-2.748936
Mg19	2.559074	-3.137685	-0.791156
Mg20	-5.899281	1.239937	-0.520396
Mg21	4.791678	-2.413145	1.188939
Mg22	3.673829	0.200801	2.237886
Mg23	0.197627	1.762587	-2.862411
Mg24	1.027921	0.250226	3.667337
Mg25	4.303178	2.259442	0.027873
Mg26	-1.365458	-0.884360	-2.781914
Mg27	1.832679	3.742540	-1.089124
Mg28	-6.366070	-1.481391	0.561791

@mg28-isomer28 bp86/6-31G(d) Etot=-5602.667217 Eb=-16.04

Mg1	-1.917529	0.092878	0.148572
Mg2	1.113109	0.272130	-0.255196
Mg3	-1.093945	2.045150	2.541412
Mg4	-4.853537	0.769445	-0.362902
Mg5	3.818067	-0.380228	-1.780151
Mg6	-0.003090	-2.268193	1.082347
Mg7	-3.284639	3.119145	0.792692
Mg8	5.588085	-0.396110	0.673570
Mg9	-3.511444	0.026117	-3.035906
Mg10	-3.746087	-2.320957	-1.024938
Mg11	-0.878223	-1.430228	-2.285431
Mg12	-4.155921	1.182849	2.814948
Mg13	-4.665674	-1.501830	1.816075
Mg14	3.012823	-1.781300	1.128848
Mg15	2.141516	2.366745	-2.246196
Mg16	-3.209071	2.780140	-2.151728
Mg17	-0.691335	1.409025	-3.214053
Mg18	-0.563696	2.892072	-0.544370
Mg19	-1.962601	-0.978406	3.156992
Mg20	1.687143	-0.395715	-3.796831
Mg21	1.751919	-2.721954	-1.673600
Mg22	8.659736	-0.970076	0.679901
Mg23	4.130188	2.247705	-0.088212
Mg24	3.752532	0.867373	2.614812
Mg25	1.694538	2.870101	1.576293
Mg26	0.977564	-0.081582	3.084613
Mg27	-1.113891	-4.113687	-1.080184
Mg28	-2.676537	-3.600609	1.428626

@mg28-isomer29 bp86/6-31G(d) Etot=-5602.666117 Eb=-16.01

Mg1	0.981012	-0.091285	0.496356
Mg2	0.569058	-1.048722	-2.486560
Mg3	-2.271954	-1.772746	2.452685
Mg4	-1.918519	0.058449	-0.206444
Mg5	3.654202	-2.385202	2.315734
Mg6	-3.364078	-3.451312	0.185465
Mg7	-1.489107	0.755988	-3.524481
Mg8	2.741672	2.438396	0.577051
Mg9	-4.908739	2.106234	0.195480
Mg10	-0.571039	2.522870	1.075223
Mg11	0.495094	2.069674	-1.764369
Mg12	4.572665	0.003181	0.747026
Mg13	5.452528	-1.593571	-1.861022
Mg14	-4.768532	-0.836473	0.811404
Mg15	2.672358	0.378557	3.144677
Mg16	-0.459883	-2.717251	-0.016850
Mg17	3.177342	0.554528	-1.970327

Mg18	-2.280061	-2.080531	-2.535840
Mg19	-3.233820	1.230355	2.556762
Mg20	-0.467393	0.487393	3.370722
Mg21	-4.239397	0.438345	-2.205131
Mg22	-5.220837	-2.359252	-1.829023
Mg23	-3.100935	4.082325	1.424923
Mg24	5.453716	2.551301	-0.875221
Mg25	7.472359	0.357343	-0.917334
Mg26	-2.422118	2.938907	-1.413394
Mg27	0.666715	-2.312960	2.898058
Mg28	2.807694	-2.324540	-0.645570

@mg28-isomer30 bp86/6-31G(d) Etot=-5602.664993 Eb=-15.99

Mg1	3.373122	-1.573503	2.999007
Mg2	1.592558	0.797763	2.808260
Mg3	0.045870	-2.022245	2.550306
Mg4	4.139420	0.746181	1.075907
Mg5	-0.063569	3.340015	2.465412
Mg6	-3.096659	-2.052224	2.115822
Mg7	4.809118	-2.406378	0.554631
Mg8	2.348941	-3.999674	1.431797
Mg9	-3.104639	3.278519	1.824886
Mg10	-4.580263	0.708380	2.169772
Mg11	-1.557063	0.684741	2.293087
Mg12	1.841694	-1.225507	0.223745
Mg13	-1.188421	4.071155	-0.404105
Mg14	-1.538374	-0.833495	-0.312920
Mg15	-0.243233	-3.583737	-0.274199
Mg16	0.535805	1.359735	-0.115867
Mg17	-4.915269	-0.987755	-0.212331
Mg18	-3.408618	-3.552942	-0.564711
Mg19	2.228545	3.831634	0.614275
Mg20	4.144217	-0.660231	-1.798554
Mg21	-3.209794	1.729046	-0.818155
Mg22	1.152918	-1.784784	-2.617889
Mg23	3.774881	2.363889	-1.412332
Mg24	-1.692845	-2.586039	-2.861643
Mg25	1.022779	3.263220	-2.315710
Mg26	-3.767979	-0.378886	-2.884024
Mg27	-0.862841	0.625797	-3.022348
Mg28	2.219699	0.847326	-3.512116

@mg28-isomer31 bp86/6-31G(d) Etot=-5602.659152 Eb=-15.86

Mg1	-1.768722	0.224435	0.194005
Mg2	1.126144	-0.481394	-0.329190
Mg3	-0.931014	-2.860312	-0.102039
Mg4	-4.626911	-0.300113	-0.941111
Mg5	3.801437	1.123576	-0.862850
Mg6	-0.045665	0.244182	2.851769
Mg7	-2.905981	-2.481532	-2.294826
Mg8	5.792329	0.076308	1.306115
Mg9	-3.458077	2.397660	-1.639186
Mg10	-4.193514	2.096264	1.215249
Mg11	-1.276238	3.973748	-0.329236
Mg12	-3.994112	-3.063100	0.465536
Mg13	-4.939606	-0.809799	2.076241
Mg14	2.897950	0.160266	2.072445
Mg15	2.220697	1.041273	-3.503538
Mg16	-2.724987	0.166931	-3.428583
Mg17	-0.431233	1.713807	-2.231374
Mg18	-0.087041	-1.381056	-2.862268
Mg19	-2.020453	-2.022248	2.619129
Mg20	2.032221	3.565814	-1.743099
Mg21	0.956627	2.280327	0.804682

Mg22	8.801036	0.639254	1.973968
Mg23	3.252160	-1.626880	-2.650237
Mg24	4.008914	-2.059672	0.245687
Mg25	1.867388	-3.699412	-1.000469
Mg26	1.191934	-2.492686	2.087046
Mg27	-1.561752	2.913024	2.397831
Mg28	-2.983532	0.661337	3.608304

@mg28-isomer32 bp86/6-31G(d) Etot=-5602.649985 Eb=-15.65

Mg1	-2.383780	-1.578426	1.125821
Mg2	-1.293534	-0.149881	-1.693894
Mg3	4.873820	1.254813	-0.962436
Mg4	5.426484	-0.400001	1.530350
Mg5	1.903153	0.777688	-1.769657
Mg6	3.782412	-1.717559	-0.585226
Mg7	4.165956	-0.675590	-3.347416
Mg8	0.413485	5.720959	0.080245
Mg9	2.806140	1.141484	1.536615
Mg10	-3.355891	2.315489	-1.910708
Mg11	-0.287077	2.793506	-1.386891
Mg12	-4.553403	0.094313	-0.131409
Mg13	1.165512	-2.188091	-2.373230
Mg14	-2.420690	4.638520	-0.144136
Mg15	-3.892829	-2.890277	-1.183637
Mg16	-0.088083	0.374047	3.190019
Mg17	0.408296	3.033033	1.658882
Mg18	-1.740226	-2.743440	-3.292450
Mg19	-3.915206	0.385118	2.927507
Mg20	1.917443	-3.949856	0.323762
Mg21	-0.051914	-2.943016	2.514851
Mg22	-2.179508	-1.591581	4.313996
Mg23	-1.990700	1.562248	0.854048
Mg24	-0.908954	-3.627429	-0.566460
Mg25	2.603587	3.465950	-0.441932
Mg26	2.918738	-1.833677	2.338776
Mg27	-3.936976	-0.503078	-3.036423
Mg28	0.613746	-0.765265	0.431033

@mg28-isomer33 bp86/6-31G(d) Etot=-5602.647896 Eb=-15.61

Mg1	-0.642329	2.700660	0.670476
Mg2	0.481087	-0.542057	-2.789702
Mg3	3.537259	-1.022521	-2.472299
Mg4	0.042923	0.909080	3.093920
Mg5	-4.052096	2.589276	0.211086
Mg6	0.419653	-1.901017	2.074771
Mg7	-4.841273	1.540928	-2.640501
Mg8	-2.365391	0.249390	1.475861
Mg9	0.671779	2.530353	-2.223682
Mg10	-4.047519	-1.320082	-1.766825
Mg11	2.097682	3.922216	0.088820
Mg12	1.448259	0.404330	0.139115
Mg13	3.710663	1.917425	-1.582984
Mg14	1.902492	3.158965	2.993024
Mg15	4.486042	-0.486514	0.399478
Mg16	5.075743	-3.209030	-0.644309
Mg17	-6.189537	0.439126	-0.190782
Mg18	-1.989750	1.134993	-1.641412
Mg19	-0.409106	-4.535439	0.603077
Mg20	-4.523181	-1.834202	1.185617
Mg21	4.249866	2.351875	1.435605
Mg22	-3.165683	-4.036310	-0.458492
Mg23	1.746547	-2.611353	-0.713378
Mg24	2.945498	0.072356	3.017044
Mg25	2.456942	1.211610	-4.269792

Mg26	-1.187063	-1.619277	-0.505832
Mg27	-5.120685	0.897910	2.644415
Mg28	3.261179	-2.912693	1.867682

@mg28-isomer34 bp86/6-31G(d) Etot=-5602.641241 Eb=-15.46

Mg1	-0.057802	0.881146	1.989414
Mg2	-2.494641	2.729146	1.291090
Mg3	0.204757	-1.267118	-0.401404
Mg4	-2.403216	-0.545205	0.910953
Mg5	1.808396	0.568872	-3.262873
Mg6	-4.969270	0.938603	0.695639
Mg7	4.078002	-0.650917	-1.551194
Mg8	-0.803862	1.364644	-1.402455
Mg9	1.559443	3.409637	-1.870865
Mg10	-2.851873	-3.434815	1.579057
Mg11	1.890724	-3.310524	0.760139
Mg12	-1.387124	4.341492	-1.107642
Mg13	2.382068	2.185627	3.094036
Mg14	2.325493	-0.904835	2.723093
Mg15	0.444784	3.694586	1.130273
Mg16	3.495414	3.568898	0.540086
Mg17	-3.697378	2.511750	-1.607170
Mg18	4.634795	0.850249	1.483158
Mg19	4.141350	-3.700537	-1.409302
Mg20	-2.122532	-2.873093	-1.452567
Mg21	1.714184	-2.430945	-2.648971
Mg22	-0.799769	-0.902858	-3.440849
Mg23	-4.905834	-2.067410	-0.253753
Mg24	-0.429366	-2.099050	2.803397
Mg25	2.073787	0.974204	-0.112331
Mg26	-4.892055	-1.336280	2.736865
Mg27	4.669919	-2.107085	1.139856
Mg28	-3.608393	-0.388181	-2.355681

@mg28-isomer35 bp86/6-31G(d) Etot=-5602.640055 Eb=-15.43

Mg1	-1.426630	2.396681	-2.101886
Mg2	0.256922	0.624102	0.296185
Mg3	2.563556	3.049318	0.757744
Mg4	-2.110465	0.141000	2.244715
Mg5	3.256403	0.720980	-1.140458
Mg6	0.567373	-0.094488	-2.634546
Mg7	6.119090	-0.491678	-1.520888
Mg8	-2.617918	2.730380	0.818430
Mg9	-0.172333	4.154903	0.150208
Mg10	0.435209	-0.177912	3.979242
Mg11	2.169010	-2.126654	-0.876675
Mg12	5.089819	-3.276761	-1.574748
Mg13	-2.425530	-0.232051	-1.085566
Mg14	1.427969	2.856139	-2.055110
Mg15	-4.836906	0.498797	0.783750
Mg16	-4.447950	2.240126	-1.728913
Mg17	4.586485	-1.570455	1.009781
Mg18	-0.725583	-2.382345	0.027379
Mg19	-3.615546	-2.327672	1.174950
Mg20	2.869867	0.546419	2.457565
Mg21	-5.990016	-0.300728	-2.298837
Mg22	5.482379	1.353524	0.798536
Mg23	-4.155711	-2.661818	-1.839995
Mg24	1.641825	-2.246301	2.091812
Mg25	-6.471749	-2.066423	0.028429
Mg26	3.601350	-1.254198	-3.395396
Mg27	-1.202353	-2.603796	2.986041
Mg28	0.131434	2.500910	2.648249

@mg28-isomer36 bp86/6-31G(d) Etot=-5602.638738 Eb=-15.40

Mg1	0.630312	1.109211	-0.072152
Mg2	-1.321415	2.193349	-2.057549
Mg3	0.092503	-1.200790	1.899850
Mg4	4.009848	-1.085393	-1.533193
Mg5	2.783381	0.706784	2.105004
Mg6	2.189916	3.539319	1.211882
Mg7	-2.850756	-0.213926	2.541751
Mg8	-2.157355	-3.177524	1.098110
Mg9	1.022938	-1.766653	-1.166040
Mg10	3.086643	-2.153035	1.416737
Mg11	3.181718	-4.066754	-0.871058
Mg12	1.570535	3.557567	-1.879215
Mg13	5.616711	-0.086091	0.958962
Mg14	-0.346122	1.986489	2.625258
Mg15	-3.931462	-3.145588	-1.472430
Mg16	-4.345814	1.870656	-1.630335
Mg17	1.878703	0.689717	-2.819974
Mg18	3.870010	1.836101	-0.652870
Mg19	5.915108	-2.942320	0.098016
Mg20	-0.704521	4.206207	0.316426
Mg21	-2.212393	-0.474418	-0.594643
Mg22	-5.486508	0.935381	1.031361
Mg23	-5.768416	-0.775982	-1.431531
Mg24	1.472229	6.164181	-0.381524
Mg25	0.679498	-4.123880	0.798956
Mg26	-4.964553	-2.041914	1.190235
Mg27	-2.857794	2.350303	0.939710
Mg28	-1.052943	-3.890996	-1.669747

@mg28-isomer37 bp86/6-31G(d) Etot=-5602.638341 Eb=-15.39

Mg1	0.571539	2.523587	-0.030988
Mg2	2.909382	-3.645613	0.140246
Mg3	3.005395	1.835910	-1.799704
Mg4	4.937250	-1.483469	0.582735
Mg5	-1.116420	-0.572050	0.289857
Mg6	5.727968	0.514005	-1.533062
Mg7	-1.974101	1.730820	-1.432167
Mg8	3.273918	1.793406	1.364244
Mg9	6.227958	1.138990	1.393713
Mg10	-4.073838	0.174815	1.694464
Mg11	0.077948	-4.061147	0.745999
Mg12	-1.962718	2.292679	1.711321
Mg13	0.317867	-1.911108	2.875924
Mg14	3.440243	-1.333235	-2.212949
Mg15	-1.891252	-0.145736	3.749105
Mg16	-4.141600	-1.545378	-0.732080
Mg17	1.847532	-0.743098	0.474422
Mg18	-4.526256	0.837546	-2.634033
Mg19	0.587483	-2.757240	-1.956062
Mg20	0.599546	1.133482	2.742775
Mg21	-6.379531	0.641741	-0.350717
Mg22	-4.546021	2.967117	-0.083659
Mg23	-2.004604	-1.231782	-2.797635
Mg24	-2.031347	4.634728	-0.245919
Mg25	-2.533601	-2.703403	1.881390
Mg26	0.600104	0.238508	-2.360467
Mg27	5.201348	3.380459	-0.376957
Mg28	-2.144192	-3.704535	-1.099795

@mg28-isomer38 bp86/6-31G(d) Etot=-5602.627346 Eb=-15.15

Mg1	-2.717305	1.783847	-1.034429
Mg2	-3.159396	3.465178	1.406889
Mg3	0.204370	1.944070	-2.223960

Mg4	-0.214133	0.270536	0.333747
Mg5	2.023809	-2.086038	1.161007
Mg6	3.806746	2.243896	-1.960600
Mg7	-1.512595	-0.684291	-2.381844
Mg8	2.170144	-0.320660	-1.405023
Mg9	5.165078	-0.760610	-1.688350
Mg10	4.976258	-3.306206	0.632682
Mg11	1.843495	0.616226	2.631775
Mg12	-0.870362	4.247588	-0.466570
Mg13	4.314619	0.979604	0.758308
Mg14	-5.365392	1.349457	0.957150
Mg15	-1.218195	-2.337471	1.534120
Mg16	1.860500	2.835362	0.411754
Mg17	-4.520065	-0.623560	-1.594813
Mg18	-2.800310	-3.187356	-1.102935
Mg19	1.753123	4.504661	-2.119249
Mg20	6.734688	-0.902015	0.919028
Mg21	4.366624	-1.199443	2.866397
Mg22	-0.403521	2.746547	2.359094
Mg23	-2.567491	0.493953	2.158859
Mg24	-7.128507	-0.905226	0.359766
Mg25	-5.845948	-3.284326	-0.925992
Mg26	-4.310813	-1.808479	1.334037
Mg27	0.189568	-2.905931	-1.162891
Mg28	3.225011	-3.169316	-1.757958

@mg28-isomer39 bp86/6-31G(d) Etot=-5602.621652 Eb=-15.02

Mg1	-1.329260	-1.061300	-1.951686
Mg2	-0.843103	1.752662	-3.441419
Mg3	-2.399505	-0.762143	3.354175
Mg4	-2.565656	2.129976	2.439101
Mg5	-1.112820	1.922125	-0.363330
Mg6	1.120594	3.729350	-1.632395
Mg7	1.480491	0.690399	-1.878470
Mg8	1.512830	-2.301852	-1.784642
Mg9	-4.530511	-2.045625	-1.386412
Mg10	0.027341	-0.684505	0.787395
Mg11	-0.142950	-2.719492	2.968047
Mg12	3.403811	-0.372143	0.194779
Mg13	-6.182244	0.513531	-0.849014
Mg14	3.940067	2.545853	-1.004678
Mg15	2.675648	4.704271	0.748154
Mg16	-2.334054	-3.960454	-1.770052
Mg17	-0.002911	1.039752	3.556014
Mg18	2.745178	-3.103048	1.129167
Mg19	-3.590715	0.941291	-2.491414
Mg20	5.983575	-1.901729	1.180460
Mg21	-0.105945	-3.844143	0.185193
Mg22	5.986294	0.209329	-1.356160
Mg23	-4.133532	2.765348	-0.145964
Mg24	-3.284196	-0.135865	0.582376
Mg25	4.658770	-2.616207	-1.466350
Mg26	1.923222	1.775426	1.328339
Mg27	-2.831835	-3.075172	1.235091
Mg28	-0.068582	3.864363	1.833697

@mg28-isomer40 bp86/6-31G(d) Etot=-5602.607458 Eb=-14.70

Mg1	-1.258331	-1.072541	-2.928690
Mg2	1.513176	-0.029811	-1.979041
Mg3	4.168000	1.077972	-1.060682
Mg4	0.312188	-0.626601	2.002887
Mg5	-0.515350	2.040845	-3.346734
Mg6	3.125734	-0.452988	1.242948
Mg7	2.060936	3.042202	-2.262648

Mg8	-1.233579	-2.621130	-0.059642
Mg9	3.636383	-2.092573	-1.662011
Mg10	-4.119003	-3.209798	1.420490
Mg11	-6.477680	-2.021699	-0.007021
Mg12	1.754357	-3.019081	0.666859
Mg13	-3.740780	-1.346372	-1.067784
Mg14	0.828058	-3.069295	-2.254067
Mg15	1.654608	2.068788	0.647300
Mg16	-1.125077	0.704314	-0.469747
Mg17	-0.464671	3.754210	-0.726323
Mg18	5.167460	-2.734962	1.005516
Mg19	-3.414470	1.389679	-2.417847
Mg20	-2.688748	-0.518031	1.880762
Mg21	6.144205	0.133819	1.585775
Mg22	6.492298	-1.098072	-1.063105
Mg23	7.983781	2.039635	3.340509
Mg24	-5.409486	0.962684	-0.006476
Mg25	-5.695805	-0.794168	2.590284
Mg26	-3.267187	3.118726	0.112323
Mg27	-1.107472	2.445251	2.083862
Mg28	-4.323547	1.928997	2.732303

@mg28-isomer41 bp86/6-31G(d) Etot=-5602.598455 Eb=-14.50

Mg1	0.646944	1.120650	-0.356795
Mg2	-0.342808	-2.102434	-0.025459
Mg3	4.551018	1.006780	-1.433189
Mg4	2.957162	3.217357	-0.125779
Mg5	-1.368611	2.497853	-2.377408
Mg6	-3.009020	4.987562	-1.545468
Mg7	-1.957534	-4.656245	1.565671
Mg8	0.150136	4.381111	-0.333293
Mg9	-1.621599	-4.846261	-1.347672
Mg10	-2.302312	2.883831	0.731303
Mg11	-0.343593	-0.511116	-2.791867
Mg12	2.341880	-1.274394	-1.168794
Mg13	2.252984	-2.346751	1.741156
Mg14	-0.955917	4.868026	2.520394
Mg15	-1.124204	0.430710	2.232800
Mg16	1.393465	-0.170448	3.738673
Mg17	-2.785390	-2.175770	-2.192861
Mg18	-0.470162	-2.521122	3.174776
Mg19	3.267090	0.572860	1.376150
Mg20	5.007992	-1.842990	-2.761013
Mg21	-4.412732	-3.944562	-0.253174
Mg22	-3.055848	-1.747136	1.369834
Mg23	-2.424049	0.282467	-0.646782
Mg24	5.066848	-1.830651	0.296726
Mg25	1.103666	2.676500	2.322230
Mg26	-4.612723	2.279353	-1.532862
Mg27	7.313190	-0.497087	-1.351074
Mg28	-5.265873	-0.738092	-0.826225

@mg28-isomer42 bp86/6-31G(d) Etot=-5602.589723 Eb=-14.30

Mg1	-0.107243	-0.747021	0.179356
Mg2	-0.753734	-3.560341	0.592986
Mg3	2.131412	-2.814155	-0.138938
Mg4	4.808711	-1.587965	0.736538
Mg5	1.901236	-0.099507	-1.936450
Mg6	-3.104977	-4.020145	2.242486
Mg7	4.339296	-1.939673	-2.156794
Mg8	2.226642	-0.434431	1.977531
Mg9	4.813518	0.949302	2.343114
Mg10	-1.950708	1.561711	-0.343674
Mg11	-0.980013	-0.305116	-2.791995

Mg12	7.465693	-0.137738	1.451476
Mg13	2.999364	1.968343	0.076945
Mg14	-2.953033	-1.545013	-0.748965
Mg15	6.890278	-0.487242	-1.469136
Mg16	-3.138756	1.962667	3.276108
Mg17	6.158411	2.110162	-0.164980
Mg18	4.545039	1.206933	-2.496831
Mg19	-4.046532	3.501801	0.727333
Mg20	-3.884475	-0.519114	-3.658650
Mg21	-0.315473	1.167419	2.587195
Mg22	-2.540170	2.140156	-3.532924
Mg23	-4.826440	1.810599	-1.710069
Mg24	-4.804807	0.539007	1.019440
Mg25	-1.314401	3.947872	1.906574
Mg26	-5.277421	-2.550189	1.090698
Mg27	-5.921517	-1.054767	-1.496147
Mg28	-2.359899	-1.063556	2.437773

@mg29-isomer01 bp86/6-31G(d) Etot=-5802.819727 Eb=-17.28

Mg1	0.447690	-1.707764	0.058232
Mg2	-2.328653	3.278424	1.134125
Mg3	0.797131	-0.175656	3.014074
Mg4	-2.565563	0.779378	-3.157893
Mg5	-1.391998	-1.901906	-2.502964
Mg6	2.435581	-2.537876	2.249575
Mg7	3.481210	0.715824	2.232142
Mg8	-1.643726	0.394543	-0.152776
Mg9	0.343924	2.686193	2.618893
Mg10	1.277785	1.171035	0.132881
Mg11	0.331825	-4.744143	1.271452
Mg12	1.801542	-2.060503	-2.607882
Mg13	-1.062171	-2.383157	2.619110
Mg14	-3.839355	-1.618397	1.782202
Mg15	-1.058718	3.108920	-1.832757
Mg16	0.367098	0.608452	-2.778354
Mg17	-4.679888	1.203417	1.201055
Mg18	0.055760	-4.463158	-1.744529
Mg19	2.734159	-4.104580	-0.390725
Mg20	3.827323	-1.195255	-0.233368
Mg21	-2.332939	-3.494087	-0.038821
Mg22	-2.002404	0.637113	2.872344
Mg23	-4.147668	2.486596	-1.322943
Mg24	2.136796	3.344862	-1.814152
Mg25	3.271369	0.596722	-2.626099
Mg26	0.347652	4.684478	0.314851
Mg27	4.638889	1.902216	-0.364932
Mg28	2.996112	3.704377	1.275060
Mg29	-4.238762	-0.916067	-1.207801

@mg29-isomer02 bp86/6-31G(d) Etot=-5802.816564 Eb=-17.21

Mg1	-1.682424	0.690819	3.236864
Mg2	0.647601	-1.021487	2.812668
Mg3	0.925546	2.172175	2.959803
Mg4	-1.767930	3.189340	1.570462
Mg5	-2.162659	-2.235186	2.572706
Mg6	3.206997	0.268808	1.950017
Mg7	4.571178	-1.647257	-0.192613
Mg8	0.722324	4.805828	0.928743
Mg9	3.068446	-2.788636	2.158758
Mg10	3.316526	3.206927	1.254785
Mg11	0.347065	-3.870500	1.492934
Mg12	0.584039	1.623140	0.026233
Mg13	3.657635	1.126303	-1.131052
Mg14	-4.113769	1.029135	1.447292

Mg15	1.256847	-1.245028	-0.230267
Mg16	2.337254	3.950702	-1.521446
Mg17	-1.600855	-0.429817	0.226749
Mg18	-2.383493	-4.002113	0.118237
Mg19	-3.488255	2.992286	-0.932048
Mg20	1.252582	1.434322	-2.971769
Mg21	-4.560646	-1.905897	0.558618
Mg22	-4.591883	0.196517	-1.529123
Mg23	2.758090	-4.134179	-0.559099
Mg24	2.813116	-1.510393	-2.699388
Mg25	-0.681827	3.920117	-1.720318
Mg26	0.017455	-3.695335	-1.761250
Mg27	-0.043309	-1.163644	-3.338284
Mg28	-2.661963	-2.036168	-2.226815
Mg29	-1.743685	1.079220	-2.501399

@mg29-isomer03 bp86/6-31G(d) Etot=-5802.808935 Eb=-17.04

Mg1	0.604391	-0.295832	-2.645343
Mg2	3.698322	0.146920	-2.087239
Mg3	-0.727578	1.722060	-0.204686
Mg4	-4.329479	-1.070373	1.303436
Mg5	0.576098	-1.382853	2.734326
Mg6	-2.208609	-3.265983	2.045373
Mg7	-3.654266	0.710311	-1.150955
Mg8	-0.351612	4.705042	-1.298375
Mg9	4.057753	2.515368	-0.040860
Mg10	-0.676318	-3.219910	-2.139389
Mg11	0.560193	-3.821555	0.784821
Mg12	3.226262	-2.446351	1.605749
Mg13	-0.181295	1.633967	2.747706
Mg14	1.653172	-0.094758	0.180999
Mg15	-1.409287	2.123995	-3.021915
Mg16	-2.219614	-0.862176	-3.181881
Mg17	2.807983	1.141085	2.599889
Mg18	-3.127831	3.769833	-0.915561
Mg19	-1.246323	-1.108282	0.122636
Mg20	-3.200978	1.880880	1.714147
Mg21	5.060801	-2.331377	-0.898563
Mg22	-3.658136	-2.677471	-1.206449
Mg23	-2.200288	-0.472049	3.276150
Mg24	5.101108	-0.082505	0.980959
Mg25	1.500345	3.661281	1.100953
Mg26	-1.459348	4.425032	1.525209
Mg27	1.685805	2.496866	-1.989868
Mg28	2.218763	-2.719615	-1.682301
Mg29	-2.100034	-5.081550	-0.258967

@mg29-isomer04 bp86/6-31G(d) Etot=-5802.803626 Eb=-16.93

Mg1	2.095681	-0.325292	-0.000025
Mg2	-0.744247	-0.140859	0.000037
Mg3	-1.700538	-1.642830	-2.773642
Mg4	1.035388	-0.299054	-3.168259
Mg5	0.781682	-2.873549	-1.540304
Mg6	1.307491	2.330151	1.565818
Mg7	-4.291801	-2.441452	1.529792
Mg8	0.781651	-2.873471	1.540135
Mg9	1.035365	-0.299123	3.168274
Mg10	-4.077348	0.216281	3.075582
Mg11	-1.195342	3.102797	0.000051
Mg12	-1.390745	1.529592	2.730666
Mg13	-3.770197	2.882642	1.525226
Mg14	5.012570	-0.649244	0.000011
Mg15	4.050088	2.364899	0.000059
Mg16	-4.077353	0.216369	-3.075607

Mg17	1.307486	2.330181	-1.565749
Mg18	-1.390731	1.529650	-2.730596
Mg19	-3.770179	2.882710	-1.525186
Mg20	3.440888	-3.355110	-0.000038
Mg21	-1.700557	-1.642954	2.773696
Mg22	-1.848006	-3.212670	-0.000051
Mg23	-4.291818	-2.441423	-1.529874
Mg24	3.796447	0.901307	-2.580717
Mg25	3.796423	0.901217	2.580780
Mg26	-3.661052	0.185843	-0.000020
Mg27	3.513731	-2.039150	2.635370
Mg28	3.513769	-2.039071	-2.635396
Mg29	2.441256	4.901613	-0.000033

@mg29-isomer05 bp86/6-31G(d) Etot=-5802.803029 Eb=-16.92

Mg1	3.311662	-0.747963	2.897731
Mg2	0.290782	-1.996475	2.517573
Mg3	1.526988	0.173552	0.482771
Mg4	0.683962	0.700232	3.695443
Mg5	4.639510	-0.970392	0.102767
Mg6	1.612586	3.147230	-3.003083
Mg7	2.607816	-1.769296	-2.042428
Mg8	1.818869	3.115533	2.285183
Mg9	-2.873295	3.531316	-0.174912
Mg10	2.995696	3.864749	-0.372964
Mg11	4.606935	-3.900664	-1.155978
Mg12	0.085303	2.834490	-0.386148
Mg13	-2.544657	-0.579930	-2.963151
Mg14	-4.339795	1.459032	-1.713226
Mg15	-2.458525	-2.988476	1.292187
Mg16	-1.385691	2.298733	2.195990
Mg17	-1.769947	2.489027	-2.812885
Mg18	-4.128147	1.155641	1.363956
Mg19	-1.542719	0.025691	0.032014
Mg20	-4.370304	-1.354155	-0.531169
Mg21	-2.210242	-0.453366	3.216995
Mg22	0.117213	-2.601748	-0.425134
Mg23	3.503255	1.161207	-1.761468
Mg24	4.287161	1.755125	1.343187
Mg25	2.765289	-3.123898	1.074485
Mg26	-2.568424	-3.446163	-1.731791
Mg27	-4.849282	-1.615911	2.481317
Mg28	0.392134	0.330511	-2.481287
Mg29	-0.204129	-2.493633	-3.425975

@mg29-isomer06 bp86/6-31G(d) Etot=-5802.801602 Eb=-16.89

Mg1	2.301390	0.180839	-0.000012
Mg2	-0.458684	-0.352837	0.000028
Mg3	-1.032201	-1.977605	-2.801468
Mg4	1.289408	-0.006697	-3.091052
Mg5	1.684114	-2.683762	-1.548356
Mg6	0.928056	2.690585	1.565252
Mg7	-3.439014	-3.325996	1.535740
Mg8	1.684048	-2.683541	1.548345
Mg9	1.289347	-0.006570	3.091135
Mg10	-3.792396	-0.753934	3.107967
Mg11	-1.675023	2.598630	-0.000077
Mg12	-1.475690	1.164039	2.749432
Mg13	-4.202426	1.890611	1.572782
Mg14	5.165187	0.601471	0.000019
Mg15	3.450498	3.358289	-0.000045
Mg16	-3.792373	-0.754014	-3.107969
Mg17	0.928091	2.690616	-1.565379
Mg18	-1.475627	1.163958	-2.749520

Mg19	-4.202388	1.890611	-1.572925
Mg20	4.248848	-2.543597	0.000074
Mg21	-1.032227	-1.977565	2.801588
Mg22	-0.822597	-3.493951	0.000047
Mg23	-3.439006	-3.326072	-1.535705
Mg24	3.666800	1.884126	-2.549449
Mg25	3.666754	1.884190	2.549402
Mg26	-3.474764	-0.628198	-0.000020
Mg27	4.083158	-1.081766	2.562860
Mg28	4.083198	-1.081837	-2.562741
Mg29	-4.154480	4.679977	0.000048

@mg29-isomer07 bp86/6-31G(d) Etot=-5802.800507 Eb=-16.86

Mg1	0.330644	-3.162279	0.006017
Mg2	2.771765	-3.347013	2.011307
Mg3	1.628072	-0.405448	0.117624
Mg4	-1.470545	-0.312599	-0.105184
Mg5	1.122223	-1.818965	-2.700467
Mg6	0.081138	-2.269260	2.901694
Mg7	3.940447	-0.641640	-2.113950
Mg8	2.558517	3.661577	-0.648205
Mg9	2.894446	-0.430551	2.938232
Mg10	-1.856094	-2.636710	-2.045055
Mg11	-2.538657	-3.096119	1.176491
Mg12	-4.697021	-2.880743	-1.068232
Mg13	-1.143993	-0.222910	-3.777103
Mg14	-4.441169	-0.630507	0.905112
Mg15	4.179675	1.344277	0.352910
Mg16	-0.075585	0.697697	2.670297
Mg17	-2.939306	1.775953	2.061140
Mg18	4.201208	2.293311	-2.728046
Mg19	4.710951	-1.529975	0.764927
Mg20	-3.901898	-0.292458	-2.407797
Mg21	2.295028	2.674508	2.289972
Mg22	1.265707	1.269831	-2.594885
Mg23	3.198772	-3.355716	-0.999181
Mg24	-0.600799	3.708757	2.512847
Mg25	-2.623697	-1.003219	3.287811
Mg26	-2.019663	2.223786	-2.325428
Mg27	-4.389234	1.990311	-0.561884
Mg28	-2.461999	4.161138	0.132915
Mg29	-0.018933	2.234966	-0.053880

@mg29-isomer08 bp86/6-31G(d) Etot=-5802.797264 Eb=-16.79

Mg1	-0.571064	2.351150	-0.627724
Mg2	-1.673235	-0.449504	0.091503
Mg3	-3.924399	0.838021	1.924530
Mg4	-4.389763	-2.280465	1.702161
Mg5	-5.064759	-0.494918	-0.621654
Mg6	2.579647	3.252369	-0.450709
Mg7	-2.512802	3.396713	1.585569
Mg8	1.207246	3.107936	-3.115868
Mg9	3.256658	1.007431	-2.412591
Mg10	-3.621667	-2.991491	-1.163621
Mg11	-1.645853	-3.426656	1.130084
Mg12	0.592554	-1.766629	2.605421
Mg13	4.256038	0.950729	0.790191
Mg14	0.117847	0.194286	-2.839980
Mg15	1.444887	-0.020723	0.045980
Mg16	-2.191574	-1.097369	3.342083
Mg17	-0.832663	-2.577077	-2.117022
Mg18	2.744654	0.117266	3.470428
Mg19	3.661124	-2.004272	1.567728
Mg20	0.329665	4.184447	1.584308

Mg21	-3.653037	2.117829	-0.966758
Mg22	4.868576	-1.227877	-1.184944
Mg23	-0.244900	1.220132	2.493393
Mg24	2.261774	-1.932676	-2.512868
Mg25	-3.007447	-0.463760	-2.877864
Mg26	4.058852	-4.044503	-0.697511
Mg27	-1.990658	2.339470	-3.385828
Mg28	2.755675	2.879976	2.581724
Mg29	1.188625	-3.179834	0.059837

@mg29-isomer09 bp86/6-31G(d) Etot=-5802.796897 Eb=-16.78

Mg1	4.867346	0.367836	-0.444642
Mg2	3.357952	-0.939678	-2.712000
Mg3	4.335103	-2.524077	-0.121745
Mg4	3.054594	2.334696	-1.887855
Mg5	1.229068	0.913584	-3.856307
Mg6	2.056621	-3.567395	-1.632724
Mg7	3.321844	2.357148	1.213246
Mg8	3.551694	-0.689740	2.193568
Mg9	1.633461	-0.231575	-0.204196
Mg10	1.520135	4.509324	-0.180037
Mg11	0.072635	-1.586393	-2.608712
Mg12	-3.234683	2.336734	-1.129924
Mg13	-0.085884	2.266695	-1.594959
Mg14	1.824026	-3.333197	1.387885
Mg15	-1.547229	4.493202	0.299487
Mg16	0.164319	2.153960	1.499152
Mg17	-0.828659	-3.649531	-0.589263
Mg18	-1.347655	-0.229993	0.020823
Mg19	1.997963	1.411011	3.698299
Mg20	-1.870916	0.649346	-3.346196
Mg21	-3.099416	2.084093	1.866227
Mg22	0.370408	-0.995649	2.633890
Mg23	-1.204625	-3.472107	2.362310
Mg24	-4.496067	-0.228307	0.258442
Mg25	-1.186929	1.201665	3.992992
Mg26	-3.632270	-3.110551	0.728960
Mg27	-3.003788	-1.947853	-1.997701
Mg28	-4.846706	0.355883	-2.707024
Mg29	-2.972342	-0.929131	2.858006

@mg29-isomer10 bp86/6-31G(d) Etot=-5802.796049 Eb=-16.77

Mg1	-0.150845	5.628666	-1.068226
Mg2	1.472350	1.743204	-2.603002
Mg3	2.575329	4.051015	-0.875769
Mg4	-1.607119	1.523977	-2.503220
Mg5	-2.703054	4.067015	-1.086806
Mg6	0.083737	2.520197	-0.061911
Mg7	-2.522259	2.483257	1.582550
Mg8	-3.077646	-1.206372	-2.323932
Mg9	4.116320	1.300541	-0.974200
Mg10	0.180535	-0.982752	-2.389534
Mg11	-5.052159	1.059181	2.077894
Mg12	3.137295	-0.743179	-3.051448
Mg13	-4.088608	1.319701	-0.869060
Mg14	2.961502	2.369714	1.695852
Mg15	1.731153	-0.142807	0.288325
Mg16	-1.322127	-0.327810	0.209991
Mg17	0.128863	1.282003	2.695833
Mg18	4.807843	-0.147750	1.617086
Mg19	2.110528	-3.552193	-2.581921
Mg20	-1.071820	-3.715486	-2.011517
Mg21	-2.583993	-0.445519	2.989713
Mg22	2.652312	-0.001419	3.663457

Mg23	-3.829821	-3.905719	-1.026446
Mg24	-4.406601	-1.419379	0.570388
Mg25	4.031001	-2.194745	-0.578704
Mg26	0.937253	-3.019340	0.197383
Mg27	0.266172	-1.719905	2.863426
Mg28	3.215488	-2.580113	2.256918
Mg29	-1.991629	-3.243983	1.296880

@mg29-isomer11 bp86/6-31G(d) Etot=-5802.795166 Eb=-16.75

Mg1	3.171155	3.268645	-1.116082
Mg2	1.667386	-2.061743	2.857731
Mg3	-4.512799	0.578393	-0.466221
Mg4	-2.960311	-1.142414	-2.494401
Mg5	3.048771	0.685029	-2.688606
Mg6	0.948264	0.879705	2.871067
Mg7	3.823937	0.142522	3.073186
Mg8	2.206508	-3.559973	-0.286698
Mg9	1.532282	-0.515949	0.002455
Mg10	-3.721092	-1.831167	1.598608
Mg11	2.150627	-2.223996	-3.173582
Mg12	0.018793	0.066137	-2.641523
Mg13	-2.989876	-3.678395	-0.676074
Mg14	4.498899	-1.889300	-1.557512
Mg15	-3.913285	0.973326	2.550828
Mg16	-5.446838	-2.208220	-0.952036
Mg17	0.848932	2.936237	-2.877631
Mg18	-1.393605	4.518849	-1.469121
Mg19	-0.385353	-2.756165	-1.787147
Mg20	-1.452950	-0.742361	3.432232
Mg21	3.018696	2.804018	1.834551
Mg22	-0.682176	-2.727006	1.181284
Mg23	0.361528	2.416744	0.151975
Mg24	-3.096230	3.095915	0.465927
Mg25	4.385050	0.687278	0.062979
Mg26	-1.551803	0.070364	0.211388
Mg27	-2.459082	1.897291	-2.353710
Mg28	-1.444729	2.567951	2.862164
Mg29	4.329301	-2.251716	1.383972

@mg29-isomer12 bp86/6-31G(d) Etot=-5802.794868 Eb=-16.74

Mg1	2.910093	2.079505	2.794851
Mg2	1.622801	-0.002705	-0.368469
Mg3	3.444465	-0.794463	2.106632
Mg4	3.895593	-3.751925	1.630474
Mg5	-0.243473	2.414610	-0.208431
Mg6	-1.448165	-0.321820	-0.069648
Mg7	-1.185976	-3.358712	0.552686
Mg8	0.059969	3.367851	2.692162
Mg9	0.412137	0.336720	2.463287
Mg10	-3.502118	2.005679	-0.537152
Mg11	-1.710352	2.706459	-2.841957
Mg12	-2.058604	-1.491143	2.881537
Mg13	-4.382927	-0.419756	1.162769
Mg14	2.491197	-1.967660	-3.067427
Mg15	2.389369	3.947065	0.625748
Mg16	2.261356	2.704320	-2.079338
Mg17	-2.500418	4.241338	1.154277
Mg18	-4.045850	-3.397992	1.557942
Mg19	4.035581	0.488224	-2.881280
Mg20	-3.480389	-2.471088	-1.272352
Mg21	1.741655	-3.022150	-0.318250
Mg22	-0.492309	-2.265766	-2.348109
Mg23	-2.590186	-0.144567	-3.135635
Mg24	0.471872	0.491335	-3.224559

Mg25	4.434997	-1.662906	-0.745559
Mg26	4.233168	1.493775	0.076495
Mg27	-5.241024	-0.135444	-1.759012
Mg28	0.999021	-2.648066	2.634832
Mg29	-2.521480	1.579284	2.523487

@mg29-isomer13 bp86/6-31G(d) Etot=-5802.793616 Eb=-16.71

Mg1	1.319982	-1.260556	-0.130937
Mg2	0.820231	1.544617	0.171558
Mg3	1.283161	-0.188712	2.831564
Mg4	1.092171	4.991065	0.375769
Mg5	1.412717	0.234910	-3.773578
Mg6	3.858195	0.570787	1.379101
Mg7	-1.147537	1.682860	2.637128
Mg8	-0.928225	1.437454	-2.466904
Mg9	-1.722581	-0.178115	0.057161
Mg10	-0.989170	-3.414240	-0.025360
Mg11	0.897872	-3.254723	2.266646
Mg12	-1.512564	3.687193	-0.061231
Mg13	-3.428406	-2.966571	-1.728758
Mg14	4.655294	-1.851971	-0.495834
Mg15	-3.755812	2.194052	-1.533075
Mg16	-3.718779	-2.779664	1.247469
Mg17	-4.861737	-0.424817	-0.323494
Mg18	-4.042914	-0.134204	2.608569
Mg19	3.615943	3.291664	0.093961
Mg20	3.600598	0.669407	-1.691181
Mg21	2.674257	-4.161725	-0.080708
Mg22	2.625771	-2.258690	-2.668137
Mg23	1.757635	2.978392	-2.304891
Mg24	-3.380833	-0.359496	-3.029866
Mg25	-0.610299	-1.679144	-2.608400
Mg26	2.013137	2.829622	2.651833
Mg27	-3.825269	2.529460	1.451412
Mg28	-1.403967	-1.475795	2.888184
Mg29	3.701130	-2.253059	2.261996

@mg29-isomer14 bp86/6-31G(d) Etot=-5802.791606 Eb=-16.67

Mg1	-2.527457	4.329675	-0.836075
Mg2	-0.512175	0.670580	2.557635
Mg3	0.100273	-2.199326	2.114469
Mg4	0.009911	4.984155	0.637873
Mg5	-3.828400	0.047852	1.964045
Mg6	4.160389	1.695674	1.532123
Mg7	2.626950	-3.285622	1.034587
Mg8	-2.484086	2.916657	1.882526
Mg9	4.259158	0.774252	-1.417949
Mg10	-3.430372	-0.517139	-2.978999
Mg11	4.765758	-1.147316	1.209710
Mg12	-0.311724	2.035228	-0.236904
Mg13	0.965887	-2.798769	-1.512009
Mg14	2.680040	3.352355	-0.482406
Mg15	-4.728447	-1.471017	-0.502012
Mg16	-3.763222	1.493818	-0.683315
Mg17	4.189684	-2.355334	-1.405706
Mg18	1.493846	2.801323	2.288480
Mg19	2.416488	-0.295679	3.061290
Mg20	-2.192745	-1.457240	3.875942
Mg21	2.614975	-0.914709	-3.378355
Mg22	-1.390658	-0.707053	-0.161985
Mg23	-0.602079	-4.584488	0.358469
Mg24	-1.742757	1.979114	-2.852508
Mg25	1.413312	1.754946	-2.692532
Mg26	-0.412248	-0.725585	-3.137026

Mg27	-3.057177	-3.021571	1.400012
Mg28	-2.388044	-3.145530	-1.682296
Mg29	1.674919	-0.209252	0.042914

@mg29-isomer15 bp86/6-31G(d) Etot=-5802.791207 Eb=-16.66

Mg1	-2.139760	1.723333	-3.665512
Mg2	-1.588822	-0.260523	0.157367
Mg3	-2.489958	-1.217872	-2.829808
Mg4	-2.545156	-4.038932	-2.025338
Mg5	-0.045040	2.467062	0.143794
Mg6	1.691540	-0.030599	0.173625
Mg7	0.267750	-2.599351	-1.009189
Mg8	0.754055	3.241352	-2.694539
Mg9	0.108790	0.288605	-2.375859
Mg10	4.311565	1.613529	0.821218
Mg11	2.099519	2.835587	2.380881
Mg12	2.563284	-1.419005	-2.918077
Mg13	4.581628	-1.048503	-0.796661
Mg14	-2.954533	-1.528402	2.707940
Mg15	-2.344069	3.667439	-1.512257
Mg16	-2.914016	2.581040	1.228626
Mg17	2.719166	3.844322	-0.449610
Mg18	3.233811	-3.838650	-1.376870
Mg19	-3.371446	1.253889	3.864197
Mg20	2.809665	-2.733794	1.321711
Mg21	-1.975029	-3.645687	0.813830
Mg22	0.076318	-1.920993	2.238789
Mg23	2.412833	-0.062330	3.151100
Mg24	-0.496706	1.023953	2.913183
Mg25	-4.240268	-2.030331	-0.366604
Mg26	-4.001390	1.030054	-1.325511
Mg27	5.124381	-0.991579	2.159719
Mg28	-4.938080	0.287380	1.476409
Mg29	3.289969	1.509006	-2.206556

@mg29-isomer16 bp86/6-31G(d) Etot=-5802.790130 Eb=-16.64

Mg1	-4.168921	0.040977	0.238597
Mg2	-0.826940	1.424773	0.217819
Mg3	-3.782740	-0.835323	-2.556951
Mg4	-3.667738	2.970799	1.112595
Mg5	-1.777962	4.675009	-0.384509
Mg6	1.555630	-0.257973	-0.317693
Mg7	4.321765	-0.336281	-2.326418
Mg8	0.213424	2.761710	-2.280512
Mg9	2.216690	2.247235	1.531294
Mg10	0.262063	0.426424	3.089812
Mg11	-1.618619	-3.042214	-2.021185
Mg12	-0.726447	3.342163	2.360921
Mg13	-3.006153	2.139551	-1.863268
Mg14	-2.726296	0.634392	2.796003
Mg15	3.133316	2.381724	-1.410783
Mg16	1.183712	4.572608	-0.015059
Mg17	3.242820	0.041906	3.340999
Mg18	1.501850	-2.180183	2.138405
Mg19	1.946595	0.745301	-3.677842
Mg20	-1.196784	-1.454029	0.647529
Mg21	0.754845	-3.809148	-0.249746
Mg22	-2.113971	-4.380329	0.807681
Mg23	-0.780789	-0.135058	-2.483324
Mg24	1.483597	-2.127689	-2.737523
Mg25	-3.788695	-2.248375	2.309259
Mg26	4.660407	-2.277011	2.189251
Mg27	-4.412136	-2.988168	-0.524388
Mg28	3.607536	-2.663007	-0.511908

Mg29	4.509941	0.330215	0.580942
@mg29-isomer17 bp86/6-31G(d) Etot=-5802.789324 Eb=-16.62			
Mg1	0.550367	0.228958	0.111226
Mg2	1.873366	1.506305	2.858233
Mg3	-2.899133	-0.692631	3.387973
Mg4	3.025898	-0.903556	1.477311
Mg5	5.911795	1.460452	-0.601735
Mg6	-1.326056	-2.579518	-1.487389
Mg7	-2.395832	-0.273468	0.224061
Mg8	-2.011079	-2.994262	1.568555
Mg9	-1.883960	2.657837	-0.326022
Mg10	-0.255088	-0.124749	-2.906400
Mg11	3.159774	2.360704	0.140358
Mg12	-4.647474	2.347098	-1.644295
Mg13	0.815085	2.560461	-1.895702
Mg14	-2.007023	2.301427	-3.270990
Mg15	0.102302	-1.149014	2.855393
Mg16	-5.973483	-0.038676	-0.686462
Mg17	-3.440569	-0.320644	-2.631668
Mg18	6.065525	-1.117945	0.881476
Mg19	0.902196	-2.985807	0.514491
Mg20	4.986096	1.288593	2.366041
Mg21	5.792401	-1.058096	-2.180412
Mg22	-4.392127	1.551045	1.457759
Mg23	-1.182038	1.608288	2.477872
Mg24	1.489895	-2.565519	-2.492985
Mg25	0.617665	3.598916	1.070808
Mg26	-4.322360	-2.563025	-0.650804
Mg27	-5.349463	-1.418810	1.888171
Mg28	2.961955	0.121433	-1.835329
Mg29	3.831366	-2.805798	-0.669534
@mg29-isomer18 bp86/6-31G(d) Etot=-5802.789323 Eb=-16.62			
Mg1	0.272579	-2.120880	-2.610751
Mg2	4.578909	-2.317699	0.634500
Mg3	1.584969	0.923569	3.013759
Mg4	-1.543501	1.050486	3.384508
Mg5	-1.287032	-1.939606	0.005595
Mg6	-1.224820	0.941849	0.391092
Mg7	-0.562311	-4.752753	-1.146338
Mg8	-4.290005	0.854858	1.817286
Mg9	0.720417	2.814705	-1.452425
Mg10	0.121133	3.269987	1.699242
Mg11	2.064216	0.396271	-3.058482
Mg12	2.953575	2.519549	0.638249
Mg13	-4.512451	-1.630670	0.035344
Mg14	3.648041	2.902319	-2.387532
Mg15	4.509437	0.341137	-1.035547
Mg16	-2.304243	3.412888	-2.150493
Mg17	1.613686	-3.324934	0.519929
Mg18	4.420975	0.328457	2.012297
Mg19	2.879541	-1.995585	3.013468
Mg20	1.509187	-0.262589	0.000770
Mg21	-3.871198	0.942585	-1.350914
Mg22	-0.972566	5.291531	-0.304853
Mg23	3.203726	-2.221881	-1.945862
Mg24	-2.965088	-1.810255	-2.568684
Mg25	-3.053523	3.432903	0.846504
Mg26	-3.036161	-1.647732	2.640091
Mg27	-0.959320	0.563008	-2.599067
Mg28	-3.492584	-4.383410	-0.728334
Mg29	-0.005586	-1.578108	2.686647

@mg29-isomer19 bp86/6-31G(d) Etot=-5802.778519 Eb=-16.39

Mg1	-0.826588	0.333625	0.319073
Mg2	-3.833311	-1.679989	1.861122
Mg3	-1.269066	3.354835	-2.282164
Mg4	0.209633	-2.224668	-1.398625
Mg5	3.466587	-2.478211	-1.736336
Mg6	1.786319	-0.748484	-3.529832
Mg7	-1.400093	-0.597807	3.187721
Mg8	-2.758199	-1.603407	-1.157921
Mg9	-0.693304	2.486748	2.653792
Mg10	0.767238	3.093548	-0.004246
Mg11	-3.478118	1.506225	-1.297340
Mg12	4.355976	0.466625	-2.684783
Mg13	-1.219761	-3.141919	1.108736
Mg14	-5.312311	-0.641187	-2.545513
Mg15	2.539372	2.818903	2.365963
Mg16	3.861411	2.395141	-0.350099
Mg17	1.812693	-4.200744	0.245872
Mg18	2.073047	0.030285	-0.346625
Mg19	1.668694	2.188117	-2.711712
Mg20	-3.529320	1.359252	1.918770
Mg21	1.324553	0.565798	3.788768
Mg22	5.654276	-0.357745	-0.198053
Mg23	1.293547	-1.755983	1.983507
Mg24	-5.496802	-2.788575	-0.464271
Mg25	-2.301051	3.721100	0.432650
Mg26	4.301975	-2.726118	1.133325
Mg27	-5.950162	0.116298	0.293318
Mg28	3.849643	0.103649	2.208411
Mg29	-0.896880	0.404690	-2.793506

@mg29-isomer20 bp86/6-31G(d) Etot=-5802.774381 Eb=-16.30

Mg1	-1.048356	0.811042	0.097208
Mg2	-0.058761	-2.008735	1.455960
Mg3	-1.218472	3.935421	-1.268107
Mg4	-0.402984	-1.538491	-1.737766
Mg5	2.584509	-2.373466	-2.069718
Mg6	1.336086	-0.055101	-3.714748
Mg7	-2.605451	-1.502521	2.912208
Mg8	-3.335804	-0.426064	-1.447736
Mg9	-0.383988	0.863508	3.003577
Mg10	0.797132	3.077921	1.110501
Mg11	-3.882635	2.606880	-1.039326
Mg12	3.924029	0.537031	-2.332118
Mg13	-2.575021	-3.039687	0.107146
Mg14	-6.109552	0.487247	-0.624333
Mg15	2.615257	1.783194	3.036754
Mg16	3.721808	2.426913	0.228955
Mg17	0.556192	-4.233450	-0.545499
Mg18	1.871200	-0.041886	0.084734
Mg19	1.356388	2.316058	-1.839058
Mg20	-3.799574	0.957037	1.665183
Mg21	1.973638	-1.079669	3.333840
Mg22	6.255471	0.902274	-0.486715
Mg23	2.920511	-2.920706	0.898214
Mg24	-5.536848	-2.429597	-1.584065
Mg25	-2.251267	3.516259	1.435885
Mg26	5.223460	-1.869741	-0.742372
Mg27	-5.123766	-1.710616	1.243671
Mg28	4.477730	-0.377248	1.748606
Mg29	-1.280934	1.386191	-2.930880

@mg29-isomer21 bp86/6-31G(d) Etot=-5802.770890 Eb=-16.22

Mg1	0.918082	-2.935120	1.445651
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Mg2	2.931307	0.384480	-0.552755
Mg3	-2.043260	-2.584900	1.334805
Mg4	3.731230	-2.198295	0.858877
Mg5	-0.004760	-0.341567	-0.012361
Mg6	4.906565	-1.334590	-2.132352
Mg7	-3.486968	-0.366188	2.970331
Mg8	5.183073	0.122138	2.281115
Mg9	6.682517	-1.422832	0.252876
Mg10	-4.922178	-2.125366	0.574270
Mg11	-3.286199	-2.119444	-2.155102
Mg12	1.139284	2.860131	0.307725
Mg13	-1.609930	2.902279	-0.530363
Mg14	-2.835093	0.097269	0.009794
Mg15	-0.530849	-1.061637	3.473783
Mg16	-5.891200	0.596722	1.194370
Mg17	-2.625963	0.999533	-2.891393
Mg18	-0.745323	-3.307138	-1.214387
Mg19	-0.618957	-1.135959	-3.314022
Mg20	2.055069	0.246183	2.395340
Mg21	-5.613105	-0.268521	-1.735057
Mg22	5.924639	1.265483	-0.792048
Mg23	4.041094	2.632620	1.227715
Mg24	-4.669772	2.408607	-0.985378
Mg25	3.417983	2.971745	-1.895793
Mg26	-3.601636	2.535912	1.853659
Mg27	1.933141	-2.068841	-1.815405
Mg28	0.420244	1.618616	-2.433868
Mg29	-0.799034	1.628681	2.279973

@mg29-isomer22 bp86/6-31G(d) Etot=-5802.769734 Eb=-16.20

Mg1	0.067289	-0.201842	-0.290535
Mg2	-2.028703	1.714982	-1.421558
Mg3	2.216680	-1.208490	-2.608379
Mg4	2.861463	-0.063849	0.143598
Mg5	-1.032263	3.487246	1.012450
Mg6	3.380987	-2.120993	2.363597
Mg7	-0.917710	-3.510850	-0.581541
Mg8	1.890944	-3.001840	-0.134015
Mg9	-1.530065	-1.331339	-2.660360
Mg10	4.211171	2.455896	-0.197518
Mg11	-4.957065	2.707752	-1.361379
Mg12	0.022789	-2.166161	2.096251
Mg13	5.279801	0.061334	-2.138000
Mg14	-3.620538	2.075814	1.296211
Mg15	-2.683853	-0.961110	0.503176
Mg16	-6.325318	0.797782	0.557967
Mg17	4.242990	0.928332	2.709929
Mg18	4.859043	-2.350330	-0.463772
Mg19	-4.552173	-0.222281	-1.876689
Mg20	-3.762527	-3.120217	-1.572614
Mg21	1.549565	2.239807	1.840149
Mg22	0.272908	0.945031	-3.394736
Mg23	3.106865	1.802788	-3.010967
Mg24	-1.161546	0.751882	2.605026
Mg25	1.018750	2.704509	-1.097021
Mg26	1.535620	-0.116049	3.655097
Mg27	-5.664895	-2.052477	0.540504
Mg28	-4.521005	-0.365266	2.817958
Mg29	6.240797	0.119940	0.667173

@mg29-isomer23 bp86/6-31G(d) Etot=-5802.769678 Eb=-16.20

Mg1	1.290594	-0.909817	-0.176800
Mg2	1.204808	-2.118767	2.587875
Mg3	3.314470	3.674985	-0.516757

Mg4	-3.693905	-2.121224	-2.252646
Mg5	-0.784998	-1.156352	-2.632209
Mg6	4.018781	-2.335524	-1.638004
Mg7	2.097623	-0.281595	-3.177841
Mg8	1.059313	1.841609	3.973841
Mg9	-3.677915	0.178696	2.366551
Mg10	0.496391	3.554510	1.287617
Mg11	3.017978	2.638847	-3.305362
Mg12	-2.272169	3.069413	2.266777
Mg13	-1.846171	-2.156049	2.765489
Mg14	-2.207749	-0.499744	-0.173709
Mg15	-0.486579	0.598946	1.828258
Mg16	0.954029	1.818244	-1.173974
Mg17	2.506342	-3.939883	0.404478
Mg18	-3.644609	1.022603	-2.485464
Mg19	3.323158	-0.308489	3.972540
Mg20	1.285506	-3.319249	-2.297743
Mg21	-0.728368	-3.271485	0.176068
Mg22	-0.902348	1.872052	-3.475698
Mg23	4.130419	0.663165	-1.114149
Mg24	-3.787662	-3.037689	0.713553
Mg25	-1.834882	2.995240	-0.736462
Mg26	-4.443629	2.195570	0.253942
Mg27	2.856237	1.427003	1.522450
Mg28	-5.304927	-0.623881	-0.276617
Mg29	4.060263	-1.471137	1.313997

@mg29-isomer24 bp86/6-31G(d) Etot=-5802.766757 Eb=-16.13

Mg1	-0.732420	1.185164	-0.189641
Mg2	-3.920019	1.910698	0.013284
Mg3	1.933801	-0.128187	0.199220
Mg4	0.737220	3.774983	-1.113970
Mg5	0.457477	1.313991	-3.017298
Mg6	-0.188985	-1.678634	-1.174398
Mg7	1.180537	2.244321	2.109220
Mg8	-1.586005	-0.674279	-3.814004
Mg9	-1.907755	2.716447	2.147022
Mg10	-3.591858	-0.694111	-1.610900
Mg11	-2.390245	2.153264	-2.606087
Mg12	-2.336868	-3.352300	-2.538322
Mg13	2.038706	-1.013635	3.148076
Mg14	-0.664274	0.267032	3.536859
Mg15	-5.279622	-1.001071	0.965173
Mg16	-4.200709	0.995388	3.102704
Mg17	2.657605	-0.668289	-2.830232
Mg18	2.158779	-3.449736	0.785633
Mg19	-0.333387	-2.474704	1.977876
Mg20	-3.164546	-3.291399	0.323596
Mg21	-2.150803	4.520276	-0.530049
Mg22	4.109466	1.088842	2.372809
Mg23	4.568526	-1.761025	1.636864
Mg24	-2.413091	-0.613523	1.308903
Mg25	3.436638	3.255379	0.352337
Mg26	3.149832	2.335460	-2.416661
Mg27	-0.518523	-4.756295	-0.253056
Mg28	4.158427	-2.642606	-1.230340
Mg29	4.792094	0.438551	-0.654616

@mg29-isomer25 bp86/6-31G(d) Etot=-5802.765626 Eb=-16.11

Mg1	-0.853645	-0.652867	0.079177
Mg2	-3.276899	0.139576	-1.614383
Mg3	-0.885811	2.241525	-1.626797
Mg4	1.094573	-1.928597	2.615698
Mg5	2.496174	-2.618249	-2.021948

Mg6	-1.005268	-2.696753	-2.234067
Mg7	2.189732	-0.230707	0.106644
Mg8	3.685967	0.045348	-2.934394
Mg9	0.610222	-0.199752	-2.695770
Mg10	2.178982	2.363064	-1.574474
Mg11	-2.736086	1.997410	1.065157
Mg12	-1.081013	0.158884	3.063874
Mg13	1.958664	0.861528	3.350679
Mg14	0.733537	-3.529289	0.161078
Mg15	5.150951	1.551302	-0.792864
Mg16	4.760805	-0.068957	1.773850
Mg17	-1.696766	4.855117	0.048442
Mg18	0.287865	2.170613	1.165392
Mg19	-3.859137	-0.708181	1.623048
Mg20	-3.752115	3.229581	-1.540137
Mg21	1.282342	4.790696	0.053335
Mg22	-1.807101	-2.944942	1.881194
Mg23	5.330690	-1.469156	-0.886504
Mg24	-6.314422	-1.115949	-0.288044
Mg25	-1.855184	-5.061708	-0.385502
Mg26	-3.708882	-2.747257	-0.639310
Mg27	3.568182	-2.883717	0.959753
Mg28	3.324366	2.727848	1.264783
Mg29	-5.820727	1.723588	0.022090

@mg29-isomer26 bp86/6-31G(d) Etot=-5802.764349 Eb=-16.08

Mg1	0.875879	-0.048695	-0.147608
Mg2	2.300733	-2.003523	-2.314210
Mg3	-3.099489	-0.876286	-2.616723
Mg4	3.437196	0.771869	-1.189271
Mg5	5.948336	-0.128357	0.437288
Mg6	-0.512261	2.810481	0.620967
Mg7	-2.025716	0.007000	0.173784
Mg8	-1.936652	1.969257	-2.207118
Mg9	-2.547849	-1.856276	3.057762
Mg10	1.387436	1.493999	2.635485
Mg11	1.707338	-3.315839	0.420130
Mg12	-4.513403	0.087691	2.024533
Mg13	0.338654	-1.379537	2.612698
Mg14	-1.584428	1.049445	3.039369
Mg15	0.000238	-0.156386	-3.301708
Mg16	-6.439250	1.575791	0.305922
Mg17	-3.596256	2.629702	0.430116
Mg18	5.408428	-1.052753	-2.417856
Mg19	0.943004	2.454957	-2.030942
Mg20	4.551217	-2.809944	-0.246999
Mg21	4.417732	1.852008	2.250361
Mg22	-3.549255	-2.462901	0.091359
Mg23	-0.674270	-2.506538	-1.498932
Mg24	2.475109	3.357365	0.470291
Mg25	-1.125628	-3.856401	1.225357
Mg26	-4.914247	1.563086	-2.227406
Mg27	-5.936352	-1.090404	-1.025548
Mg28	3.240747	-0.914708	1.764797
Mg29	5.423010	2.835897	-0.335897

@mg29-isomer27 bp86/6-31G(d) Etot=-5802.759251 Eb=-15.97

Mg1	-1.976826	0.126307	0.105238
Mg2	1.109062	-2.325650	1.907159
Mg3	-0.098507	0.904584	-2.576863
Mg4	0.943937	0.252313	0.250584
Mg5	-4.247884	-1.578207	2.032562
Mg6	-1.772621	-2.994815	1.240135
Mg7	-3.069390	3.049983	0.075365

Mg8	-3.053855	0.168638	-2.711800
Mg9	-0.264762	-2.030866	-1.450313
Mg10	2.487822	-0.598868	-2.334530
Mg11	-3.698290	-2.255499	-0.972870
Mg12	-2.038414	3.203552	-2.781917
Mg13	-5.035065	0.433764	-0.224382
Mg14	-4.943065	2.675840	-2.271500
Mg15	5.331196	-1.612922	-1.408673
Mg16	0.517857	-4.802218	0.152806
Mg17	2.730166	-3.037694	-0.638601
Mg18	1.537983	0.635352	3.196112
Mg19	-1.402912	-0.623381	3.189590
Mg20	3.664891	-0.802183	1.206911
Mg21	-2.206761	-4.904159	-1.184711
Mg22	1.752836	3.530741	1.976764
Mg23	0.015959	3.127156	-0.516456
Mg24	3.108028	2.092253	-0.640102
Mg25	4.225981	1.948901	2.338911
Mg26	5.089466	1.030638	-2.754041
Mg27	6.045103	0.887804	0.021611
Mg28	-3.815487	1.241037	2.472317
Mg29	-0.936447	2.257599	2.300695

@mg29-isomer28 bp86/6-31G(d) Etot=-5802.758669 Eb=-15.96

Mg1	1.056871	-2.537242	1.749098
Mg2	6.102444	-2.318180	0.541918
Mg3	-5.011825	0.155371	1.278318
Mg4	2.646050	2.208173	1.584615
Mg5	3.471342	-0.677419	1.143899
Mg6	4.805386	-1.212936	-1.760741
Mg7	-2.793561	1.259045	-3.062131
Mg8	-1.348515	-1.371136	-2.494866
Mg9	-4.532866	-0.904392	-1.674462
Mg10	-1.910131	-2.031056	0.946247
Mg11	3.182778	-3.393217	-0.314488
Mg12	-2.236233	0.681998	-0.182390
Mg13	-3.005248	-3.698779	-1.384804
Mg14	0.224972	1.419965	-2.505251
Mg15	6.017242	0.861603	0.118127
Mg16	4.827530	3.552132	-0.011423
Mg17	-5.086129	-2.741551	0.597320
Mg18	0.723741	0.405104	3.196285
Mg19	-4.978351	2.204028	-1.027601
Mg20	1.456243	3.720089	-0.679161
Mg21	0.608053	-0.016567	0.155441
Mg22	-0.463449	2.710374	1.553021
Mg23	3.122958	1.268863	-1.363157
Mg24	1.760645	-1.373803	-2.403159
Mg25	-2.351412	0.636505	2.848942
Mg26	-1.103668	-1.878346	3.874202
Mg27	0.109881	-3.491718	-0.981430
Mg28	-1.705204	3.500762	-1.111612
Mg29	-3.589545	3.062331	1.369243

@mg29-isomer29 bp86/6-31G(d) Etot=-5802.753038 Eb=-15.84

Mg1	-0.742522	-1.848221	-1.432262
Mg2	0.650235	-1.317860	1.409825
Mg3	2.275137	-2.029188	-1.340248
Mg4	-4.632270	-0.686627	1.488734
Mg5	-1.599570	0.698477	0.150355
Mg6	-4.462081	1.341707	-0.955109
Mg7	-3.958800	2.103224	1.926596
Mg8	-1.363964	3.216743	2.793477
Mg9	1.385746	0.931273	-0.496472

Mg10	-3.706826	-1.585921	-1.301172
Mg11	-2.471024	3.790132	-0.107392
Mg12	5.177925	-2.437987	-0.559466
Mg13	7.267472	-0.362770	-0.377969
Mg14	-2.158640	-2.389455	1.366525
Mg15	3.741360	-0.355332	1.353232
Mg16	-2.264144	0.344039	-3.114777
Mg17	0.368625	-4.272477	0.223101
Mg18	6.242389	2.285239	0.341126
Mg19	0.769634	0.043089	-3.313716
Mg20	4.399468	0.500597	-1.539390
Mg21	3.054275	-3.436583	1.335829
Mg22	1.013881	1.434004	2.577064
Mg23	-4.944235	-3.615917	0.565186
Mg24	-0.427108	2.703117	-2.262299
Mg25	0.524085	3.709277	0.534067
Mg26	3.394413	2.763389	1.120406
Mg27	-2.467636	-4.933845	-0.465930
Mg28	-3.286189	3.249769	-3.064126
Mg29	-1.779635	0.158109	3.144806

@mg29-isomer30 bp86/6-31G(d) Etot=-5802.748146 Eb=-15.73

Mg1	1.104832	-1.477040	-2.223880
Mg2	2.355806	0.079643	0.148588
Mg3	0.376083	-2.413200	1.020504
Mg4	-3.554701	0.007464	-1.609439
Mg5	5.267546	-1.553445	0.985744
Mg6	1.813862	2.539062	1.832579
Mg7	4.595989	0.736311	2.788919
Mg8	-0.913751	0.896574	-3.086757
Mg9	2.138856	0.995008	4.420217
Mg10	-6.661903	-0.450175	-1.195229
Mg11	-7.651815	1.179309	1.169284
Mg12	-5.333286	-0.582821	1.725924
Mg13	3.059640	-3.109012	-0.065757
Mg14	2.063358	1.228529	-3.032462
Mg15	5.531720	1.185654	-0.018629
Mg16	-3.023003	1.461037	1.702643
Mg17	-1.754991	-2.429455	-1.402909
Mg18	-4.666620	-2.605993	-0.493094
Mg19	0.482849	2.938635	-0.963580
Mg20	-2.479431	2.776202	-1.130095
Mg21	4.215425	-1.188771	-2.041721
Mg22	5.034995	1.566340	-2.970870
Mg23	3.384575	3.082008	-0.899958
Mg24	0.710043	-4.348338	-1.390598
Mg25	-0.144178	0.182559	2.815822
Mg26	2.606805	-1.622043	2.813670
Mg27	-0.681419	0.250015	-0.125362
Mg28	-5.296505	2.207606	-0.346295
Mg29	-2.580778	-1.531665	1.572741

@mg29-isomer31 bp86/6-31G(d) Etot=-5802.745616 Eb=-15.67

Mg1	-0.665960	-2.034615	-0.936970
Mg2	0.351635	1.943308	2.187627
Mg3	2.634324	-1.705166	-0.835102
Mg4	-1.631656	2.290495	-2.787801
Mg5	0.691169	-0.988265	1.653436
Mg6	-2.071815	0.509718	0.066472
Mg7	5.592324	-2.456802	-0.316918
Mg8	-1.987530	-2.208436	1.883560
Mg9	0.725793	0.793733	-1.098538
Mg10	-0.528065	3.445427	-0.160802
Mg11	-4.769219	-0.833735	-0.838888

Mg12	4.805158	-1.394270	-3.014203
Mg13	-4.638959	1.606973	-2.631659
Mg14	3.275323	0.619955	1.281815
Mg15	-4.596509	-3.317183	0.813465
Mg16	-2.482937	-0.551972	-3.001824
Mg17	3.812281	-2.201150	2.036019
Mg18	-2.939879	2.508919	2.283945
Mg19	-3.391983	-3.265060	-2.005951
Mg20	-1.568690	0.191635	3.675033
Mg21	-4.347792	-0.442931	2.219341
Mg22	-5.502851	1.740662	0.444671
Mg23	-1.918295	-4.617250	0.123530
Mg24	2.433405	3.388085	0.205390
Mg25	3.754668	1.110205	-1.698293
Mg26	6.184364	-0.261289	1.772698
Mg27	5.576307	2.428910	0.474421
Mg28	6.677970	0.231393	-1.169718
Mg29	-3.472581	3.468705	-0.624759

@mg29-isomer32 bp86/6-31G(d) Etot=-5802.739179 Eb=-15.54

Mg1	0.222557	-0.886935	1.281689
Mg2	2.026949	1.482945	1.512998
Mg3	5.229345	1.398874	1.584132
Mg4	0.395655	0.795681	-1.311449
Mg5	2.316080	-1.432177	-2.164869
Mg6	4.764307	-2.283014	-0.639457
Mg7	-1.582579	-3.255301	1.052024
Mg8	-0.540868	-2.210927	-1.613678
Mg9	3.635048	1.088998	-1.105083
Mg10	-2.535926	-0.182724	0.021449
Mg11	-2.033628	-0.993218	3.252375
Mg12	-1.892150	2.757790	-1.373943
Mg13	3.332172	-1.243665	1.725297
Mg14	-4.317984	-2.472563	2.014517
Mg15	-4.015497	2.284102	-3.396414
Mg16	1.662924	-3.349079	0.150344
Mg17	6.749357	0.240705	-0.791993
Mg18	-1.184997	1.949273	1.618113
Mg19	-2.075009	-0.064771	-3.065505
Mg20	5.136306	-0.547834	-3.159747
Mg21	-3.610876	-2.568476	-1.380020
Mg22	-4.688659	1.959807	-0.405335
Mg23	-2.457026	1.818232	4.358056
Mg24	6.415358	-1.322980	1.800442
Mg25	-4.455645	0.665463	2.360662
Mg26	0.729774	3.693701	-0.186917
Mg27	-5.138139	-0.343514	-2.725288
Mg28	-5.871869	-0.796802	0.132995
Mg29	3.785020	3.818409	0.454604

@mg29-isomer33 bp86/6-31G(d) Etot=-5802.735053 Eb=-15.45

Mg1	-0.440219	0.883492	1.316375
Mg2	-0.838628	1.600523	-1.724934
Mg3	-2.828302	2.975828	0.320498
Mg4	2.046292	-0.624478	0.363789
Mg5	2.295052	-2.826284	-1.905729
Mg6	2.739729	-3.222732	1.874084
Mg7	4.905941	-2.497803	-0.086012
Mg8	-2.817023	-0.881872	2.778599
Mg9	2.159530	2.204430	-1.333887
Mg10	-0.092064	-2.119171	2.111157
Mg11	0.384783	-4.350801	0.085358
Mg12	-0.506863	-1.560095	-1.143502
Mg13	-2.921726	-0.053617	-0.084538

Mg14	-5.276824	-1.974584	1.010006
Mg15	-5.042140	1.050197	1.900083
Mg16	5.141239	2.812692	-0.943746
Mg17	0.074859	3.888863	0.252356
Mg18	2.291266	2.076588	1.745152
Mg19	5.032377	3.434998	1.942527
Mg20	-2.451230	-3.160008	0.512098
Mg21	1.449902	-0.156784	-2.929375
Mg22	-5.883809	2.933246	-0.278437
Mg23	4.822924	0.374642	1.049773
Mg24	3.042751	4.814965	0.194061
Mg25	-4.099803	1.498027	-2.255853
Mg26	-6.486220	0.077289	-0.713031
Mg27	4.284233	-0.083605	-1.873500
Mg28	-4.347711	-1.888660	-1.903121
Mg29	3.361686	-5.225285	-0.280252

@mg29-isomer34 bp86/6-31G(d) Etot=-5802.730264 Eb=-15.34

Mg1	0.177865	-0.057409	-0.513279
Mg2	1.386474	-2.211277	1.559577
Mg3	-0.218849	0.050472	-3.444154
Mg4	0.724341	2.951404	0.865488
Mg5	-1.992898	1.586517	0.709143
Mg6	-1.140573	4.734212	-1.032543
Mg7	4.888462	-1.270524	1.796729
Mg8	2.655211	0.628003	0.780145
Mg9	1.486242	-4.368559	-0.761789
Mg10	-0.910803	-2.616380	-1.557182
Mg11	2.808233	0.413134	-2.572027
Mg12	-3.908691	3.685491	-0.408002
Mg13	2.908898	0.053026	3.675878
Mg14	5.359725	0.414697	-0.849463
Mg15	-3.600844	-3.302572	-0.144353
Mg16	-3.066788	-0.402680	-1.355964
Mg17	0.168112	0.527027	2.718330
Mg18	-1.569745	-1.676533	1.429651
Mg19	-2.206647	2.291245	-2.545822
Mg20	3.461875	-2.050215	-0.745533
Mg21	-1.084179	-4.880422	0.629295
Mg22	-4.577252	2.337590	2.166712
Mg23	-2.704958	0.300832	3.593871
Mg24	3.720590	3.052451	-0.815606
Mg25	1.623475	-2.380959	-3.143620
Mg26	-4.503279	-0.633333	1.401030
Mg27	5.362525	1.755876	1.758721
Mg28	-6.041360	-1.602016	-1.035735
Mg29	0.794837	2.670903	-2.159497

@mg29-isomer35 bp86/6-31G(d) Etot=-5802.703339 Eb=-14.76

Mg1	0.132835	-2.479285	-0.157983
Mg2	-2.788066	-3.386398	-0.968264
Mg3	2.586285	-2.402857	-2.050091
Mg4	-5.230613	-1.414688	-1.907505
Mg5	-4.965558	-2.311395	0.984861
Mg6	-0.707134	-2.594396	-2.987798
Mg7	0.983442	-1.855547	2.591351
Mg8	-6.360476	0.303863	0.358983
Mg9	-0.803151	0.364554	1.194562
Mg10	-2.064262	-2.493876	1.900710
Mg11	2.953950	-3.423112	0.813842
Mg12	4.066573	-1.138064	2.619079
Mg13	6.833386	-0.259109	1.862467
Mg14	3.841894	0.487752	-1.946931
Mg15	2.183026	-0.100188	0.484154

Mg16	6.681569	0.829526	-0.943562
Mg17	-4.759339	1.572968	-2.164246
Mg18	0.677887	0.018333	-2.156685
Mg19	-6.289639	3.314709	-0.203581
Mg20	4.456931	1.687588	1.324590
Mg21	-1.018894	2.453781	-1.316657
Mg22	-2.478875	-0.312167	-1.267886
Mg23	5.086168	-1.789808	-0.380154
Mg24	1.910131	2.723586	-1.085986
Mg25	-3.431883	2.091237	0.504467
Mg26	-5.903553	2.254625	2.564965
Mg27	3.259115	4.462707	1.046182
Mg28	-3.853744	0.001004	2.539120
Mg29	5.001997	3.394657	-1.252003

@mg30-isomer01 bp86/6-31G(d) Etot=-6002.925318 Eb=-17.45

Mg1	0.394453	3.368586	1.999272
Mg2	2.676450	-4.285335	-0.221516
Mg3	-3.476898	-1.156641	2.585357
Mg4	1.384401	2.588481	-2.591176
Mg5	1.508783	0.634701	3.082484
Mg6	-1.757000	-2.519472	-2.227637
Mg7	3.584058	-1.383281	-0.716295
Mg8	4.273108	0.109240	1.804268
Mg9	-4.586735	1.880658	-1.140729
Mg10	0.453837	-4.429623	1.820687
Mg11	-1.809978	0.179830	0.002310
Mg12	1.143524	1.092673	0.042256
Mg13	-1.715588	2.426936	-2.287037
Mg14	-4.518295	-1.154828	-0.337342
Mg15	-2.258872	-3.245262	0.737192
Mg16	1.535141	-2.695886	-2.732363
Mg17	2.871317	0.009465	-3.233943
Mg18	-0.488610	-1.635054	2.814905
Mg19	2.519809	-2.232080	2.231723
Mg20	-4.684020	1.316638	1.737721
Mg21	-1.530786	1.193933	2.919017
Mg22	3.438862	2.894916	2.028169
Mg23	0.486993	-1.757734	-0.098026
Mg24	-2.509576	3.228410	0.737372
Mg25	-0.169409	-4.801213	-1.114175
Mg26	-0.117664	-0.065460	-2.792132
Mg27	2.740893	4.346745	-0.376351
Mg28	-0.200022	4.496988	-0.781133
Mg29	-3.308344	-0.067659	-2.954681
Mg30	4.120169	1.661327	-0.938196

@mg30-isomer02 bp86/6-31G(d) Etot=-6002.924048 Eb=-17.43

Mg1	2.183154	4.408556	0.435256
Mg2	-0.633795	-1.831354	2.498185
Mg3	-3.018046	-2.734577	0.794375
Mg4	2.168350	2.315924	2.786875
Mg5	-5.040059	-0.428871	0.620269
Mg6	-2.659497	3.706486	-0.902164
Mg7	4.348890	2.343040	0.627092
Mg8	1.135802	1.269747	0.180718
Mg9	-0.708415	1.125281	3.002311
Mg10	-3.539399	2.193189	1.582807
Mg11	1.667339	-0.513270	3.706796
Mg12	1.149398	0.818333	-2.977834
Mg13	-1.831206	1.441696	-2.903614
Mg14	-0.626650	3.677492	1.406052
Mg15	-3.324144	-0.491681	2.980938
Mg16	-1.706573	0.227782	0.084912

Mg17	2.142299	-3.119645	2.008372
Mg18	1.599391	-4.626195	-0.879536
Mg19	2.045276	-2.239774	-2.912663
Mg20	3.609950	-0.444381	1.513091
Mg21	0.697171	-1.528930	-0.350822
Mg22	-1.267905	-3.686583	-1.654129
Mg23	-3.513839	-1.323157	-1.992095
Mg24	3.165453	2.995690	-2.051228
Mg25	3.910572	-2.761754	-0.539656
Mg26	-0.808687	-1.298130	-3.350238
Mg27	-0.492326	-4.593601	1.199915
Mg28	0.184035	3.556634	-1.845155
Mg29	3.731259	0.070223	-1.575522
Mg30	-4.567798	1.471830	-1.493309

@mg30-isomer03 bp86/6-31G(d) Etot=-6002.921530 Eb=-17.37

Mg1	-1.590302	0.084460	0.039371
Mg2	4.273859	2.404486	-0.898284
Mg3	1.191490	1.263828	0.141814
Mg4	2.416954	4.305780	0.534021
Mg5	0.226971	-1.165395	-3.485058
Mg6	0.836953	-1.598256	-0.316320
Mg7	-0.291737	-1.523583	2.667782
Mg8	-1.508006	-3.038079	-1.952420
Mg9	-0.345175	1.604462	-2.613368
Mg10	1.231244	-4.058676	2.067741
Mg11	3.536148	-3.551866	0.278370
Mg12	-4.475641	0.806126	1.140262
Mg13	-3.355710	-1.574450	2.543914
Mg14	-1.832448	1.037888	3.109561
Mg15	0.156332	3.254624	2.269913
Mg16	4.006302	-0.547333	-0.289441
Mg17	2.564982	0.575774	-2.760376
Mg18	0.876261	-4.660698	-0.871485
Mg19	-2.752035	3.354654	1.336195
Mg20	-1.650454	-3.745427	1.005320
Mg21	1.958747	3.573702	-2.334385
Mg22	-2.670092	-0.381154	-2.894996
Mg23	2.762846	-1.349418	2.382301
Mg24	3.530417	1.703505	2.036047
Mg25	1.144393	0.829567	3.649223
Mg26	-0.540342	4.080379	-0.696366
Mg27	-3.137749	2.381543	-1.497244
Mg28	-3.956155	-1.942349	-0.409227
Mg29	2.789413	-2.506936	-2.461356
Mg30	-5.397465	0.382843	-1.721509

@mg30-isomer04 bp86/6-31G(d) Etot=-6002.917483 Eb=-17.29

Mg1	-1.289679	-1.216916	-0.014203
Mg2	-3.638349	-1.752509	-2.165135
Mg3	-3.091966	1.359716	1.950508
Mg4	-1.602746	-4.105988	1.503751
Mg5	1.716507	-0.377909	0.098276
Mg6	-1.640494	0.245725	-3.142393
Mg7	-4.448560	-1.072867	0.748859
Mg8	-1.493975	-3.934347	-1.674807
Mg9	-2.484966	-1.469584	2.935727
Mg10	-3.679103	1.190910	-1.208696
Mg11	-3.243966	3.828421	0.243837
Mg12	0.551787	-2.167983	2.541486
Mg13	-4.069775	-3.927852	-0.074209
Mg14	1.070488	-3.640033	0.001758
Mg15	-0.548688	1.621196	-0.031116
Mg16	-0.229337	0.677764	2.835941

Mg17	-0.945138	5.584270	-0.222359
Mg18	3.648516	-2.274851	1.475451
Mg19	-0.818763	3.756095	2.173019
Mg20	1.023269	1.374377	-2.696459
Mg21	4.604079	0.688495	1.697294
Mg22	3.418770	-3.000671	-1.616468
Mg23	3.378427	-0.410975	-3.064958
Mg24	-1.513724	3.254497	-2.311074
Mg25	1.380391	3.972938	-1.038033
Mg26	0.588888	-1.730755	-2.521656
Mg27	3.607722	1.876156	-0.957577
Mg28	2.529645	-0.080033	3.505769
Mg29	2.020807	2.519776	1.795560
Mg30	5.199933	-0.787063	-0.768093

@mg30-isomer05 bp86/6-31G(d) Etot=-6002.915117 Eb=-17.24

Mg1	-1.641947	0.818542	0.120760
Mg2	-0.148552	-1.707498	-0.160698
Mg3	-0.322894	2.109933	2.642930
Mg4	0.249457	-3.820239	-2.485135
Mg5	1.195092	-2.997501	2.265168
Mg6	1.507394	0.809487	0.077755
Mg7	-3.288266	3.005636	-1.320782
Mg8	4.485434	1.022625	1.874081
Mg9	4.208548	-0.550407	-0.914595
Mg10	-1.804898	-3.744985	1.855887
Mg11	-2.972813	3.592101	1.627377
Mg12	2.382433	3.276940	1.558538
Mg13	0.069344	-5.194899	0.069966
Mg14	-2.667754	-3.300159	-1.116299
Mg15	-0.459660	3.711824	-0.023209
Mg16	-4.874393	1.385663	0.757132
Mg17	2.089506	3.869385	-1.514452
Mg18	-3.644515	-1.374008	1.337033
Mg19	-0.940011	-0.885704	2.775146
Mg20	-4.013179	-0.418505	-1.589095
Mg21	-0.005979	1.590404	-2.493717
Mg22	1.699979	-1.112384	-2.632216
Mg23	4.620026	2.585858	-0.578185
Mg24	3.136998	1.444253	-2.908584
Mg25	-1.362712	-1.203943	-2.969280
Mg26	-2.759950	1.277444	-3.700239
Mg27	2.618440	-3.338411	-0.613681
Mg28	-3.182120	1.035398	3.154006
Mg29	1.910282	0.020784	3.092912
Mg30	3.916711	-1.907633	1.811476

@mg30-isomer06 bp86/6-31G(d) Etot=-6002.907495 Eb=-17.08

Mg1	-3.110838	-2.762634	-2.238108
Mg2	-3.536274	-2.611955	0.895356
Mg3	2.732455	1.392645	2.304439
Mg4	-0.930388	1.880854	-2.674420
Mg5	-0.227453	0.126648	2.427903
Mg6	-0.759253	-3.198608	-0.522168
Mg7	4.187967	-3.475098	0.037335
Mg8	-3.869487	1.907087	-1.507005
Mg9	4.340792	-1.110813	-1.853488
Mg10	-2.085220	2.883510	0.607583
Mg11	1.599514	-4.366327	0.996713
Mg12	4.543250	-0.694998	1.155374
Mg13	2.187536	3.691558	-2.204065
Mg14	1.483944	-1.060984	0.005650
Mg15	3.872914	1.632981	-0.687270
Mg16	-2.941426	-1.109038	3.400076

Mg17	2.753722	4.059008	0.729685
Mg18	-5.029543	-0.871660	-1.196304
Mg19	-2.466693	1.890684	3.427404
Mg20	-0.727301	-2.861489	2.432048
Mg21	2.348617	-1.831918	2.825770
Mg22	2.021705	0.651339	-2.922795
Mg23	-0.391779	-1.222193	-2.851621
Mg24	0.048538	4.866481	-0.415923
Mg25	0.260764	3.187040	2.531660
Mg26	-4.252328	0.611982	1.329952
Mg27	0.715106	1.756692	-0.150358
Mg28	-3.143846	-0.092146	-3.518042
Mg29	2.087220	-3.038274	-2.132741
Mg30	-1.712217	-0.230373	-0.232640

@mg30-isomer07 bp86/6-31G(d) Etot=-6002.905436 Eb=-17.04

Mg1	3.853930	1.815090	0.385566
Mg2	2.947945	-3.235861	-1.614673
Mg3	-0.897772	0.525386	3.909642
Mg4	1.550425	-0.199971	0.137721
Mg5	-1.669776	-0.485699	-0.183009
Mg6	-0.504072	4.303352	-0.930505
Mg7	-4.921649	-1.276438	1.094389
Mg8	-3.340107	1.162072	2.129338
Mg9	4.378116	-0.391122	2.497701
Mg10	-0.530954	1.975316	1.172857
Mg11	0.704307	-1.321819	-2.855490
Mg12	-0.009082	1.489898	-1.981289
Mg13	-2.414111	-0.113069	-3.197164
Mg14	4.083674	-1.632447	-3.763765
Mg15	-4.239279	0.952861	-0.887503
Mg16	-0.226615	-1.858899	2.209880
Mg17	-4.438531	-2.021749	-1.762568
Mg18	-3.031354	-1.606971	3.349140
Mg19	4.611471	-1.052381	-0.493692
Mg20	-2.691089	2.892799	-2.651888
Mg21	2.051631	1.523264	2.922359
Mg22	-3.141062	3.519548	0.260041
Mg23	1.919126	3.990264	1.184198
Mg24	2.094319	-1.252422	4.154243
Mg25	-1.887429	-3.095335	-2.588585
Mg26	0.203585	-3.085922	-0.407297
Mg27	3.057311	0.812030	-2.454035
Mg28	2.422871	3.617198	-1.693887
Mg29	2.787288	-2.717040	1.468416
Mg30	-2.723118	-3.231933	0.589860

@mg30-isomer08 bp86/6-31G(d) Etot=-6002.905422 Eb=-17.04

Mg1	-1.074931	-1.085938	-0.660147
Mg2	-1.193242	-1.936521	-3.646371
Mg3	3.142216	-2.395226	1.812046
Mg4	-3.156257	-3.030461	0.860993
Mg5	-0.674513	4.716364	-1.665678
Mg6	-1.435859	3.977095	1.342262
Mg7	1.594869	-0.211525	0.354223
Mg8	-3.898696	2.161742	1.736564
Mg9	-4.381944	-0.820972	2.517132
Mg10	0.576578	0.511867	-3.146966
Mg11	3.530184	2.473366	0.363334
Mg12	0.884699	-0.692848	3.423671
Mg13	2.023855	-4.478481	-0.215550
Mg14	-0.986723	-4.099505	-1.259202
Mg15	-3.635009	-2.612417	-2.093551
Mg16	5.071605	-0.165786	0.482213

Mg17	-0.421470	1.839438	-0.667634
Mg18	4.188250	-2.488509	-1.141918
Mg19	0.097034	-2.920211	1.502922
Mg20	1.975795	3.162031	-2.206047
Mg21	3.534978	0.660234	2.827495
Mg22	1.015783	2.314781	2.281038
Mg23	-1.876568	-2.047434	3.540916
Mg24	-3.279646	3.038799	-1.099440
Mg25	1.420861	-2.214882	-2.187520
Mg26	-1.408599	0.499655	1.908896
Mg27	1.454768	4.825373	0.382427
Mg28	-2.445405	0.690701	-2.871433
Mg29	-4.064537	-0.074608	-0.370148
Mg30	3.421922	0.403878	-2.104525

@mg30-isomer09 bp86/6-31G(d) Etot=-6002.905371 Eb=-17.04

Mg1	0.346635	1.651019	0.242136
Mg2	0.808954	-1.231097	-0.118874
Mg3	3.328520	1.048537	-0.471781
Mg4	1.300777	1.561121	-2.881253
Mg5	-1.527719	1.175298	2.917949
Mg6	-2.146949	-0.126508	0.079284
Mg7	-2.846569	2.807090	0.705921
Mg8	3.664348	-1.396362	1.666085
Mg9	1.160887	-1.517843	-3.131865
Mg10	3.590787	1.505968	2.554959
Mg11	3.383184	-4.357636	0.713063
Mg12	1.120066	-0.208852	2.929396
Mg13	3.872393	0.125915	-3.303470
Mg14	-0.138431	4.705901	0.632341
Mg15	-1.291972	0.222748	-2.776402
Mg16	3.673518	-2.179171	-1.355820
Mg17	1.892579	4.176954	-1.630407
Mg18	-1.121760	3.294987	-2.001406
Mg19	-3.882540	-2.576530	0.496913
Mg20	-3.834421	1.804725	-2.034084
Mg21	0.895323	2.898322	2.934448
Mg22	-5.336861	0.227740	0.034812
Mg23	-1.505789	-2.751517	-1.930054
Mg24	2.963823	4.048939	1.050623
Mg25	-4.130006	-0.286934	2.592252
Mg26	1.236413	-3.234608	2.381451
Mg27	1.200267	-4.129341	-1.308202
Mg28	-1.133229	-4.239240	0.698655
Mg29	-1.452559	-1.849070	2.585320
Mg30	-4.089665	-1.170555	-2.271990

@mg30-isomer10 bp86/6-31G(d) Etot=-6002.902279 Eb=-16.97

Mg1	-2.042853	-3.967299	0.452073
Mg2	0.735220	-2.875091	1.520703
Mg3	-2.513711	-3.258156	-2.637443
Mg4	-3.737846	-2.073357	2.220993
Mg5	-1.021616	-1.259588	3.435685
Mg6	0.154536	-3.035794	-1.467811
Mg7	-4.551704	-2.719863	-0.575651
Mg8	3.048277	-3.069006	-0.667475
Mg9	-3.297222	0.787400	3.113254
Mg10	-3.872793	-0.599509	-2.588216
Mg11	-1.471882	-0.818642	0.186830
Mg12	1.870217	-0.228293	3.165068
Mg13	-0.818082	-0.327337	-2.839446
Mg14	1.936471	-1.434923	-3.292743
Mg15	-4.356390	0.346922	0.265615
Mg16	5.669791	-2.028762	0.256984

Mg17	-0.495220	1.514613	2.317446
Mg18	1.561388	-0.286528	-0.076297
Mg19	-3.048697	2.211290	-1.928472
Mg20	4.242057	0.419953	1.338510
Mg21	4.272915	-0.332060	-1.808606
Mg22	3.659079	-2.520516	2.356601
Mg23	-0.316332	1.912828	-0.687392
Mg24	-2.868905	3.060224	1.117160
Mg25	3.728079	2.433245	-0.948078
Mg26	1.693974	1.629025	-2.990353
Mg27	2.158826	2.683023	1.582616
Mg28	-1.620644	4.808673	-1.119143
Mg29	-0.138014	4.690927	1.442487
Mg30	1.441080	4.336599	-1.144899

@mg30-isomer11 bp86/6-31G(d) Etot=-6002.898747 Eb=-16.90

Mg1	-4.286038	1.825532	0.124774
Mg2	-3.419590	-0.294321	2.292632
Mg3	0.416889	-1.620977	-1.770380
Mg4	4.960248	1.596688	-0.857524
Mg5	3.006181	3.132453	0.784734
Mg6	3.019305	-0.119475	-2.686419
Mg7	2.644174	-2.633306	0.933933
Mg8	-0.606557	0.454590	3.154816
Mg9	-1.529426	-5.517597	1.004165
Mg10	-2.259461	-0.699579	-2.974040
Mg11	-3.182945	-3.239222	1.825484
Mg12	4.892637	-1.358705	-0.627368
Mg13	-0.371012	-1.979562	1.304010
Mg14	-1.366267	0.680025	-0.083700
Mg15	-2.412045	4.271062	0.243001
Mg16	4.145510	0.219425	1.820326
Mg17	0.030907	3.082588	1.829857
Mg18	-2.113366	-3.368118	-1.282493
Mg19	-2.427590	2.532526	-2.358374
Mg20	-2.841535	2.642804	2.715365
Mg21	2.800318	2.891907	-2.405680
Mg22	1.545633	0.472799	0.163227
Mg23	0.217496	3.511815	-1.114307
Mg24	-4.070873	-1.248552	-0.505359
Mg25	2.210237	1.730464	3.459134
Mg26	-4.866675	0.775645	-2.696486
Mg27	0.281167	1.166918	-2.938198
Mg28	1.874569	-1.217438	3.400970
Mg29	0.714916	-4.544192	-0.655245
Mg30	2.993193	-3.146197	-2.100854

@mg30-isomer12 bp86/6-31G(d) Etot=-6002.896354 Eb=-16.85

Mg1	1.724565	-1.514793	-3.074917
Mg2	3.102939	-0.271006	2.193582
Mg3	1.483966	1.722070	-2.848200
Mg4	-0.120998	-0.991051	2.656589
Mg5	4.565329	-3.115391	1.443801
Mg6	-1.864744	1.434490	2.698810
Mg7	-4.450643	0.933872	1.285479
Mg8	-3.272468	-1.630204	2.501418
Mg9	1.144715	-1.172751	-0.151695
Mg10	0.160684	4.077170	1.947261
Mg11	1.069466	1.549752	3.548482
Mg12	-0.739306	-3.566793	1.251989
Mg13	-0.732601	-3.175051	-1.872339
Mg14	-3.321437	-3.819607	-0.215257
Mg15	-5.159209	-1.470247	-0.248392
Mg16	-0.886375	0.011846	-2.561517

Mg17	1.890158	4.001372	-0.719730
Mg18	3.457620	1.291125	-0.522828
Mg19	-3.456310	-1.912803	-2.641159
Mg20	-2.563490	3.105200	0.283243
Mg21	4.185908	-1.649409	-1.048402
Mg22	4.150202	0.371085	-3.318966
Mg23	-3.729899	0.981342	-1.818246
Mg24	1.896942	-3.201700	2.573307
Mg25	-1.988493	-0.857421	0.026030
Mg26	2.133197	-4.019398	-0.575356
Mg27	3.044793	2.929478	1.951742
Mg28	0.212619	1.512472	0.247850
Mg29	-1.190657	3.027959	-2.387332
Mg30	-0.746475	5.418395	-0.605247

@mg30-isomer13 bp86/6-31G(d) Etot=-6002.892973 Eb=-16.78

Mg1	0.057667	0.650540	0.336318
Mg2	-2.594972	-0.297119	-0.118130
Mg3	-3.292160	-2.250348	2.521659
Mg4	-3.976088	-1.653972	-2.394036
Mg5	2.480150	-3.022205	1.057436
Mg6	-3.795883	1.425441	-2.728622
Mg7	3.064956	-2.777355	-1.974824
Mg8	4.583405	-0.915725	2.366629
Mg9	1.538023	-0.822825	-3.604334
Mg10	-5.345584	-2.157068	0.365759
Mg11	-5.916737	0.436752	-0.767190
Mg12	-4.144498	2.837102	-0.167839
Mg13	0.679167	2.270366	3.085298
Mg14	-1.476091	0.053877	3.137635
Mg15	-1.901383	2.891026	1.672139
Mg16	3.396543	1.974585	1.990493
Mg17	2.733419	-0.198608	-0.168619
Mg18	5.305049	-2.255042	-0.120013
Mg19	4.336677	0.126905	-2.600991
Mg20	-2.636568	-3.479179	-0.256562
Mg21	-1.113049	0.188802	-2.853305
Mg22	1.286527	3.488817	0.303926
Mg23	3.928475	2.698231	-0.963524
Mg24	0.071234	-2.164194	-1.162701
Mg25	1.628493	-0.584613	2.821478
Mg26	-1.392954	2.893615	-1.374453
Mg27	1.387047	1.923609	-2.361203
Mg28	-4.379428	0.603993	2.094500
Mg29	-0.433310	-2.582288	1.761042
Mg30	5.921871	0.696879	0.102033

@mg30-isomer14 bp86/6-31G(d) Etot=-6002.891706 Eb=-16.75

Mg1	0.792210	3.857691	0.820470
Mg2	2.192485	-0.482268	3.836590
Mg3	-1.186062	-3.739804	1.230837
Mg4	-4.574521	-0.150598	0.125157
Mg5	-1.433155	2.466513	-0.971583
Mg6	3.429313	1.922326	-2.803942
Mg7	-3.029945	0.798914	2.727337
Mg8	1.215209	-1.806853	1.211451
Mg9	-1.407255	-0.346245	0.380391
Mg10	0.712459	0.684027	-3.150498
Mg11	-3.519998	-2.206090	2.179193
Mg12	-2.089910	-0.167422	-2.705680
Mg13	-0.898878	-1.524911	3.431103
Mg14	4.799342	1.163282	-0.324286
Mg15	-4.129257	2.754569	0.581110
Mg16	3.503887	3.896735	-0.458587

Mg17	-4.258924	1.888686	-2.271348
Mg18	-3.032048	-2.619933	-0.962729
Mg19	0.049096	-2.107070	-1.615538
Mg20	3.126184	1.938878	2.165827
Mg21	0.085965	1.284253	2.581564
Mg22	-1.834229	3.593504	2.284237
Mg23	-4.940507	-1.029791	-2.811275
Mg24	4.078239	-1.015383	1.580271
Mg25	1.384607	0.992094	-0.219887
Mg26	3.522964	-3.617453	0.065754
Mg27	2.293751	-3.875328	-2.676990
Mg28	3.091376	-1.031553	-1.688294
Mg29	0.938868	-5.219687	-0.294709
Mg30	1.118736	3.698917	-2.245946

@mg30-isomer15 bp86/6-31G(d) Etot=-6002.889867 Eb=-16.71

Mg1	0.081056	0.742709	0.289400
Mg2	1.703670	1.216213	-2.685273
Mg3	-1.967174	1.355306	2.761944
Mg4	3.277443	2.198204	1.701690
Mg5	-2.553037	-0.194638	-0.197614
Mg6	0.119213	-2.377620	-0.159104
Mg7	0.527341	3.132408	2.372950
Mg8	5.814084	0.842307	0.174401
Mg9	-3.706637	-0.302973	-2.883470
Mg10	1.197038	3.427618	-0.578515
Mg11	-4.445198	2.239775	1.387353
Mg12	-2.336188	-3.017702	-1.966411
Mg13	-4.209632	-0.942391	2.105557
Mg14	2.355612	-2.047315	-2.433114
Mg15	3.977815	2.789116	-1.213267
Mg16	1.312466	0.265159	3.144458
Mg17	-2.678663	-3.515733	0.966893
Mg18	2.720438	-0.233040	-0.117391
Mg19	-1.835844	3.330080	0.338179
Mg20	4.630872	0.163463	-2.602587
Mg21	-5.925299	0.327335	-0.362530
Mg22	5.394153	-1.975549	-0.568279
Mg23	-1.208397	-1.493889	2.578593
Mg24	1.487006	-2.726150	2.671909
Mg25	-0.472408	-0.858045	-2.788405
Mg26	-1.222870	2.037527	-2.369726
Mg27	4.027061	-1.039935	2.384632
Mg28	-4.073526	2.480741	-1.533732
Mg29	2.991102	-3.455576	0.253382
Mg30	-4.981497	-2.367407	-0.671923

@mg30-isomer16 bp86/6-31G(d) Etot=-6002.887779 Eb=-16.67

Mg1	0.777066	1.203444	-0.394336
Mg2	2.023830	1.183990	-3.185462
Mg3	1.588041	-1.894335	-0.486373
Mg4	-0.653632	3.416403	-2.115132
Mg5	-3.651908	2.076121	-1.710356
Mg6	-1.933992	3.229548	0.752980
Mg7	-0.985472	0.525729	-3.016029
Mg8	0.665879	4.811900	0.263366
Mg9	-3.575441	-3.160327	-0.252762
Mg10	2.164706	-2.243073	2.884850
Mg11	3.933401	-1.430137	-2.400308
Mg12	0.775378	0.197932	4.345497
Mg13	-5.273095	-0.604794	-0.181454
Mg14	-0.111683	-0.722382	1.776324
Mg15	3.988512	1.119461	-0.770617
Mg16	4.363315	-1.761207	0.690389

Mg17	0.496064	-4.754681	-1.117789
Mg18	-4.368388	1.631243	1.454575
Mg19	2.511282	3.753233	-1.794521
Mg20	1.061207	-1.613156	-3.541339
Mg21	-3.234954	-1.470502	2.240274
Mg22	-1.985729	1.246564	3.262673
Mg23	-0.860820	-3.572478	1.449613
Mg24	0.579121	2.577743	2.441862
Mg25	2.942769	0.549303	2.090143
Mg26	-1.210928	-2.403069	-1.882404
Mg27	-3.813041	-0.926105	-2.660600
Mg28	-2.102569	0.029507	-0.210286
Mg29	2.706559	-4.448915	0.911369
Mg30	3.184521	3.453040	1.155852

@mg30-isomer17 bp86/6-31G(d) Etot=-6002.886171 Eb=-16.63

Mg1	-0.167170	0.069404	0.088827
Mg2	3.324713	2.874870	0.829085
Mg3	2.750596	-0.041168	-0.242578
Mg4	-3.143054	-0.188661	-0.489625
Mg5	-4.206487	0.690854	-3.187153
Mg6	1.796113	0.726061	2.640425
Mg7	3.127360	-2.003261	2.075892
Mg8	3.737970	-3.079257	-0.843690
Mg9	-1.506789	-2.736179	-0.039417
Mg10	0.016969	-1.768862	2.653958
Mg11	-6.189039	-0.796425	-1.496916
Mg12	5.847122	1.507510	-0.446488
Mg13	0.983356	-2.288936	-1.807209
Mg14	3.633930	2.193283	-2.251477
Mg15	-2.012695	2.550269	0.406431
Mg16	1.145412	0.480697	-2.984287
Mg17	5.917665	-1.434089	0.259373
Mg18	1.205461	-3.830526	0.715531
Mg19	4.908051	0.586684	2.186822
Mg20	4.716949	-0.644998	-2.427767
Mg21	-3.039749	-1.228618	2.379145
Mg22	0.860410	2.832182	-0.997895
Mg23	-4.665085	-2.790121	0.092727
Mg24	-1.486225	1.830395	-2.566967
Mg25	-5.980086	-0.437602	1.454848
Mg26	-1.522451	-1.139008	-2.990914
Mg27	0.506291	3.290868	1.939325
Mg28	-1.220885	1.048874	3.096050
Mg29	-4.159054	1.703239	2.381623
Mg30	-5.179598	2.022519	-0.427679

@mg30-isomer18 bp86/6-31G(d) Etot=-6002.885756 Eb=-16.63

Mg1	1.088792	-2.634133	1.951855
Mg2	0.869898	0.254462	3.027961
Mg3	-1.458946	-3.278989	0.372900
Mg4	-1.667798	-1.384302	2.783597
Mg5	-2.231656	0.146076	0.107468
Mg6	-4.408366	0.431353	2.239282
Mg7	0.725674	-0.173970	-0.111268
Mg8	1.240903	-3.191406	-1.245365
Mg9	2.725757	2.309044	1.884509
Mg10	3.835065	-1.644820	-1.585299
Mg11	-0.212699	2.750798	0.871424
Mg12	-4.118246	-2.659677	1.560123
Mg13	-1.302154	0.833765	-3.705262
Mg14	0.580274	2.427381	-2.101082
Mg15	3.365085	1.318268	-1.391720
Mg16	3.472775	-0.635746	1.416282

Mg17	5.251966	3.214737	0.265861
Mg18	3.522914	-3.719422	0.600097
Mg19	6.202097	-2.466221	0.500008
Mg20	-3.216255	3.391910	1.312444
Mg21	-1.300793	-1.801608	-2.275143
Mg22	-5.121157	2.025607	-0.450165
Mg23	2.393737	4.070751	-0.407762
Mg24	6.154045	0.438793	-0.108709
Mg25	-5.779622	-0.899414	-0.201429
Mg26	-2.403232	2.803345	-1.548643
Mg27	-1.763409	1.628855	3.212687
Mg28	-3.928272	-3.036360	-1.379832
Mg29	1.394087	-0.485168	-3.139202
Mg30	-3.910465	-0.033907	-2.455617

@mg30-isomer19 bp86/6-31G(d) Etot=-6002.885403 Eb=-16.62

Mg1	0.082841	0.643923	-2.848567
Mg2	1.642792	-2.112797	-2.794801
Mg3	-1.369041	3.580710	-2.768271
Mg4	-3.097892	1.135335	-2.610817
Mg5	3.213433	0.459995	-3.146942
Mg6	-1.482494	-1.829883	-2.373817
Mg7	-4.417514	-1.478582	-1.969781
Mg8	3.117661	-4.304457	-1.208439
Mg9	1.870927	3.129446	-2.823620
Mg10	0.241491	-3.659010	-0.502432
Mg11	4.059704	-1.436269	-0.899803
Mg12	0.093024	2.447589	-0.300786
Mg13	-4.926903	0.770048	-0.072379
Mg14	-2.997220	3.240304	-0.289800
Mg15	-1.209458	3.439551	2.223001
Mg16	-2.890539	-3.044800	0.117008
Mg17	1.111929	-0.554614	-0.004881
Mg18	-1.908916	0.103800	0.129315
Mg19	3.204325	1.781679	-0.407587
Mg20	-5.801109	-2.100010	0.621262
Mg21	2.606777	-3.075566	1.465279
Mg22	6.180230	0.999595	0.288531
Mg23	4.530493	2.567800	2.267874
Mg24	-0.688462	-2.204654	1.978476
Mg25	-3.692748	1.908937	2.403566
Mg26	-3.640117	-1.127811	2.456875
Mg27	1.587178	1.724307	2.271446
Mg28	-1.025152	0.534475	3.238800
Mg29	1.604100	-1.065905	3.576944
Mg30	4.000660	-0.473137	1.984344

@mg30-isomer20 bp86/6-31G(d) Etot=-6002.884954 Eb=-16.61

Mg1	2.679994	3.760247	-0.855568
Mg2	0.015465	2.228043	-0.600658
Mg3	4.019328	-3.566700	1.144526
Mg4	1.123535	-2.759824	-0.022960
Mg5	3.786907	-0.378101	-3.937859
Mg6	-3.762906	-0.207042	-2.633052
Mg7	4.226041	2.530147	1.310931
Mg8	1.425135	3.325016	1.971897
Mg9	-3.643112	-2.691528	1.800113
Mg10	2.955343	0.999149	3.401218
Mg11	-2.958381	0.126211	2.794960
Mg12	-4.645618	2.547551	1.624506
Mg13	-0.815653	-2.505357	2.572231
Mg14	4.388107	1.224387	-1.437647
Mg15	-6.122540	2.313775	-0.974757
Mg16	2.169770	-1.820643	2.744386

Mg17	4.758915	-0.623659	1.322047
Mg18	1.906069	1.921998	-3.118882
Mg19	-1.007889	0.856312	-3.153377
Mg20	2.011180	0.216152	0.191411
Mg21	-3.005365	2.318999	-1.057959
Mg22	-1.647285	-4.079464	0.076144
Mg23	-4.554062	-0.215522	0.271281
Mg24	0.072493	0.531529	2.500220
Mg25	3.903737	-1.945397	-1.321014
Mg26	1.213278	-1.054361	-2.499052
Mg27	-1.424239	-2.470665	-2.598512
Mg28	-1.321162	-0.599982	-0.080398
Mg29	-1.763965	2.836841	1.763347
Mg30	-3.983118	-2.818111	-1.197524

@mg30-isomer21 bp86/6-31G(d) Etot=-6002.884068 Eb=-16.59

Mg1	0.014388	-4.388520	0.175883
Mg2	-0.277851	0.366527	2.716971
Mg3	4.935839	0.718216	1.058953
Mg4	-0.106777	3.711160	-0.304234
Mg5	2.750824	2.867286	0.481526
Mg6	2.670105	0.841807	3.068252
Mg7	1.248515	-2.276107	2.380273
Mg8	4.442102	1.495123	-1.771838
Mg9	-0.098169	-0.061553	-3.484935
Mg10	-1.637293	-2.382949	-2.245664
Mg11	-4.401677	-2.149545	-1.225795
Mg12	0.591407	3.185065	2.573284
Mg13	-3.226377	0.365740	-2.608220
Mg14	-3.973883	0.286800	0.460521
Mg15	-2.298428	5.297789	0.986948
Mg16	1.840433	0.033282	0.270752
Mg17	4.383811	-1.498344	-1.046813
Mg18	1.315937	-2.167067	-1.609894
Mg19	-1.373330	-1.796961	0.870745
Mg20	-4.181374	-2.677399	1.746389
Mg21	-2.474491	2.429865	2.041914
Mg22	2.959055	-3.707680	0.423845
Mg23	-3.184500	-0.400868	3.361519
Mg24	2.911053	-0.352175	-3.462290
Mg25	4.216459	-1.788435	2.320557
Mg26	-0.903020	0.829332	-0.458329
Mg27	1.593338	2.158282	-2.374523
Mg28	-1.463204	2.716460	-3.118733
Mg29	-3.347291	2.995954	-0.813844
Mg30	-2.925600	-4.651084	-0.413218

@mg30-isomer22 bp86/6-31G(d) Etot=-6002.882314 Eb=-16.55

Mg1	1.478552	0.224854	0.031686
Mg2	3.135878	-2.098465	1.710906
Mg3	3.185639	-2.696529	-1.207909
Mg4	-1.509498	-0.341618	0.023110
Mg5	-2.242911	-3.073993	1.682133
Mg6	-2.563183	-0.651741	3.480512
Mg7	1.520987	3.414665	1.887958
Mg8	1.607969	3.873043	-1.036952
Mg9	4.903789	-0.055209	-1.164481
Mg10	5.500716	0.121779	1.808417
Mg11	0.429989	-1.779793	-2.455852
Mg12	0.175342	1.320421	-2.556907
Mg13	-4.561268	-0.897251	1.293789
Mg14	-4.693927	-3.549253	-0.068531
Mg15	3.890587	2.291011	0.503414
Mg16	-4.474052	-0.962395	-1.694706

Mg17	-2.992682	1.796090	-2.112621
Mg18	2.671706	0.706149	2.910923
Mg19	-0.396201	1.342836	2.695287
Mg20	-2.102296	-0.690497	-3.490692
Mg21	-0.997939	2.790428	0.092377
Mg22	-3.828249	3.875575	-0.108529
Mg23	-3.362136	1.885616	2.041150
Mg24	2.877943	-0.541172	-3.409360
Mg25	-2.118191	-3.069250	-1.463343
Mg26	0.492125	-2.932797	0.256940
Mg27	5.942145	-2.469896	0.368247
Mg28	3.349590	2.177007	-2.592861
Mg29	0.323453	-1.531934	2.858330
Mg30	-5.643879	1.522318	-0.282435

@mg30-isomer23 bp86/6-31G(d) Etot=-6002.881354 Eb=-16.53

Mg1	-0.478068	1.043529	0.124958
Mg2	-3.408092	1.515951	1.876691
Mg3	0.602221	3.866936	-0.670122
Mg4	1.314584	0.548424	2.941373
Mg5	1.012211	1.510332	-2.684360
Mg6	2.174701	3.181176	1.801381
Mg7	-4.371342	-1.517597	2.692766
Mg8	-5.194379	-2.983716	0.174345
Mg9	3.726705	0.428502	-3.208962
Mg10	2.227239	-0.302629	-0.184844
Mg11	4.490489	-2.164977	1.051681
Mg12	1.382568	-1.568016	-2.879144
Mg13	-4.821097	-1.119480	-2.279939
Mg14	4.490468	-2.250734	-2.141161
Mg15	4.144450	0.903989	1.858489
Mg16	-2.412263	3.875786	0.186647
Mg17	-3.856650	1.598929	-1.254323
Mg18	-1.551654	-0.239840	-2.513356
Mg19	3.629381	-1.387778	3.877572
Mg20	-1.662275	3.037581	-2.612761
Mg21	-1.229225	-1.023882	2.633123
Mg22	-0.796640	2.855976	2.565114
Mg23	1.433605	-2.502686	2.222170
Mg24	-0.301155	-2.214494	-0.293868
Mg25	-2.770364	-3.310958	-1.754560
Mg26	5.505543	0.178891	-0.786527
Mg27	-6.029749	-0.048141	0.576349
Mg28	2.349381	-3.506013	-0.566282
Mg29	-2.909105	-0.908077	0.147130
Mg30	3.308511	2.503018	-0.899579

@mg30-isomer24 bp86/6-31G(d) Etot=-6002.880621 Eb=-16.52

Mg1	0.348446	-0.288528	-0.170159
Mg2	3.069354	-1.410594	2.199955
Mg3	3.735392	-3.395807	-0.068043
Mg4	1.974906	1.452946	1.760724
Mg5	1.568547	-2.459767	-1.964988
Mg6	3.421064	-0.279053	-0.747790
Mg7	-0.674092	2.765040	0.581933
Mg8	-1.249177	-1.133581	-2.809107
Mg9	0.141771	-1.011180	2.880429
Mg10	4.279017	3.131771	0.113665
Mg11	-2.522406	0.257337	0.119197
Mg12	-2.769485	-0.380248	3.400333
Mg13	5.993861	-1.604180	0.728296
Mg14	-6.289792	-0.998375	-1.188320
Mg15	-1.107110	-3.824481	-1.288638
Mg16	-4.025126	0.603910	-2.502538

Mg17	4.215844	1.787252	-2.780625
Mg18	-2.016077	-2.516953	1.278740
Mg19	-5.024187	-0.958659	1.505501
Mg20	-5.821717	1.628118	0.053953
Mg21	-3.472829	3.166238	-0.808922
Mg22	1.449255	0.356020	-3.107025
Mg23	-3.656023	-2.329921	-1.365622
Mg24	0.956188	-3.367192	0.987507
Mg25	-1.077562	1.872641	-2.362500
Mg26	-3.670511	2.271047	2.132671
Mg27	6.306029	1.090468	-0.700160
Mg28	1.620181	2.774165	-1.323113
Mg29	-0.742081	1.820204	3.384567
Mg30	5.038322	0.981362	2.060079

@mg30-isomer25 bp86/6-31G(d) Etot=-6002.880273 Eb=-16.51

Mg1	-0.475779	2.369268	-2.540751
Mg2	-1.555094	3.520303	0.088731
Mg3	0.116280	0.533273	-0.092377
Mg4	-1.583575	-0.698453	-2.567975
Mg5	-3.381254	2.079635	-1.798477
Mg6	1.321758	-1.554595	-2.116814
Mg7	5.550565	1.351791	-1.102100
Mg8	-0.804009	-2.868400	-0.425838
Mg9	1.465254	3.988733	-0.791182
Mg10	-5.992008	1.010538	-0.143497
Mg11	-2.841958	-0.312974	0.106104
Mg12	0.803423	3.215206	2.068916
Mg13	3.736599	-3.225387	-0.750632
Mg14	-3.520761	-3.144932	1.484495
Mg15	-5.849007	-1.968084	0.087176
Mg16	-1.591671	1.388718	2.407938
Mg17	-4.783857	-0.506687	-2.430644
Mg18	6.224658	-1.474126	-0.308098
Mg19	1.511574	0.193437	2.655037
Mg20	1.494437	-2.691326	1.410565
Mg21	3.415333	2.524904	0.964171
Mg22	4.454086	-2.227971	2.083478
Mg23	-1.044682	-1.590649	2.397885
Mg24	3.109256	-0.341619	0.130071
Mg25	-4.099294	2.665049	1.342686
Mg26	-4.604655	-0.263245	2.405819
Mg27	5.604089	0.536427	1.872612
Mg28	2.507278	1.551434	-2.152561
Mg29	4.404999	-0.932641	-2.692502
Mg30	-3.591986	-3.127628	-1.592236

@mg30-isomer26 bp86/6-31G(d) Etot=-6002.878540 Eb=-16.47

Mg1	0.729692	-0.721766	-2.893466
Mg2	0.404042	1.900538	2.348392
Mg3	-0.330437	-3.191443	1.461115
Mg4	-0.058544	-0.205400	0.091450
Mg5	4.723181	2.312384	0.289940
Mg6	0.740288	-0.977538	3.273938
Mg7	2.822785	-0.112803	-0.127061
Mg8	4.764189	-2.747101	-0.457166
Mg9	-1.430287	-2.522901	-1.362418
Mg10	-3.337000	-3.091802	0.956074
Mg11	-5.990174	-1.857056	-0.257407
Mg12	-5.206901	-0.049236	-2.514366
Mg13	-2.090201	0.343353	-2.774217
Mg14	-3.926028	2.202623	1.665038
Mg15	1.645516	-2.909737	-0.878067
Mg16	2.945317	3.829727	2.161342

Mg17	1.632657	2.754393	-0.298828
Mg18	3.150604	1.416473	-2.670761
Mg19	5.526232	-0.490135	1.434862
Mg20	-3.249779	-0.241367	-0.205215
Mg21	-1.412721	2.523577	-0.193251
Mg22	-4.163662	2.571822	-1.364906
Mg23	0.180537	2.270374	-2.873708
Mg24	-6.364655	1.133817	0.135995
Mg25	-2.034648	-0.370708	2.491313
Mg26	3.173935	0.802603	2.833520
Mg27	2.877626	-2.376574	1.885201
Mg28	-5.066084	-0.570856	2.287864
Mg29	5.735440	0.010603	-1.486991
Mg30	3.609080	-1.635863	-2.958217

@mg30-isomer27 bp86/6-31G(d) Etot=-6002.876543 Eb=-16.43

Mg1	5.866880	1.868589	0.872890
Mg2	5.546899	-0.129817	-1.214567
Mg3	1.079224	2.042167	-2.383328
Mg4	-2.519408	-0.772959	1.714784
Mg5	2.241265	-3.230986	1.436644
Mg6	-1.316978	-4.030818	-2.073540
Mg7	-5.144578	1.057381	1.404519
Mg8	-2.585335	2.256890	2.317520
Mg9	-0.626024	-3.127794	2.665812
Mg10	1.501297	4.100369	-0.109978
Mg11	2.933220	1.942820	1.458338
Mg12	-0.008376	-0.911914	-2.672018
Mg13	-2.879593	-3.762365	0.653870
Mg14	4.417030	-2.834319	-0.645688
Mg15	1.706360	-3.480996	-1.662186
Mg16	-5.245680	-1.814684	0.413035
Mg17	-3.566776	3.155526	-0.429333
Mg18	4.252398	-0.851762	1.657675
Mg19	-4.989246	0.620341	-1.466868
Mg20	3.955217	2.656053	-1.327075
Mg21	-0.600022	1.319428	0.061190
Mg22	-2.224540	1.382866	-2.587357
Mg23	-2.856042	-1.516083	-1.617634
Mg24	-0.244073	-1.870054	0.045950
Mg25	-1.091536	4.151883	-1.872751
Mg26	2.349631	-0.299647	-0.893246
Mg27	-0.105465	-5.093024	0.424988
Mg28	-1.343156	4.724929	1.000257
Mg29	0.388610	2.807305	2.557231
Mg30	1.108796	-0.359325	2.270866

@mg30-isomer28 bp86/6-31G(d) Etot=-6002.871432 Eb=-16.33

Mg1	-0.776560	0.788232	-0.167857
Mg2	-3.614228	1.790876	1.319003
Mg3	-0.427896	-2.081939	0.737254
Mg4	-1.150381	3.317795	2.106206
Mg5	-2.207751	3.481418	-0.860334
Mg6	0.863786	-1.794271	3.406681
Mg7	0.941763	1.073488	2.792073
Mg8	0.572644	3.079533	-2.241835
Mg9	3.254262	1.796431	-2.069133
Mg10	0.944723	0.119572	-3.066297
Mg11	-3.256937	-1.177655	0.401503
Mg12	0.958280	-2.634128	-1.878771
Mg13	-1.835635	-1.326978	-2.395116
Mg14	3.556409	-4.191900	-1.654706
Mg15	1.639153	2.881583	0.522626
Mg16	4.665171	3.448020	-0.017465

Mg17	3.884567	1.890192	2.392510
Mg18	-5.180743	-0.514748	2.668260
Mg19	2.066735	-0.257543	0.101669
Mg20	-1.749044	1.655114	-3.374237
Mg21	-3.958524	1.009494	-1.633539
Mg22	5.068455	-2.494529	0.217220
Mg23	-6.546842	0.090963	-0.095526
Mg24	-4.918398	-1.880186	-2.103441
Mg25	-1.762887	-0.168747	2.884694
Mg26	3.783466	-1.189152	-2.335337
Mg27	3.778126	-1.120596	2.653648
Mg28	5.165059	0.436393	-0.001739
Mg29	2.294100	-3.357132	1.037833
Mg30	-6.050873	-2.669601	0.654152

@mg30-isomer29 bp86/6-31G(d) Etot=-6002.871389 Eb=-16.33

Mg1	0.601557	-0.187909	0.071558
Mg2	1.368447	-3.617827	0.348996
Mg3	0.492864	-2.476118	2.900796
Mg4	1.477799	2.319377	-1.912950
Mg5	4.284988	0.859112	-2.300093
Mg6	0.155025	-2.360066	-2.213677
Mg7	-1.053117	2.556021	-0.189112
Mg8	3.183366	-1.734069	-1.123457
Mg9	6.122431	-1.110406	1.739732
Mg10	-1.531292	-0.197841	2.553220
Mg11	-0.969881	0.582792	-2.634503
Mg12	-3.500973	2.282351	1.940513
Mg13	-2.824895	-1.964003	-2.561762
Mg14	-4.616215	-2.453529	-0.132513
Mg15	-3.743254	2.305362	-1.975727
Mg16	1.466765	0.335619	3.063109
Mg17	4.134252	3.255076	-0.536355
Mg18	-4.778561	-0.406718	2.175031
Mg19	1.757725	-0.188284	-3.500236
Mg20	-5.379033	-0.261253	-2.155268
Mg21	-1.474753	-2.586313	0.378738
Mg22	-5.848799	1.779459	0.143949
Mg23	-7.240592	-0.793041	0.294710
Mg24	3.600708	0.570875	0.877623
Mg25	6.569899	1.382333	0.019890
Mg26	1.617650	2.819259	1.081887
Mg27	3.354258	-2.161774	2.179372
Mg28	-0.694735	2.674801	2.916829
Mg29	6.304736	-1.270571	-1.260337
Mg30	-2.836371	0.047285	-0.189961

@mg30-isomer30 bp86/6-31G(d) Etot=-6002.870013 Eb=-16.30

Mg1	0.051057	-0.429754	-2.989217
Mg2	2.655627	1.252430	-2.924947
Mg3	5.143020	1.869717	-0.965784
Mg4	1.539594	-2.356176	1.820007
Mg5	-2.276412	-2.124604	-1.590974
Mg6	-1.363622	-2.872094	1.194393
Mg7	-0.490041	0.211109	0.023083
Mg8	-3.329661	-0.126405	1.017886
Mg9	-2.912768	3.133684	-0.323352
Mg10	2.451576	2.973445	-0.305427
Mg11	-4.338794	-3.022201	0.585144
Mg12	-0.100889	2.512482	-2.028337
Mg13	0.709040	-2.673109	-1.040464
Mg14	-5.610518	1.701134	-0.205809
Mg15	-6.382702	-0.833604	1.459043
Mg16	2.513536	-0.140970	-0.138583

Mg17	-2.809126	0.785732	-2.079339
Mg18	5.353821	-0.708598	-2.474455
Mg19	-8.248224	-0.192241	-0.661782
Mg20	4.315483	1.370463	1.939998
Mg21	-5.343735	-0.999597	-1.493246
Mg22	-0.584280	-0.500808	3.001888
Mg23	6.297797	-0.495100	0.368268
Mg24	-1.928416	2.165595	2.301713
Mg25	4.098977	-2.690695	-0.458512
Mg26	2.694551	-1.811633	-3.133157
Mg27	1.199756	1.903278	2.246508
Mg28	2.384762	-0.262633	3.880454
Mg29	-0.222190	4.037616	0.581420
Mg30	4.532779	-1.676463	2.393579

@mg30-isomer31 bp86/6-31G(d) Etot=-6002.869157 Eb=-16.28

Mg1	0.708191	-1.611147	-2.945895
Mg2	-0.680310	-0.465256	-0.167850
Mg3	2.343819	-0.147963	0.139824
Mg4	-2.262771	-1.306431	-2.732922
Mg5	0.102003	1.313604	-2.537449
Mg6	-0.524435	-3.508799	-0.965249
Mg7	0.822754	2.528206	0.191442
Mg8	-2.131188	2.238160	1.300821
Mg9	2.900820	-1.358617	3.316088
Mg10	-5.423718	-1.264808	-2.184090
Mg11	3.071825	-2.635317	-1.469077
Mg12	4.623977	-2.633829	1.152256
Mg13	-6.107633	-1.239696	0.844930
Mg14	-3.459593	-2.598345	-0.153351
Mg15	1.564394	-2.985432	1.182235
Mg16	-3.434327	0.722453	-0.958884
Mg17	-3.158688	-0.579678	2.151773
Mg18	0.144054	3.002228	3.076690
Mg19	5.250274	0.144757	1.957820
Mg20	3.068979	0.202948	-2.992817
Mg21	2.485712	3.131703	-2.327020
Mg22	-5.194018	1.609271	1.717028
Mg23	4.149087	2.382912	0.115602
Mg24	5.354559	2.165464	-2.574682
Mg25	-6.620032	1.201266	-0.938070
Mg26	-4.492702	3.559551	-0.505987
Mg27	5.379007	-0.430594	-1.022414
Mg28	2.734408	1.641146	2.748178
Mg29	0.149566	-0.067843	2.678088
Mg30	-1.364012	-3.009918	1.902981

@mg30-isomer32 bp86/6-31G(d) Etot=-6002.868481 Eb=-16.26

Mg1	0.748766	-0.988150	0.150768
Mg2	-1.615131	-2.879578	-0.125193
Mg3	-4.043008	-1.805539	1.408786
Mg4	3.277682	0.118010	1.713740
Mg5	5.923707	-1.146181	0.397002
Mg6	1.004249	-1.525295	3.120052
Mg7	0.540453	-0.290487	-2.912704
Mg8	-4.045900	-2.024454	-1.782709
Mg9	4.089861	2.500869	-1.438241
Mg10	1.534652	-3.279774	-1.767234
Mg11	-4.600784	1.297740	1.430563
Mg12	-1.217279	-2.652336	-3.028953
Mg13	-1.599732	-3.044677	2.882489
Mg14	-1.949877	0.348879	-0.128900
Mg15	-2.009256	-0.153799	3.017383
Mg16	1.254773	1.842984	-0.988522

Mg17	-1.508084	2.619296	-2.136845
Mg18	2.945872	3.126398	1.293423
Mg19	5.838904	1.821455	0.929937
Mg20	6.349954	0.577505	-2.009281
Mg21	3.365952	-0.629298	-1.566957
Mg22	-0.343434	3.896623	0.481377
Mg23	-4.489893	1.636243	-1.731560
Mg24	0.465747	1.404894	2.189504
Mg25	3.437539	-2.839173	0.641824
Mg26	-2.456542	0.024169	-3.320811
Mg27	0.919801	-4.084407	1.275394
Mg28	-2.260301	2.768379	2.480483
Mg29	-6.129531	-0.505819	-0.435047
Mg30	-3.429161	3.865524	-0.039764

@mg30-isomer33 bp86/6-31G(d) Etot=-6002.867980 Eb=-16.25

Mg1	-0.941186	-0.795794	-0.228491
Mg2	-1.764573	-3.769418	1.777438
Mg3	-0.043379	0.147740	-3.084024
Mg4	0.048293	-1.308762	2.846130
Mg5	-2.978351	-1.044502	2.128669
Mg6	-0.105205	2.233756	-0.772799
Mg7	1.123698	-2.556652	-2.288879
Mg8	1.918353	3.185435	1.471476
Mg9	1.856313	1.044428	3.568452
Mg10	-3.011492	1.984476	0.180252
Mg11	-0.789320	1.458298	2.163277
Mg12	-5.236429	-0.227307	0.215652
Mg13	-5.382869	2.053954	-1.880585
Mg14	1.870570	0.153723	0.183379
Mg15	-6.168020	2.555730	1.014063
Mg16	4.345442	1.355216	1.853466
Mg17	3.058458	-1.539308	2.449678
Mg18	-3.541672	-2.717584	-0.541939
Mg19	-1.129390	-4.509349	-1.037052
Mg20	1.689882	4.739254	-1.120759
Mg21	5.836006	-1.423832	1.473308
Mg22	1.055489	-3.140183	0.667220
Mg23	3.021344	-0.125196	-2.850433
Mg24	-1.855449	-2.506399	-3.086144
Mg25	1.735736	2.589497	-3.248395
Mg26	3.766739	2.667186	-1.016677
Mg27	3.683562	-2.322100	-0.642038
Mg28	-3.197690	0.053319	-2.277051
Mg29	-4.173302	1.545389	3.001792
Mg30	5.308444	0.218984	-0.918986

@mg30-isomer34 bp86/6-31G(d) Etot=-6002.866008 Eb=-16.21

Mg1	-0.466377	1.276568	1.457173
Mg2	1.229134	-0.911511	2.876532
Mg3	-0.763947	-1.658652	0.667871
Mg4	1.929649	2.026933	3.214059
Mg5	3.549499	-2.685607	3.364666
Mg6	-2.074678	3.129450	-0.318058
Mg7	-3.237965	-0.263927	2.834549
Mg8	-3.086609	0.104228	0.014977
Mg9	-5.985493	-0.540231	1.515093
Mg10	0.480834	-2.250564	-2.113740
Mg11	4.206377	0.199675	2.475825
Mg12	0.803405	4.094583	1.367198
Mg13	-4.662713	2.308962	1.211008
Mg14	5.245204	0.490606	-0.451833
Mg15	2.076160	0.028343	0.018851
Mg16	-0.745839	0.539099	-1.801748

Mg17	4.024460	2.585066	-2.238120
Mg18	3.489375	-1.970378	-1.870231
Mg19	3.557470	2.808116	0.771504
Mg20	-6.845571	1.326940	-0.617138
Mg21	-1.500536	-4.335358	-0.658197
Mg22	1.973022	0.329345	-3.165823
Mg23	-2.623383	-1.842666	-2.208404
Mg24	-5.541887	-1.204840	-1.512227
Mg25	4.859685	-2.196830	0.793067
Mg26	5.041763	0.090085	-3.442428
Mg27	1.159851	2.737649	-1.247932
Mg28	-3.876570	-2.764291	0.556207
Mg29	-4.114870	1.617189	-2.139578
Mg30	1.900553	-3.067983	0.646879

@mg30-isomer35 bp86/6-31G(d) Etot=-6002.854883 Eb=-15.98

Mg1	-0.293494	-1.337016	-0.708317
Mg2	-2.143233	-2.214667	1.503184
Mg3	2.292421	0.143383	0.229325
Mg4	-1.653400	-0.158562	-3.172879
Mg5	-3.651102	-1.348917	-1.136918
Mg6	3.856664	3.101357	1.447346
Mg7	-5.139022	-2.309517	1.491431
Mg8	0.907184	-2.064987	-3.466886
Mg9	1.033778	-2.308705	1.805229
Mg10	-6.789606	-2.113744	-1.040848
Mg11	2.292581	1.032020	3.293453
Mg12	-0.484353	0.405361	2.121640
Mg13	2.520290	2.925013	-1.175646
Mg14	-2.250515	3.010737	1.311473
Mg15	-6.071406	0.759802	-1.605878
Mg16	3.621977	-1.662687	3.077334
Mg17	2.329667	-3.002543	-1.009451
Mg18	3.564811	-4.168227	1.426220
Mg19	5.170553	1.218415	-0.773037
Mg20	4.237385	1.782942	-3.580344
Mg21	4.935341	-1.746638	0.167859
Mg22	0.859681	3.095965	1.684010
Mg23	3.897118	-1.017503	-2.627821
Mg24	5.227725	0.583219	2.117302
Mg25	-6.901229	0.112110	1.210627
Mg26	1.406863	0.778120	-2.992617
Mg27	-0.332680	1.772835	-0.793167
Mg28	-3.280206	1.657312	-1.339864
Mg29	-5.441501	2.722597	0.835537
Mg30	-3.722292	0.352523	1.701705

@mg30-isomer36 bp86/6-31G(d) Etot=-6002.847352 Eb=-15.82

Mg1	-1.742909	-0.458481	1.412844
Mg2	0.939785	0.050739	-0.419432
Mg3	1.343231	-3.134595	-0.564327
Mg4	4.269653	-2.565627	-1.096135
Mg5	-4.716890	-0.866077	2.051306
Mg6	0.859991	0.034090	-3.490943
Mg7	2.338237	-2.700988	-3.512217
Mg8	1.021208	0.067726	2.714590
Mg9	-3.793554	1.740430	0.674403
Mg10	3.043249	-2.053382	1.658434
Mg11	-4.982955	-0.458996	-0.967559
Mg12	-2.941807	-3.219855	2.711126
Mg13	-0.639369	2.322814	0.711509
Mg14	4.246061	-2.326746	4.563954
Mg15	0.192691	-2.794082	2.362125
Mg16	-2.854848	4.460541	1.566550

Mg17	-2.001686	0.122289	-1.642460
Mg18	-3.657419	-2.634568	-2.497774
Mg19	4.115398	0.290039	-0.035894
Mg20	-0.055871	5.505217	1.641810
Mg21	2.593731	2.193445	-1.976643
Mg22	-4.735745	-3.324997	0.257467
Mg23	-0.478343	2.635590	-2.455894
Mg24	-1.605122	5.305327	-1.017659
Mg25	2.339373	2.492168	1.208492
Mg26	3.884351	-0.257874	-3.084527
Mg27	3.971349	0.560823	3.017740
Mg28	-1.743658	-3.120049	-0.122783
Mg29	1.365659	4.626142	-0.836793
Mg30	-0.573791	-2.491062	-2.831310

@mg30-isomer37 bp86/6-31G(d) Etot=-6002.838061 Eb=-15.63

Mg1	2.083367	-0.250419	0.145379
Mg2	0.418567	-3.234137	-1.762682
Mg3	0.433794	1.939045	-1.190855
Mg4	-0.338213	1.454233	1.923028
Mg5	-0.875996	-0.709786	-0.298374
Mg6	2.112009	3.045057	1.373804
Mg7	-3.734499	-0.185543	-1.155207
Mg8	1.344048	-0.528004	-2.841584
Mg9	-5.483799	2.043033	0.197562
Mg10	-2.447014	2.403059	-0.234996
Mg11	2.225455	0.886730	3.519925
Mg12	3.555242	2.142270	-1.225807
Mg13	-3.338204	0.519741	2.199168
Mg14	-2.636857	-3.084944	-1.414064
Mg15	1.742101	4.888582	-1.042954
Mg16	-1.065497	4.565982	-1.974796
Mg17	3.925649	-1.403385	2.293847
Mg18	-3.528737	-2.384662	1.508759
Mg19	-6.170827	-0.656757	1.281746
Mg20	5.274458	-0.439940	-0.518240
Mg21	-6.867892	0.033915	-1.619384
Mg22	-0.805801	-3.697825	0.965310
Mg23	2.164720	-3.426084	0.683043
Mg24	5.165354	-3.336096	0.293150
Mg25	3.417885	-2.584854	-2.033760
Mg26	-0.566282	4.665502	0.920839
Mg27	4.606855	1.462063	1.686001
Mg28	4.375442	0.029313	-3.367069
Mg29	-5.530574	-2.645925	-0.896204
Mg30	0.545244	-1.510163	2.584416

@mg30-isomer38 bp86/6-31G(d) Etot=-6002.813045 Eb=-15.10

Mg1	-0.259267	2.221742	-1.603086
Mg2	1.976695	-0.042521	-1.734717
Mg3	-0.984319	2.814659	1.502669
Mg4	-3.855809	1.969848	1.773022
Mg5	-6.954404	2.024464	1.455490
Mg6	1.850555	2.473762	0.583420
Mg7	4.581765	1.972188	2.458365
Mg8	-0.677886	-1.298545	-2.306628
Mg9	-0.103969	-0.024253	0.575110
Mg10	-1.490583	-3.052257	0.179382
Mg11	2.788408	-0.295137	1.483703
Mg12	1.440150	-2.850545	-0.590509
Mg13	-2.886087	0.207335	-0.708985
Mg14	-3.062761	-3.196131	-2.350691
Mg15	-5.132645	-0.964803	-2.525668
Mg16	2.591716	2.747969	-2.714058

Mg17	-7.062066	-0.579915	-0.185674
Mg18	0.541889	-2.419270	2.398850
Mg19	4.800363	0.383437	-3.083233
Mg20	-5.439492	1.784895	-1.254413
Mg21	7.088154	-0.365702	-1.028822
Mg22	-2.911138	3.455775	-0.737560
Mg23	7.306455	1.526788	1.334409
Mg24	4.553757	1.426519	-0.403464
Mg25	-5.508898	-0.539516	2.461192
Mg26	-2.469671	-0.836732	2.222578
Mg27	5.823268	-1.098634	1.697956
Mg28	3.572764	-3.211786	1.793681
Mg29	-4.501606	-2.386158	0.248099
Mg30	4.384664	-1.847476	-0.940418

@mg30-isomer39 bp86/6-31G(d) Etot=-6002.806706 Eb=-14.97

Mg1	2.929798	-0.413179	2.114079
Mg2	0.569559	-0.203306	0.004869
Mg3	3.631689	-0.383630	-0.862574
Mg4	-0.338330	-3.438119	-0.495313
Mg5	1.502251	-2.049191	-2.351459
Mg6	-0.051562	1.023884	2.600510
Mg7	5.915618	-1.379878	-2.477425
Mg8	-2.627509	-1.888021	0.517004
Mg9	1.437407	0.949685	-2.698344
Mg10	-1.400557	-0.863346	-2.180315
Mg11	-2.779702	-0.241570	3.060305
Mg12	2.426280	-3.009684	0.463160
Mg13	-2.403318	2.834894	2.681067
Mg14	5.441014	-2.573813	0.479994
Mg15	1.228979	3.884107	-2.053580
Mg16	-0.392401	3.218701	0.437515
Mg17	2.475195	2.275039	0.176752
Mg18	-5.134015	1.754138	2.029549
Mg19	5.167933	1.803270	1.292619
Mg20	-4.651748	-0.671002	-1.523881
Mg21	-7.271537	0.687394	-0.043689
Mg22	-1.288000	2.298582	-2.442986
Mg23	0.025659	-2.123122	2.314884
Mg24	5.253543	1.950032	-1.759995
Mg25	-7.306996	-2.268582	-0.621698
Mg26	-5.371254	-1.174818	1.583670
Mg27	-7.361979	-0.362688	-2.892313
Mg28	-2.635546	1.132426	-0.016114
Mg29	7.067920	-0.046126	-0.069869
Mg30	5.941610	-0.722079	2.733576

@mg30-isomer40 bp86/6-31G(d) Etot=-6002.802573 Eb=-14.89

Mg1	1.066117	1.946011	-1.448798
Mg2	-1.399624	2.596827	0.773071
Mg3	3.163105	0.073222	0.485075
Mg4	-4.196601	2.291389	2.117757
Mg5	3.755693	0.811986	-2.347793
Mg6	-2.869424	-0.262579	1.080450
Mg7	6.097586	2.221172	-0.551204
Mg8	1.609412	2.453739	1.687389
Mg9	-4.146012	-0.976535	-1.792124
Mg10	1.080792	-1.017606	-2.028609
Mg11	4.592769	2.500285	2.059875
Mg12	-1.477627	0.535115	-1.662643
Mg13	-3.999900	2.119908	-1.015687
Mg14	5.992983	-0.160815	1.670987
Mg15	-6.397048	0.782915	0.453287
Mg16	3.799757	-2.299732	-1.721426

Mg17	0.247944	-0.158609	0.977231
Mg18	6.358709	-3.034631	0.457054
Mg19	0.524434	4.768327	-0.215605
Mg20	-5.322560	-0.503651	2.854513
Mg21	-7.619231	-1.863701	1.404242
Mg22	-4.714200	-2.590758	0.590907
Mg23	-7.154995	-1.815590	-1.462403
Mg24	3.960647	-4.707761	0.221649
Mg25	-6.453903	0.963047	-2.481220
Mg26	6.268199	-0.627165	-1.312867
Mg27	3.807883	-2.305089	2.140369
Mg28	1.436452	-2.952876	0.296986
Mg29	-1.464829	-2.352308	-0.598033
Mg30	3.453473	3.565464	-0.632430

@mg31-isomer01 bp86/6-31G(d) Etot=-6203.036228 Eb=-17.72

Mg1	-3.138603	-3.479491	-1.969888
Mg2	-1.020375	-1.536763	-0.065164
Mg3	1.657504	-0.000120	-0.000034
Mg4	-0.623805	4.783683	0.939008
Mg5	-4.091403	-1.515260	0.320688
Mg6	0.031202	-0.612372	2.726972
Mg7	1.846674	-3.106894	-0.601814
Mg8	-1.019995	1.537068	0.065219
Mg9	-0.233285	-2.411530	-2.915424
Mg10	5.099620	-0.384936	2.469992
Mg11	-2.888429	-0.588399	-2.465694
Mg12	2.644435	2.121252	-2.270058
Mg13	0.031257	0.612368	-2.726957
Mg14	1.847172	3.106646	0.601857
Mg15	-4.091074	1.515751	-0.320689
Mg16	-2.551157	2.319507	-2.886508
Mg17	0.069807	3.698596	-1.918554
Mg18	4.418468	1.565080	0.291554
Mg19	-0.624526	-4.783589	-0.939011
Mg20	2.644125	-2.121608	2.270009
Mg21	2.546399	-1.153723	-2.889236
Mg22	2.546616	1.153334	2.889245
Mg23	0.069177	-3.698566	1.918494
Mg24	-2.551525	-2.319169	2.886581
Mg25	-2.888260	0.588780	2.465625
Mg26	4.418251	-1.565742	-0.291594
Mg27	-2.938815	-4.422928	0.876212
Mg28	5.099654	0.384168	-2.470021
Mg29	-0.232864	2.411585	2.915506
Mg30	-2.938164	4.423379	-0.876194
Mg31	-3.138082	3.479890	1.969876

@mg31-isomer02 bp86/6-31G(d) Etot=-6203.032421 Eb=-17.65

Mg1	2.828154	0.475353	3.493122
Mg2	0.281592	1.779600	2.629022
Mg3	0.273404	-1.170709	3.207694
Mg4	3.134183	2.873602	1.516633
Mg5	-2.388035	0.331895	3.038425
Mg6	-2.168870	3.495186	2.258386
Mg7	0.674084	-4.070164	2.097926
Mg8	2.759583	-1.940787	1.608759
Mg9	-2.161820	-2.794672	2.376921
Mg10	-4.548866	2.014673	1.562565
Mg11	4.851074	0.328976	1.418587
Mg12	0.231759	3.871090	0.427086
Mg13	1.580527	0.718594	-0.032177
Mg14	-0.596543	-5.333042	-0.202256
Mg15	-3.856535	-0.910625	0.683120

Mg16	-1.512954	1.084549	-0.037224
Mg17	2.673548	3.733378	-1.385291
Mg18	-0.297035	-1.649350	0.119541
Mg19	2.033533	-3.800832	-0.750404
Mg20	-2.863119	3.727683	-0.718177
Mg21	3.855019	-1.170923	-1.074350
Mg22	-2.975236	-3.585196	-0.492508
Mg23	-4.723934	1.300640	-1.265672
Mg24	0.039830	2.779795	-2.367329
Mg25	2.582447	1.015879	-3.012686
Mg26	-0.675176	-3.247274	-2.503497
Mg27	-0.218864	-0.177334	-2.813825
Mg28	-2.637646	1.759180	-3.189570
Mg29	4.835305	1.785698	-1.126164
Mg30	2.018126	-2.064895	-3.214441
Mg31	-3.027537	-1.159968	-2.252216

@mg31-isomer03 bp86/6-31G(d) Etot=-6203.032281 Eb=-17.64

Mg1	2.365421	3.012396	-2.589925
Mg2	4.631054	2.112809	-1.003018
Mg3	2.172280	3.495180	0.526464
Mg4	-3.526256	-1.812040	-0.374473
Mg5	1.394014	1.743261	2.977577
Mg6	-1.494372	0.918409	0.123745
Mg7	-2.213359	-4.630968	0.323768
Mg8	-2.598210	2.400717	-2.876930
Mg9	4.509447	-0.698681	0.094794
Mg10	-2.209577	-2.197570	2.382349
Mg11	1.654618	0.463500	0.118606
Mg12	0.130059	0.978465	-2.634839
Mg13	0.080676	-4.237301	2.096428
Mg14	-3.797184	2.781642	2.012836
Mg15	2.550274	-2.783767	1.169139
Mg16	-4.284542	-0.068657	1.999112
Mg17	-0.286040	-1.748605	-0.285806
Mg18	2.933598	-2.692366	-1.733361
Mg19	0.536954	-1.139735	2.739466
Mg20	3.504551	-0.632847	3.063292
Mg21	-3.164651	4.078081	-0.501722
Mg22	3.064450	0.062610	-2.788571
Mg23	4.370592	1.907298	1.948620
Mg24	0.644591	-4.607080	-0.960303
Mg25	-0.793686	3.492097	1.644167
Mg26	-1.971931	-3.501474	-2.402967
Mg27	0.539092	-1.924064	-3.272919
Mg28	-4.434791	1.205686	-0.824371
Mg29	-0.281069	3.737787	-1.340299
Mg30	-2.423778	-0.586695	-2.884991
Mg31	-1.602226	0.871910	3.254131

@mg31-isomer04 bp86/6-31G(d) Etot=-6203.032240 Eb=-17.64

Mg1	-1.827214	0.000365	-2.771522
Mg2	1.872551	-0.000246	0.050971
Mg3	-0.815106	4.370016	1.740478
Mg4	-3.833107	2.153530	-1.635649
Mg5	-0.858211	-1.555874	-0.103835
Mg6	-2.459907	4.690055	-0.675516
Mg7	-0.857661	1.556059	-0.103943
Mg8	0.749396	-4.099240	-1.007395
Mg9	-3.833871	-2.152245	-1.635854
Mg10	1.718269	2.759515	1.624593
Mg11	1.717350	-2.760055	1.624357
Mg12	-2.461427	-4.689161	-0.675753
Mg13	4.372033	1.469730	1.843310

Mg14	-0.816500	-4.369909	1.740234
Mg15	-1.414551	3.084324	-2.981593
Mg16	4.371581	-1.471224	1.843195
Mg17	-3.605321	0.000501	0.300239
Mg18	1.947424	-0.000400	3.169531
Mg19	5.415851	-0.000825	-0.558154
Mg20	-0.706484	1.518739	2.992589
Mg21	1.086252	-1.530613	-2.711370
Mg22	3.464910	2.451477	-0.951313
Mg23	-3.370868	0.000399	3.259959
Mg24	3.703389	-0.000479	-2.885157
Mg25	-3.368534	2.710936	1.583356
Mg26	3.464119	-2.452465	-0.951472
Mg27	-0.706969	-1.518834	2.992752
Mg28	-1.415542	-3.083723	-2.981727
Mg29	1.086881	1.530632	-2.711502
Mg30	0.750707	4.099063	-1.007135
Mg31	-3.369439	-2.710049	1.583326

@mg31-isomer05 bp86/6-31G(d) Etot=-6203.031901 Eb=-17.64

Mg1	2.228869	2.964067	-0.749668
Mg2	-0.135011	-0.391337	-2.775817
Mg3	3.225776	2.747703	2.110777
Mg4	-3.431706	-3.320068	2.010507
Mg5	0.894117	0.759015	2.474774
Mg6	1.610704	-0.527374	-0.209252
Mg7	4.366209	0.911853	-0.025844
Mg8	-2.772855	-2.137148	-2.871203
Mg9	3.837926	0.031098	3.077949
Mg10	2.436253	-3.497885	-0.277918
Mg11	-2.646136	3.695194	-1.913630
Mg12	0.145322	2.613540	-3.012174
Mg13	-3.964457	-0.473921	2.455349
Mg14	-1.103320	-1.414141	3.198636
Mg15	-0.607804	1.675031	-0.225028
Mg16	4.667352	-1.494633	-1.815479
Mg17	-0.152006	4.996443	-0.910744
Mg18	-2.908167	-4.218432	-0.694830
Mg19	-4.455496	-1.446179	-0.427337
Mg20	-2.849829	0.809361	-2.509831
Mg21	0.414692	3.791502	1.860033
Mg22	-0.189247	-3.267362	-1.749479
Mg23	-1.461140	-1.102194	0.161419
Mg24	1.781357	-2.185917	2.477819
Mg25	-2.426732	4.342232	1.022083
Mg26	-3.739258	1.600656	0.248566
Mg27	-1.937557	1.745845	2.712060
Mg28	2.236471	-2.196652	-3.168999
Mg29	4.619600	-1.969355	1.135674
Mg30	2.764158	0.841564	-2.867396
Mg31	-0.448086	-3.882507	1.258983

@mg31-isomer06 bp86/6-31G(d) Etot=-6203.031292 Eb=-17.62

Mg1	0.689608	-0.647172	2.840204
Mg2	3.239298	-2.277138	2.520204
Mg3	0.638389	-3.671207	2.063181
Mg4	-2.078410	-4.553594	0.920489
Mg5	-2.028277	-1.939669	2.634228
Mg6	-1.704974	1.262461	3.181209
Mg7	3.604487	0.683098	2.879981
Mg8	-3.587715	-2.008952	-0.108477
Mg9	-4.128621	0.045729	1.979155
Mg10	-3.955222	2.969556	1.634612
Mg11	0.363882	-4.936270	-0.806591

Mg12	2.464105	-2.743688	-0.419621
Mg13	-2.198194	-3.974075	-2.060779
Mg14	1.059841	2.360315	2.721709
Mg15	4.547481	-0.653732	0.206971
Mg16	1.616472	0.572033	0.097304
Mg17	-0.455216	-1.702363	-0.128972
Mg18	-1.477149	1.065279	0.066291
Mg19	-1.153625	3.960510	1.267910
Mg20	-4.372403	0.936199	-0.969085
Mg21	4.291603	2.399323	0.541305
Mg22	1.734268	3.936759	0.283604
Mg23	5.288485	1.216810	-2.088361
Mg24	-2.386460	-1.070176	-2.726450
Mg25	2.969458	-0.704358	-2.620974
Mg26	0.512804	-2.564195	-2.908991
Mg27	-3.283796	3.894821	-1.061708
Mg28	0.162747	0.497319	-2.738419
Mg29	2.558720	2.387179	-2.234141
Mg30	-0.350155	3.353922	-1.774589
Mg31	-2.581430	1.905275	-3.191201

@mg31-isomer07 bp86/6-31G(d) Etot=-6203.030465 Eb=-17.61

Mg1	2.424215	2.802946	-0.312991
Mg2	-0.015672	0.761180	2.927183
Mg3	3.064693	1.720460	-3.049634
Mg4	-3.446431	-3.859157	-1.055757
Mg5	0.679181	-0.193067	-2.520154
Mg6	1.562061	-0.559559	0.376690
Mg7	4.353263	0.490918	-0.493176
Mg8	-2.962238	-0.428567	2.591745
Mg9	3.609157	-1.211218	-3.086922
Mg10	2.292881	-3.374530	1.361018
Mg11	-1.834332	5.260557	1.267876
Mg12	0.715761	3.645352	2.117160
Mg13	-4.070603	-1.241437	-2.301378
Mg14	-1.272371	-2.543569	-2.815002
Mg15	-0.500471	1.644411	-0.019651
Mg16	4.623076	-1.278807	2.020132
Mg17	0.319274	5.065135	-0.673883
Mg18	-2.995416	-3.484743	1.876978
Mg19	-4.876445	-1.669931	0.549780
Mg20	-2.448935	2.533347	2.242111
Mg21	0.266474	2.854181	-2.765744
Mg22	-0.322079	-2.206708	2.499406
Mg23	-1.533656	-1.149279	-0.162365
Mg24	1.592831	-3.005453	-1.731129
Mg25	-2.459301	3.683754	-1.303934
Mg26	-3.772651	1.111748	-0.136479
Mg27	-2.171787	0.988553	-2.757787
Mg28	2.235979	-1.138286	3.620637
Mg29	4.469970	-2.565084	-0.635757
Mg30	3.033277	1.481299	2.341700
Mg31	-0.559707	-4.134446	0.029326

@mg31-isomer08 bp86/6-31G(d) Etot=-6203.030266 Eb=-17.60

Mg1	2.056150	-0.584778	-3.759210
Mg2	1.549178	2.083019	-2.400675
Mg3	4.397804	0.466462	-2.388318
Mg4	-0.756448	0.289303	-2.943184
Mg5	-1.398806	3.391419	-2.314799
Mg6	0.216937	-2.521121	-2.567958
Mg7	3.274664	-2.380915	-1.642646
Mg8	0.814263	4.116824	-0.227202
Mg9	-2.987297	-1.747918	-2.382687

Mg10	3.548409	2.404940	-0.227039
Mg11	1.603591	-0.240550	-0.079283
Mg12	-3.567775	1.294938	-2.423592
Mg13	-1.849144	-4.468785	-1.356166
Mg14	4.822705	-0.445205	0.438215
Mg15	-2.014764	5.329579	-0.096597
Mg16	0.962656	-3.968020	-0.047914
Mg17	-1.106912	-1.525858	0.076800
Mg18	-0.942471	1.417946	-0.044420
Mg19	3.274279	-2.787260	1.395217
Mg20	0.449779	-2.494474	2.630801
Mg21	-1.688987	-4.450492	1.640012
Mg22	2.571594	-0.403297	3.030823
Mg23	4.653242	1.680554	2.554373
Mg24	-3.768631	2.957056	0.144455
Mg25	1.616982	2.329279	2.063729
Mg26	-1.268230	3.495167	2.166983
Mg27	-3.971393	-0.122461	0.187105
Mg28	-0.435345	0.357729	2.850813
Mg29	-3.974983	-3.142999	0.292124
Mg30	-2.763399	-1.700935	2.715854
Mg31	-3.317650	1.370854	2.714385

@mg31-isomer09 bp86/6-31G(d) Etot=-6203.030063 Eb=-17.60

Mg1	-2.299101	2.267159	-2.716665
Mg2	2.129712	-1.537333	-3.130199
Mg3	-3.066902	-0.796286	-3.446691
Mg4	0.860255	2.587860	-2.979573
Mg5	3.547022	1.152695	-2.693987
Mg6	2.566166	3.542909	-0.629630
Mg7	-0.377392	0.006252	-2.464848
Mg8	5.128156	1.562257	-0.261971
Mg9	-3.826367	3.544133	-0.504525
Mg10	-0.598959	-2.904346	-2.797001
Mg11	1.724338	0.626264	-0.175472
Mg12	-0.640109	4.081434	-0.747208
Mg13	4.000546	-1.344670	-0.755196
Mg14	-4.150973	0.473699	-0.851614
Mg15	3.566970	2.535051	2.084534
Mg16	-1.387305	1.184668	0.227828
Mg17	1.857204	-3.697814	-1.005066
Mg18	-3.085710	-2.493807	-0.944668
Mg19	0.617822	2.969200	1.798946
Mg20	-0.251861	-1.703474	0.182541
Mg21	4.509620	-0.270129	2.104765
Mg22	-4.264196	1.785655	1.987135
Mg23	-1.115067	-5.023764	-0.714345
Mg24	1.542796	0.296398	2.949685
Mg25	-2.237105	3.948067	1.981616
Mg26	2.391835	-2.340227	1.718473
Mg27	-3.144794	-1.006862	1.712572
Mg28	-1.475613	1.100922	3.301408
Mg29	-2.470415	-3.954197	1.794597
Mg30	0.500478	-4.660771	1.767270
Mg31	-0.551050	-1.930944	3.207290

@mg31-isomer10 bp86/6-31G(d) Etot=-6203.029869 Eb=-17.60

Mg1	-2.709393	1.634132	-2.842932
Mg2	-3.078854	2.804014	1.983363
Mg3	1.925965	-3.343050	1.765871
Mg4	3.201873	1.772094	2.905579
Mg5	-2.149912	-1.344013	-3.577234
Mg6	-1.722304	-0.103726	2.899698
Mg7	2.224869	3.656646	0.608197

Mg8	1.303175	-0.634734	3.048760
Mg9	-0.726025	4.485760	0.904341
Mg10	-3.076406	-2.624068	1.454437
Mg11	0.126025	0.442024	-2.617672
Mg12	1.708682	0.623669	0.068407
Mg13	-4.739116	1.957754	-0.588180
Mg14	-0.648454	-2.893204	3.171232
Mg15	-2.100825	-3.621656	-1.490292
Mg16	0.860185	-4.660108	-0.869647
Mg17	-0.304641	-1.620604	0.116427
Mg18	3.083842	2.298894	-2.103834
Mg19	0.561592	-2.492032	-2.969900
Mg20	-1.208239	-4.995315	1.167269
Mg21	4.850411	-0.042201	-1.309692
Mg22	2.788784	-2.257544	-0.917476
Mg23	-3.519685	-0.866564	-0.986998
Mg24	0.123907	3.335643	-1.773869
Mg25	4.873814	2.197247	0.574900
Mg26	-1.393086	1.213387	-0.014614
Mg27	0.207762	2.187109	2.602462
Mg28	-2.892875	4.104360	-1.085036
Mg29	2.853663	-0.513114	-3.429593
Mg30	4.011884	-0.841942	1.552718
Mg31	-4.436618	0.141140	1.753304

@mg31-isomer11 bp86/6-31G(d) Etot=-6203.028964 Eb=-17.58

Mg1	3.821176	-0.634815	-1.998561
Mg2	0.077514	3.177358	-2.047358
Mg3	-0.324760	-1.780801	-0.197168
Mg4	2.301843	3.657495	0.044948
Mg5	-0.911248	-4.266145	-2.098974
Mg6	4.979840	-0.446618	0.911239
Mg7	2.545222	-0.617499	2.845547
Mg8	-0.861799	4.054470	0.740733
Mg9	1.002084	2.390615	2.574453
Mg10	-2.869251	3.866993	-1.617975
Mg11	4.950046	2.010861	-0.721354
Mg12	-1.989159	1.673593	-3.605382
Mg13	-4.320125	1.332880	-1.870938
Mg14	3.971643	2.055692	2.123119
Mg15	1.403775	-4.937040	-0.279628
Mg16	-1.293207	1.149140	-0.220902
Mg17	-3.862524	2.611272	1.019772
Mg18	0.468402	0.047307	-2.728608
Mg19	-3.725267	-0.565436	0.331204
Mg20	1.671830	-2.777386	-2.503187
Mg21	2.772813	2.098418	-2.674842
Mg22	-0.522855	-0.141210	2.532764
Mg23	-3.289921	-3.394566	-0.550973
Mg24	1.737746	0.591252	0.093146
Mg25	-3.521868	0.338045	3.155442
Mg26	-1.864608	2.755230	3.281722
Mg27	2.876840	-2.438004	0.332564
Mg28	0.754562	-3.138919	2.384728
Mg29	-2.366559	-2.465015	2.284833
Mg30	-1.261700	-5.079282	0.924916
Mg31	-2.350487	-1.127887	-2.465277

@mg31-isomer12 bp86/6-31G(d) Etot=-6203.028904 Eb=-17.58

Mg1	1.676914	-2.502406	2.051181
Mg2	-3.590998	-2.426591	0.110853
Mg3	-0.032617	0.402107	-2.646999
Mg4	4.917808	0.838502	-1.452130
Mg5	-1.260428	-4.290034	-1.517766

Mg6	3.042866	0.139764	2.810521
Mg7	5.645573	0.582850	1.423946
Mg8	-1.134460	1.534093	0.120605
Mg9	4.089544	-1.711637	0.270259
Mg10	-2.853023	1.524593	-3.275338
Mg11	-4.014336	2.715390	1.548515
Mg12	1.859500	-3.445754	-0.928281
Mg13	1.697416	0.372715	0.041891
Mg14	-3.976884	0.542664	-0.665102
Mg15	-1.554344	4.436803	1.421287
Mg16	0.903193	3.956039	-0.312256
Mg17	0.959706	2.656111	2.358875
Mg18	2.352253	2.272920	-2.421708
Mg19	-1.845190	2.301286	3.494471
Mg20	-0.625108	-1.503070	-0.123897
Mg21	2.866436	-1.023312	-2.596007
Mg22	-1.445616	-2.811339	2.574177
Mg23	-2.536120	-1.383867	-2.607151
Mg24	-3.037053	-0.163025	2.140322
Mg25	-2.658285	-5.121955	0.962880
Mg26	-3.105865	3.698602	-1.177032
Mg27	-0.063365	-0.122060	2.804857
Mg28	-0.526895	3.368589	-2.821500
Mg29	0.362124	-2.549653	-3.343879
Mg30	0.293168	-5.016034	1.130563
Mg31	3.594083	2.727705	0.623842

@mg31-isomer13 bp86/6-31G(d) Etot=-6203.027110 Eb=-17.54

Mg1	-0.947839	2.752522	-2.322916
Mg2	-0.372591	4.936817	0.253203
Mg3	-3.951465	1.755538	-1.919785
Mg4	-2.262297	0.188657	-3.671280
Mg5	-0.153625	-0.023404	2.702921
Mg6	3.660788	-0.555516	-2.045414
Mg7	-1.181641	-2.438579	-2.410824
Mg8	2.492943	2.128589	-2.924464
Mg9	1.779806	-2.727347	-2.981833
Mg10	2.639134	1.364434	2.631091
Mg11	-0.137680	-3.038622	2.230455
Mg12	-1.643383	-0.224217	-0.159525
Mg13	2.844380	-3.914500	1.625272
Mg14	3.765014	1.840519	-0.134497
Mg15	-0.268683	3.022394	2.747611
Mg16	-2.445105	2.800765	0.453392
Mg17	0.664681	1.711481	0.057948
Mg18	-2.342871	-3.325120	0.151722
Mg19	-2.791929	1.407030	3.104664
Mg20	2.374273	4.192510	1.555140
Mg21	-5.174034	-2.384356	0.805567
Mg22	-4.550501	0.517447	0.798721
Mg23	2.392257	-1.541936	3.325038
Mg24	0.676581	-4.288160	-0.552753
Mg25	-4.099832	-1.370773	-1.794719
Mg26	1.278904	-1.296198	0.063136
Mg27	0.515050	0.016083	-2.691089
Mg28	3.868265	-3.451759	-1.047124
Mg29	-2.849821	-1.572649	2.590689
Mg30	4.249851	-1.051686	0.986731
Mg31	1.971368	4.570038	-1.427078

@mg31-isomer14 bp86/6-31G(d) Etot=-6203.026355 Eb=-17.52

Mg1	-1.541089	2.365226	2.955992
Mg2	-2.403426	-0.895268	2.887571
Mg3	1.428734	2.899778	2.820117

Mg4	-0.188513	-2.905175	3.061588
Mg5	2.697900	-1.980657	3.110641
Mg6	0.508952	0.073877	2.751855
Mg7	1.804210	-3.926151	1.001128
Mg8	3.587011	0.812895	2.300585
Mg9	-2.519014	-3.809402	1.434616
Mg10	-4.116288	1.373161	1.829842
Mg11	4.002447	-1.759359	0.412451
Mg12	-0.523344	-1.664769	0.167322
Mg13	-3.695540	-1.132034	0.202064
Mg14	-3.200187	-3.676640	-1.502403
Mg15	-0.485567	-4.664436	-0.841703
Mg16	-1.199961	1.241760	0.119283
Mg17	-3.213948	4.029951	0.881468
Mg18	1.756498	0.268200	-0.263131
Mg19	-0.150603	4.271122	0.625698
Mg20	2.881083	3.140117	0.211836
Mg21	5.137663	1.025435	-0.283851
Mg22	1.838991	-2.625381	-1.728249
Mg23	-4.036615	1.685595	-1.236425
Mg24	4.163693	-0.830336	-2.473982
Mg25	-0.912684	-2.039091	-2.914220
Mg26	-3.752330	-0.985773	-2.788262
Mg27	0.753209	2.717039	-1.948513
Mg28	-2.029208	3.896549	-1.810262
Mg29	3.620885	2.084003	-2.591303
Mg30	-1.522872	1.020497	-3.036304
Mg31	1.309914	-0.010733	-3.355449

@mg31-isomer15 bp86/6-31G(d) Etot=-6203.025887 Eb=-17.51

Mg1	-1.856293	0.526231	3.043749
Mg2	0.121768	-1.734695	2.661368
Mg3	-0.170063	-2.883958	-2.419617
Mg4	-0.062819	0.073506	-2.735625
Mg5	1.097727	1.065086	3.164013
Mg6	-3.011195	-1.181952	-2.716676
Mg7	-1.700448	-0.670253	-0.000038
Mg8	-3.085465	2.220156	0.873005
Mg9	-4.810811	0.596244	-1.020151
Mg10	-0.765423	3.623264	2.303472
Mg11	4.154224	-0.065823	-1.463716
Mg12	3.095461	-1.307403	3.328756
Mg13	-1.749399	4.402772	-0.614888
Mg14	3.529736	0.858703	1.313350
Mg15	1.448193	-1.069911	-0.102872
Mg16	-2.689061	-3.740242	-0.969670
Mg17	-2.803439	-2.608681	1.999012
Mg18	2.677545	-3.848829	-1.170131
Mg19	0.195386	1.676460	0.151975
Mg20	1.000496	5.125068	-0.082577
Mg21	2.530964	1.272575	-3.540622
Mg22	2.449497	-3.828768	1.938093
Mg23	-4.599432	-0.158001	1.970650
Mg24	-0.116298	-3.815580	0.484446
Mg25	-2.398543	1.886795	-2.188890
Mg26	4.482900	-2.114143	0.699567
Mg27	0.302334	3.215576	-2.548374
Mg28	2.959254	2.830206	-0.954108
Mg29	2.476581	-1.764627	-3.268569
Mg30	-5.025949	-2.185614	-0.182280
Mg31	2.322572	3.605839	2.047348

@mg31-isomer16 bp86/6-31G(d) Etot=-6203.025884 Eb=-17.51

Mg1	0.150710	1.774335	-0.047665
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Mg2	1.915738	0.158379	3.072361
Mg3	-2.267212	1.609586	-2.519387
Mg4	-2.057132	4.133539	-0.993444
Mg5	-3.438935	-3.024707	-1.130387
Mg6	-1.620856	-0.746615	-0.089026
Mg7	-0.822033	1.304196	2.862142
Mg8	3.458720	1.456036	0.833991
Mg9	4.325300	-3.260428	-0.151527
Mg10	1.426266	-1.010233	0.045209
Mg11	-2.558456	-1.252355	-3.518297
Mg12	4.785015	-0.515816	-1.015960
Mg13	1.580658	3.374505	2.257535
Mg14	2.764714	1.300509	-2.237986
Mg15	-0.521716	-1.677688	2.793295
Mg16	2.826404	3.906126	-0.683228
Mg17	-3.239350	1.683292	0.650276
Mg18	4.373173	-1.210347	1.993840
Mg19	-0.469293	-2.910647	-2.346784
Mg20	0.491605	5.380441	0.054922
Mg21	2.080832	-3.198587	2.052252
Mg22	-3.262853	-0.286219	3.221415
Mg23	-4.535586	-0.127913	-1.739439
Mg24	-4.932502	-1.099680	0.950430
Mg25	0.162163	0.002924	-2.861341
Mg26	2.651571	-1.910318	-2.642688
Mg27	-1.435894	4.041979	1.926299
Mg28	-3.205162	-3.113919	2.172008
Mg29	0.489318	3.302318	-2.606802
Mg30	-0.817279	-3.750952	0.576718
Mg31	1.702074	-4.331744	-0.878732

@mg31-isomer17 bp86/6-31G(d) Etot=-6203.025806 Eb=-17.51

Mg1	-4.304539	-2.861367	0.580453
Mg2	-4.948137	-0.113691	1.139899
Mg3	-4.211557	-0.625606	-1.813704
Mg4	-2.775861	-3.480927	-1.816470
Mg5	-3.215732	1.932246	-0.163085
Mg6	-2.634340	-1.399310	2.750379
Mg7	-1.873468	-1.383414	-3.597850
Mg8	-3.299323	1.640999	2.929099
Mg9	-1.500415	-0.751764	-0.194778
Mg10	-1.941368	1.571957	-2.869521
Mg11	-1.389232	-3.645196	0.932741
Mg12	-1.734100	4.263914	-1.504837
Mg13	-1.389652	3.668826	1.655234
Mg14	0.644645	5.183658	0.002250
Mg15	0.944920	3.188010	-2.687640
Mg16	0.598918	0.024560	-2.863005
Mg17	0.240048	1.726950	-0.213262
Mg18	-0.439074	0.771736	2.585785
Mg19	0.356957	-2.964848	-1.691529
Mg20	0.415755	-2.044523	2.964541
Mg21	1.599652	-0.924026	0.194233
Mg22	1.708311	3.014952	2.289091
Mg23	2.359147	0.277691	3.558125
Mg24	3.074019	3.640876	-0.426501
Mg25	3.195562	1.086945	-1.887396
Mg26	1.530759	-4.157984	1.202871
Mg27	3.001929	-1.782516	-2.952039
Mg28	3.860884	1.118932	1.164093
Mg29	3.747160	-2.105908	2.093916
Mg30	3.540514	-3.737493	-0.792679
Mg31	4.837618	-1.133680	-0.568415

@mg31-isomer18 bp86/6-31G(d) Etot=-6203.025239 Eb=-17.50

Mg1	3.044179	-0.694871	3.242480
Mg2	0.822262	3.983926	2.383177
Mg3	3.016927	2.066278	1.731837
Mg4	0.496381	0.915119	3.140038
Mg5	4.962733	-0.264625	1.104395
Mg6	-1.909617	2.543138	2.542876
Mg7	3.585787	1.328599	-1.109566
Mg8	1.921768	4.132579	-0.562178
Mg9	-1.117085	4.827819	0.360143
Mg10	4.666275	-1.660133	-1.437344
Mg11	-2.128578	-0.693954	3.297131
Mg12	3.392471	-3.026741	1.145399
Mg13	-4.218431	0.726071	1.751790
Mg14	0.206416	1.731476	0.075672
Mg15	1.637809	-0.853390	-0.055428
Mg16	0.494161	-2.085446	2.602940
Mg17	1.767630	2.367185	-3.140629
Mg18	-2.932783	2.329796	-0.384829
Mg19	-1.495227	-0.794529	0.180924
Mg20	2.324814	-0.718485	-3.164098
Mg21	-2.051766	-3.590106	2.084378
Mg22	-0.905093	3.451407	-2.318942
Mg23	-4.524842	-2.237706	1.524028
Mg24	2.592300	-3.658601	-1.747471
Mg25	-0.442397	0.382996	-2.709452
Mg26	-4.412852	-0.499008	-0.985794
Mg27	0.288226	-3.896511	0.203839
Mg28	-3.228433	1.465301	-3.220344
Mg29	-0.130163	-2.568718	-2.455841
Mg30	-2.904656	-3.445227	-0.858279
Mg31	-2.818218	-1.563638	-3.220851

@mg31-isomer19 bp86/6-31G(d) Etot=-6203.025066 Eb=-17.50

Mg1	-2.128541	1.097449	-3.800338
Mg2	-3.023765	-1.655541	-2.657779
Mg3	-0.060421	-0.726823	-2.761977
Mg4	1.978785	-2.951651	-2.816525
Mg5	-0.631315	-3.525633	-1.523495
Mg6	-4.940435	-1.281034	-0.275956
Mg7	-3.489707	1.275077	-1.145614
Mg8	-3.382975	-3.775525	-0.416494
Mg9	2.953803	-0.041250	-2.853232
Mg10	0.672387	2.198678	-3.131218
Mg11	-1.863008	3.635688	-2.135056
Mg12	1.947109	-3.629950	0.280357
Mg13	-0.841451	-3.485737	1.637041
Mg14	-1.617271	-0.996399	0.077749
Mg15	-0.368124	1.664521	-0.048653
Mg16	1.614250	-0.526041	0.099405
Mg17	-3.688136	-2.417240	2.249810
Mg18	-2.590665	3.708568	0.803960
Mg19	4.432076	-2.324680	-1.285627
Mg20	-3.691067	0.655344	1.779361
Mg21	3.208998	2.729390	-1.763909
Mg22	0.838798	4.414930	-0.816228
Mg23	-1.331692	-0.822087	3.297554
Mg24	0.207742	4.137002	2.147141
Mg25	1.528375	-1.954999	2.971068
Mg26	4.309628	-2.221868	1.644301
Mg27	-1.806153	2.260909	3.385957
Mg28	2.629816	2.621056	1.145495
Mg29	0.871743	1.117501	3.065433
Mg30	3.752281	0.355625	2.928200

Mg31	4.508934	0.464723	-0.080730
@mg31-isomer20 bp86/6-31G(d) Etot=-6203.024455 Eb=-17.49			
Mg1	0.080378	2.893311	2.124930
Mg2	-0.021002	-1.687718	0.099111
Mg3	-3.944432	-0.962601	0.641930
Mg4	0.414978	0.111034	2.957870
Mg5	2.514146	-2.538200	-2.544509
Mg6	2.441699	3.781814	0.128094
Mg7	-0.438684	-3.326667	-2.548204
Mg8	-0.539184	-4.628099	1.822834
Mg9	-2.644576	0.903604	2.928292
Mg10	-0.534625	3.777117	-0.748647
Mg11	-1.833900	-2.037296	2.629144
Mg12	-4.911126	1.837083	1.000152
Mg13	-4.559204	0.839779	-1.846665
Mg14	1.843028	-4.236348	-0.098517
Mg15	3.420309	-1.555090	0.195505
Mg16	-2.728175	3.723713	1.601002
Mg17	-3.605973	3.522822	-1.238903
Mg18	4.555568	1.383775	0.530503
Mg19	-1.598046	0.957378	0.029447
Mg20	1.444051	2.554572	-2.720876
Mg21	1.659141	-2.570252	2.570301
Mg22	-2.520624	-1.219417	-2.248305
Mg23	-0.663822	-5.792372	-0.899955
Mg24	3.583813	-0.345695	3.002475
Mg25	3.588147	0.220670	-2.375120
Mg26	2.963007	2.481276	2.875530
Mg27	0.460498	-0.307828	-2.697641
Mg28	4.420552	3.012663	-2.058179
Mg29	-1.716125	1.809905	-2.957547
Mg30	1.479051	0.907860	0.071391
Mg31	-2.608868	-3.510790	-0.225444
@mg31-isomer21 bp86/6-31G(d) Etot=-6203.024211 Eb=-17.48			
Mg1	1.576481	1.985225	2.531172
Mg2	-1.165249	0.942316	3.149511
Mg3	-0.847789	4.016605	2.012450
Mg4	-1.572699	-2.090635	3.196423
Mg5	4.080025	0.029111	2.613678
Mg6	1.195893	-0.982209	3.131235
Mg7	3.422515	-2.753485	1.959890
Mg8	0.537268	-3.616577	1.670986
Mg9	-3.600560	-0.408750	1.978682
Mg10	4.034435	2.015149	0.421813
Mg11	-3.516663	2.681142	2.159744
Mg12	1.697593	4.049002	0.377243
Mg13	-2.591155	-3.957714	0.940216
Mg14	-0.891580	1.608413	0.101494
Mg15	-2.920231	4.180977	-0.328250
Mg16	4.619354	-1.090210	-0.304363
Mg17	-1.090426	-1.359417	0.022093
Mg18	1.641674	-0.066679	0.073415
Mg19	2.199302	-2.973656	-0.869935
Mg20	5.114391	1.022954	-2.356533
Mg21	-4.364946	-1.870480	-0.540486
Mg22	-0.247738	-4.787342	-1.015316
Mg23	2.334571	2.305469	-2.058292
Mg24	-0.297140	3.930725	-1.868557
Mg25	-3.991236	1.190889	-0.515049
Mg26	-2.698262	-3.620824	-2.184930
Mg27	2.675166	-0.721640	-2.895969
Mg28	-0.035995	0.774739	-2.876727

Mg29	0.003828	-2.248386	-2.880280
Mg30	-2.644504	2.446183	-2.871072
Mg31	-2.656322	-0.630892	-2.774288

@mg31-isomer22 bp86/6-31G(d) Etot=-6203.024195 Eb=-17.48

Mg1	-2.186710	-2.669156	-2.771970
Mg2	-3.400043	-2.110321	2.056237
Mg3	2.570547	2.215233	1.744895
Mg4	2.176029	-0.028121	3.656306
Mg5	-1.117323	0.408568	-2.989820
Mg6	-2.923963	0.750902	3.285969
Mg7	1.987405	-2.795394	2.113082
Mg8	-0.113858	1.946726	3.254322
Mg9	-0.904185	-3.898818	2.269424
Mg10	-3.042951	2.677415	-1.576291
Mg11	0.897904	-1.843060	-2.709721
Mg12	1.665170	-0.448558	0.040545
Mg13	-4.532502	-2.301820	-0.779694
Mg14	-2.574111	3.251559	1.605127
Mg15	-0.343842	3.344494	-2.830845
Mg16	1.958238	3.663997	-0.884512
Mg17	-0.449092	1.637354	0.061174
Mg18	3.339623	-2.967825	-0.643895
Mg19	1.744242	1.233242	-2.775887
Mg20	-1.354536	5.043704	-0.601425
Mg21	5.810266	-1.253048	-0.761621
Mg22	4.097871	1.337566	-0.743189
Mg23	-4.024065	-0.101127	-2.653683
Mg24	0.421068	-3.865485	-0.517032
Mg25	4.300786	-0.662924	1.704517
Mg26	-1.327374	-1.283893	-0.285625
Mg27	-0.487515	-0.955804	2.649694
Mg28	-2.611098	-4.360788	-0.137884
Mg29	3.788546	-0.925628	-2.849409
Mg30	-3.787325	0.529356	0.413232
Mg31	0.422801	4.431653	1.657980

@mg31-isomer23 bp86/6-31G(d) Etot=-6203.023971 Eb=-17.48

Mg1	1.112433	3.299599	-1.090654
Mg2	-0.179603	-0.994277	-2.853022
Mg3	2.760237	2.946440	1.510787
Mg4	-1.334125	-3.490237	2.247670
Mg5	0.490421	1.049248	2.410131
Mg6	1.937065	0.357738	-0.129691
Mg7	4.031427	2.631543	-1.286632
Mg8	-2.409668	-3.129849	-2.721089
Mg9	3.388923	0.269439	3.035515
Mg10	3.871910	-1.845058	0.804161
Mg11	-3.812257	2.645586	-1.978310
Mg12	-0.929369	1.985586	-3.150157
Mg13	-3.503566	-1.222520	2.646300
Mg14	-0.965483	-0.918315	4.008044
Mg15	-1.237372	1.348687	-0.194138
Mg16	4.747358	-0.203220	-1.802489
Mg17	-1.663877	4.469003	-1.195172
Mg18	-1.606609	-4.927993	-0.331767
Mg19	-3.474635	-2.366625	-0.076094
Mg20	-3.133057	-0.228826	-2.436829
Mg21	-0.500428	3.897594	1.602705
Mg22	0.372173	-4.074709	-2.396344
Mg23	-0.450032	-1.438263	0.257457
Mg24	1.504595	-2.053594	2.760087
Mg25	-3.589485	3.685700	0.927234
Mg26	-4.198704	0.696871	0.365237

Mg27	-2.466462	1.672048	2.814098
Mg28	2.526849	-2.138105	-1.963146
Mg29	5.219733	1.011988	0.896099
Mg30	2.075877	1.019092	-3.131650
Mg31	1.415731	-3.954569	0.451660

@mg31-isomer24 bp86/6-31G(d) Etot=-6203.023933 Eb=-17.48

Mg1	1.642118	-4.451318	1.197568
Mg2	4.165207	-3.165109	0.478883
Mg3	2.063023	-3.645619	-1.817318
Mg4	-4.154812	0.940340	1.443669
Mg5	1.821391	-0.093371	-2.930330
Mg6	-3.407394	-3.007021	-1.838254
Mg7	-1.691356	2.778208	0.717461
Mg8	-3.568410	-2.616448	1.144875
Mg9	3.862964	-0.012358	0.637201
Mg10	-1.256545	4.154096	-1.996158
Mg11	1.155501	-1.471875	-0.033218
Mg12	-0.595920	-2.662131	2.394104
Mg13	0.767177	5.010432	0.063101
Mg14	-3.269566	-0.436254	-3.274149
Mg15	3.222038	3.193746	0.620424
Mg16	-3.555903	1.917334	-1.461158
Mg17	0.901931	1.426915	-0.163705
Mg18	2.832207	1.286491	3.115775
Mg19	1.679036	3.321608	-2.388032
Mg20	4.080261	1.601982	-1.886899
Mg21	-5.073865	-0.719374	-0.886525
Mg22	2.471874	-1.825744	2.737873
Mg23	4.232874	-1.535540	-2.003352
Mg24	0.683511	3.260441	2.522884
Mg25	-0.600845	-1.831842	-2.652844
Mg26	-2.205871	2.106717	3.556927
Mg27	0.016561	0.240091	2.561814
Mg28	-1.734148	-0.392820	-0.078813
Mg29	-0.930514	-3.826194	-0.377873
Mg30	-2.741473	-0.831961	3.402303
Mg31	-0.811054	1.286579	-2.806235

@mg31-isomer25 bp86/6-31G(d) Etot=-6203.022486 Eb=-17.45

Mg1	1.633721	2.981096	-2.097725
Mg2	-1.691446	-0.672807	-0.491997
Mg3	0.000186	-1.281268	1.896844
Mg4	2.582623	3.955439	0.648788
Mg5	1.691572	-0.672813	-0.492170
Mg6	-0.000456	3.737979	2.418478
Mg7	0.000167	1.628721	0.258567
Mg8	1.548817	-2.209173	-3.020852
Mg9	3.976933	1.470803	-0.522180
Mg10	-2.607075	1.353247	2.178046
Mg11	0.000221	-3.492419	-0.568470
Mg12	4.693633	-1.303373	-1.764135
Mg13	-4.175607	-1.353176	1.270694
Mg14	3.132354	-3.591382	-0.747902
Mg15	-0.000442	5.038521	-0.361847
Mg16	-3.131827	-3.591863	-0.747682
Mg17	2.607161	1.353616	2.178238
Mg18	-1.926834	-3.593736	1.918184
Mg19	-4.693428	-1.304162	-1.764015
Mg20	-2.394196	-1.221142	3.719416
Mg21	-0.000069	0.513157	-2.985723
Mg22	-3.977410	1.470160	-0.522122
Mg23	2.394550	-1.220893	3.719413
Mg24	-3.020931	0.614223	-3.282518

Mg25	0.000029	0.996214	3.726065
Mg26	-1.548668	-2.209349	-3.020662
Mg27	1.927478	-3.593484	1.918025
Mg28	3.020738	0.614703	-3.282561
Mg29	-1.634192	2.980638	-2.097512
Mg30	-2.583439	3.955100	0.648739
Mg31	4.175836	-1.352576	1.270574

@mg31-isomer26 bp86/6-31G(d) Etot=-6203.020354 Eb=-17.40

Mg1	-3.843034	1.268011	2.145486
Mg2	-3.624714	-1.785871	2.280917
Mg3	-1.254541	0.568719	3.424484
Mg4	-1.853963	3.539071	1.821170
Mg5	0.824331	2.985295	3.378853
Mg6	-4.067558	-2.854018	-0.789526
Mg7	-4.971777	-0.208896	-0.188403
Mg8	1.709329	4.295778	0.397067
Mg9	-2.975552	2.071188	-0.695285
Mg10	1.740570	-0.019386	3.245287
Mg11	-0.327080	-2.270299	2.816877
Mg12	-1.002738	4.357782	-1.036741
Mg13	-1.692206	-0.683974	0.319930
Mg14	0.265418	1.640482	0.779766
Mg15	-2.038618	-3.987538	0.988644
Mg16	3.373160	2.338217	2.089583
Mg17	2.689382	-2.854453	2.543947
Mg18	1.490102	-0.997150	0.144727
Mg19	-0.143016	0.621608	-1.879538
Mg20	0.924161	-4.032013	0.302431
Mg21	-3.080923	-0.491599	-2.610976
Mg22	1.317442	3.303856	-2.596585
Mg23	-1.177255	-2.984917	-1.846858
Mg24	3.250500	1.729080	-0.856141
Mg25	4.264781	-0.505931	1.300758
Mg26	-1.729088	2.476791	-3.450659
Mg27	3.888106	-3.300151	-0.087227
Mg28	1.833397	-2.588524	-2.492912
Mg29	2.293465	0.469348	-3.519670
Mg30	-0.403065	-1.149721	-4.129379
Mg31	4.320983	-0.950784	-1.800026

@mg31-isomer27 bp86/6-31G(d) Etot=-6203.018991 Eb=-17.38

Mg1	-3.567851	0.195263	-2.964228
Mg2	-2.091532	2.810837	-2.453725
Mg3	-4.564486	1.971263	-0.804972
Mg4	-0.612760	-0.260480	-2.806735
Mg5	0.966071	2.201798	-2.405683
Mg6	-2.535773	-2.580634	-2.246454
Mg7	-3.616798	-0.821956	0.041077
Mg8	2.394222	-0.573743	-3.013251
Mg9	-3.091982	4.233840	0.284026
Mg10	3.953894	2.088951	-3.181460
Mg11	0.516543	-3.139122	-2.567382
Mg12	-1.277703	1.299955	-0.034345
Mg13	0.010752	4.108158	-0.166467
Mg14	-1.576707	-5.243712	-1.466916
Mg15	-3.697502	1.619267	2.072337
Mg16	3.095962	3.243994	-0.471196
Mg17	1.724019	0.426336	0.028904
Mg18	-2.578041	-3.666520	0.949613
Mg19	-0.440891	-1.563086	0.096541
Mg20	4.687174	0.298327	-1.021027
Mg21	2.804362	-2.432143	-0.666823
Mg22	0.522008	-4.532583	0.434169

Mg23	-1.409742	3.594867	2.576841
Mg24	-3.173299	-1.332084	2.953889
Mg25	-0.817211	0.596757	2.887913
Mg26	2.444913	-3.119352	2.275224
Mg27	-0.415068	-2.438971	3.008030
Mg28	1.434757	2.679033	2.194096
Mg29	4.520684	-1.157016	1.563821
Mg30	2.037886	-0.272446	3.113067
Mg31	4.354097	1.765202	1.791116

@mg31-isomer28 bp86/6-31G(d) Etot=-6203.017712 Eb=-17.35

Mg1	5.492514	2.241847	0.267431
Mg2	3.264776	2.069105	-1.950383
Mg3	0.732797	3.661748	-1.081011
Mg4	2.793244	3.041768	1.145939
Mg5	-1.691209	3.230486	-2.885641
Mg6	0.462965	1.127565	-2.966854
Mg7	-2.187306	4.380203	-0.119872
Mg8	4.967287	-0.313220	-1.056903
Mg9	-0.233545	3.070211	1.814230
Mg10	2.521190	-1.086152	-2.709196
Mg11	4.106673	0.081070	1.945197
Mg12	1.662428	0.403870	0.067311
Mg13	-4.188181	2.500999	-1.419616
Mg14	-1.308950	1.221507	-0.396392
Mg15	1.590935	1.158889	3.409623
Mg16	-0.353055	-1.759820	-3.575987
Mg17	-2.609577	0.273828	-3.063912
Mg18	-3.578735	2.312639	1.638194
Mg19	3.199123	-2.387272	0.037910
Mg20	-1.794762	1.665448	3.979513
Mg21	-0.418181	-1.707492	-0.491579
Mg22	-0.670137	-0.328111	2.184393
Mg23	1.799189	-1.920323	2.708570
Mg24	1.320403	-3.853813	-1.971021
Mg25	-2.916458	-2.628519	-2.164581
Mg26	1.305893	-4.482629	1.075529
Mg27	-3.545907	-0.636334	2.793043
Mg28	-3.972517	-0.301253	-0.290745
Mg29	-1.026591	-3.278970	2.567174
Mg30	-1.315470	-4.757125	-0.356671
Mg31	-3.408836	-3.000150	0.866305

@mg31-isomer29 bp86/6-31G(d) Etot=-6203.017494 Eb=-17.35

Mg1	1.600474	-2.597506	-3.130829
Mg2	2.318722	1.407040	3.202467
Mg3	-2.179275	-4.672702	-0.244831
Mg4	-3.556785	2.362256	2.354214
Mg5	4.508331	1.882888	1.415273
Mg6	1.064022	2.559512	-2.389817
Mg7	2.245513	-3.467636	2.025336
Mg8	-0.564846	1.972246	2.987617
Mg9	-3.642394	3.100882	-0.706738
Mg10	-3.621235	-2.781894	1.671024
Mg11	-1.853689	2.631040	-3.157099
Mg12	-0.094852	-0.056440	-2.847890
Mg13	-1.706436	4.460023	1.505914
Mg14	-0.775589	-3.610772	2.290247
Mg15	-1.403583	-2.806752	-2.700624
Mg16	3.950481	-0.986552	2.064494
Mg17	-1.075247	1.558723	-0.075842
Mg18	-0.857507	4.687267	-1.226176
Mg19	-3.107260	0.095428	-2.495169
Mg20	0.664687	-0.971169	2.765782

Mg21	-2.294936	-0.452154	2.959282
Mg22	3.798552	2.467452	-1.342647
Mg23	0.745275	-4.027466	-0.597478
Mg24	3.298492	-2.413414	-0.647520
Mg25	-0.974818	-1.387745	0.036478
Mg26	-3.997490	-2.438762	-1.323778
Mg27	5.225567	-0.147232	-0.697804
Mg28	1.374346	3.276714	0.736927
Mg29	1.753014	0.231300	0.024872
Mg30	-3.896778	0.111093	0.422057
Mg31	3.055242	0.014333	-2.877744

@mg31-isomer30 bp86/6-31G(d) Etot=-6203.014932 Eb=-17.29

Mg1	-1.927648	1.457490	3.089578
Mg2	1.205361	1.701821	3.419492
Mg3	-2.830149	-1.655422	2.415275
Mg4	0.085537	-0.865391	2.508742
Mg5	-0.006144	3.914131	1.760320
Mg6	-4.076691	0.865555	1.009096
Mg7	-4.325279	-1.987856	-0.092309
Mg8	-3.103172	3.783973	1.506818
Mg9	1.973792	-3.056715	3.517377
Mg10	-3.853749	3.011770	-1.300037
Mg11	-1.173520	1.482952	0.094404
Mg12	-2.842375	-4.557172	0.178784
Mg13	-1.481752	4.743948	-0.822880
Mg14	-3.300417	0.121457	-1.960841
Mg15	-1.015615	-1.537363	-0.317602
Mg16	-0.593372	-3.847243	1.946914
Mg17	2.958820	2.717528	1.316618
Mg18	3.236635	-0.501520	2.428916
Mg19	-2.635445	-3.058060	-2.479847
Mg20	1.167887	3.237473	-1.113534
Mg21	1.558285	0.212407	-0.148988
Mg22	-1.274219	2.301106	-2.911449
Mg23	1.998083	-2.983682	0.505450
Mg24	5.428647	0.927151	1.073935
Mg25	-0.793352	-0.754468	-3.397932
Mg26	-0.159973	-4.461659	-1.222032
Mg27	3.951759	1.778160	-1.461080
Mg28	4.314506	-1.371545	-0.528805
Mg29	1.558985	0.998291	-3.267268
Mg30	1.741947	-2.094926	-2.356733
Mg31	4.212631	-0.522189	-3.390383

@mg31-isomer31 bp86/6-31G(d) Etot=-6202.998982 Eb=-16.97

Mg1	0.756230	2.712569	2.389683
Mg2	3.866938	2.059187	1.695073
Mg3	4.440881	2.324837	-1.394148
Mg4	0.013441	1.071999	0.001713
Mg5	2.114570	3.770448	-0.095889
Mg6	-1.164225	0.271870	2.812339
Mg7	2.685323	-0.180141	-0.107791
Mg8	-2.644144	2.676815	1.597468
Mg9	-2.537449	-1.187559	-3.165979
Mg10	1.682256	1.950637	-2.497260
Mg11	-0.112857	-1.916721	0.334663
Mg12	0.541757	-0.784155	-2.612432
Mg13	-1.407058	1.531614	-2.806359
Mg14	1.919835	-0.085007	2.878676
Mg15	-3.712919	2.700322	-1.308338
Mg16	-4.154093	0.275023	2.785811
Mg17	-3.623267	-3.036174	-0.964552
Mg18	-5.734509	1.461865	0.535053

Mg19	-0.858692	-3.468882	-2.142040
Mg20	-2.814768	-2.414713	1.978392
Mg21	-5.585531	-1.482786	0.759589
Mg22	-0.944057	3.837614	-0.705672
Mg23	-2.702974	-0.096932	-0.119591
Mg24	2.282697	-3.029171	-1.504537
Mg25	2.707366	-2.864187	1.564463
Mg26	-5.181247	-0.171990	-1.946826
Mg27	4.909165	-0.781910	2.175988
Mg28	5.047168	-2.433611	-0.439901
Mg29	3.973976	-0.530398	-2.692154
Mg30	0.074960	-2.477677	3.264068
Mg31	6.161227	0.297215	-0.269509

@mg31-isomer32 bp86/6-31G(d) Etot=-6202.997952 Eb=-16.95

Mg1	-1.281307	-0.978433	0.314814
Mg2	0.791054	0.060637	-3.287075
Mg3	-3.894805	-0.384941	-1.716894
Mg4	1.004765	3.528102	-1.728767
Mg5	-1.100022	1.342576	-1.395582
Mg6	3.547523	-1.176970	-3.028182
Mg7	-4.318755	-0.978577	1.366910
Mg8	3.321923	1.759030	-2.388088
Mg9	-2.753569	-3.499492	2.016304
Mg10	-1.445653	-2.137256	-2.602237
Mg11	-2.160903	0.369596	-4.075513
Mg12	-1.827874	-0.868632	3.318249
Mg13	0.651851	4.837450	1.023225
Mg14	3.343259	3.121084	0.352317
Mg15	1.476792	0.672081	0.084312
Mg16	4.610885	-0.054134	-0.312297
Mg17	-3.711908	-3.204307	-0.775343
Mg18	-0.786763	2.053392	1.694566
Mg19	-0.908072	-4.206886	-0.356446
Mg20	-1.823473	4.235226	-0.526601
Mg21	0.287106	-2.848014	2.273787
Mg22	1.839745	2.914933	2.993234
Mg23	1.276511	-2.136936	-1.154434
Mg24	-3.605157	2.642666	-2.590009
Mg25	3.052487	-1.800375	1.606430
Mg26	4.015004	0.978148	2.480230
Mg27	4.271337	-3.163624	-0.925312
Mg28	1.028078	-0.015010	3.152754
Mg29	-3.657695	1.854260	0.357246
Mg30	-3.341523	1.704850	3.329695
Mg31	2.099159	-4.620443	0.498710

@mg31-isomer33 bp86/6-31G(d) Etot=-6202.986189 Eb=-16.71

Mg1	-2.054885	-0.464809	0.176415
Mg2	1.343203	-0.373878	-2.382678
Mg3	-2.365187	2.382396	-1.280059
Mg4	-0.526153	-2.721399	-1.998555
Mg5	2.523991	-3.239257	-2.130938
Mg6	0.429093	1.338660	0.097973
Mg7	0.717495	-1.687693	0.776621
Mg8	0.852912	1.038886	3.200926
Mg9	-4.628110	1.801201	0.702692
Mg10	-2.859602	4.292815	1.181757
Mg11	1.930779	4.498658	-0.770275
Mg12	4.286545	-0.898763	-1.527901
Mg13	-1.973896	-4.761477	-0.307303
Mg14	3.176471	1.986870	-1.703345
Mg15	-3.479059	-2.921901	1.595283
Mg16	5.474276	1.487205	0.208181

Mg17	-5.471315	-1.066581	0.380115
Mg18	5.996047	-1.375497	0.928175
Mg19	-1.956214	1.711483	2.423896
Mg20	3.009978	2.848651	1.421503
Mg21	-0.692912	-3.939303	2.298561
Mg22	-1.646401	-0.046255	-2.968634
Mg23	3.136974	-0.194346	1.599418
Mg24	0.115392	3.965807	1.746089
Mg25	0.287264	2.533242	-2.763457
Mg26	3.579512	-3.221496	0.678166
Mg27	-3.567592	-2.527796	-1.669267
Mg28	1.053852	-4.742911	-0.037089
Mg29	-0.950839	4.985330	-1.062934
Mg30	-1.212616	-1.091889	3.224305
Mg31	-4.529002	0.404047	-2.037641

@mg31-isomer34 bp86/6-31G(d) Etot=-6202.971330 Eb=-16.41

Mg1	1.996329	-0.416744	0.044233
Mg2	-1.101710	-0.149579	-0.233499
Mg3	0.421687	0.054215	2.769204
Mg4	-0.408181	-2.658667	1.493877
Mg5	5.035736	1.131196	1.331536
Mg6	4.690956	-1.900315	1.356493
Mg7	2.167093	-2.524586	2.876693
Mg8	3.453917	-0.001264	3.575923
Mg9	4.934791	-0.266959	-1.289790
Mg10	-0.069249	-2.641469	-1.620178
Mg11	-3.007748	-2.678802	-0.170445
Mg12	3.270986	2.558637	-0.615147
Mg13	-2.759773	-1.012245	-2.767332
Mg14	2.659851	2.646276	2.478569
Mg15	2.331257	-3.576648	-0.003981
Mg16	-2.164582	2.090410	-2.338391
Mg17	3.025765	1.002446	-3.197700
Mg18	-1.362095	4.489045	-0.694972
Mg19	5.021504	-3.300304	-1.321372
Mg20	0.160728	-0.005443	-3.050338
Mg21	-4.258870	0.496160	-0.659460
Mg22	2.707085	-1.983166	-2.723354
Mg23	0.396281	2.175465	0.568125
Mg24	-2.764692	-0.575047	2.292105
Mg25	-2.750802	2.366052	1.072429
Mg26	-5.445420	-2.017814	1.644094
Mg27	0.742005	2.914794	-2.368540
Mg28	1.374160	4.978068	0.680168
Mg29	-5.596352	-2.020955	-1.566243
Mg30	-7.281787	-0.196214	0.208966
Mg31	-5.418870	1.023457	2.228328

@mg31-isomer35 bp86/6-31G(d) Etot=-6202.960587 Eb=-16.19

Mg1	-1.890678	1.227313	3.464302
Mg2	-4.508434	0.168105	2.380330
Mg3	-4.019857	-2.691027	1.162105
Mg4	0.518762	0.041255	1.954292
Mg5	-1.692047	-1.805231	2.774648
Mg6	0.108161	3.056914	1.886506
Mg7	-2.491515	-0.024109	0.103120
Mg8	3.736951	-1.144262	2.195791
Mg9	2.847260	-2.552638	-2.046379
Mg10	-1.494912	-4.008496	0.362630
Mg11	-0.185866	1.542498	-0.792723
Mg12	-0.024443	-1.582774	-1.024035
Mg13	1.083373	-4.749101	-0.893196
Mg14	-2.859975	3.001238	1.204811

Mg15	3.705275	-3.862090	0.504144
Mg16	3.076460	1.910795	2.040689
Mg17	4.339361	1.632354	-2.058447
Mg18	5.725878	0.910343	0.791515
Mg19	1.571256	0.418068	-3.167282
Mg20	2.079922	3.434552	-0.769740
Mg21	4.860936	3.662682	0.162245
Mg22	1.088370	-2.864417	1.604212
Mg23	2.586618	-0.002455	-0.305767
Mg24	-1.454486	0.045058	-3.296875
Mg25	-2.786937	2.619569	-1.895354
Mg26	5.456325	-1.639112	-0.526698
Mg27	-5.233735	1.833400	-0.259670
Mg28	-4.435260	0.203873	-2.814039
Mg29	-2.990203	-2.357125	-1.797297
Mg30	-0.909461	4.593628	-0.555359
Mg31	-5.807098	-1.018808	-0.388477

@mg31-isomer36 bp86/6-31G(d) Etot=-6202.948608 Eb=-15.95

Mg1	1.970437	-0.052857	0.093340
Mg2	-1.135051	-0.205997	0.187756
Mg3	1.352866	0.655357	3.194343
Mg4	-1.461508	-0.429509	3.323682
Mg5	5.080909	0.996201	0.443135
Mg6	3.846388	-1.341116	2.241645
Mg7	0.757803	-2.114941	2.238141
Mg8	4.415013	1.269753	3.534916
Mg9	5.035566	-1.800059	-0.577392
Mg10	0.245911	-2.811231	-0.756567
Mg11	-2.396021	-2.790708	1.196499
Mg12	4.044259	3.233309	-1.361724
Mg13	-2.385427	-1.791117	-2.147032
Mg14	2.946143	2.836861	1.464377
Mg15	2.803179	-3.647793	0.558427
Mg16	-1.701032	1.453494	-2.380750
Mg17	3.677936	0.394875	-2.365762
Mg18	-1.215342	4.293018	-1.229741
Mg19	4.644943	-4.699008	-1.533975
Mg20	0.575109	-0.505092	-2.765770
Mg21	-4.341814	0.341141	-1.604864
Mg22	2.729521	-2.553458	-2.580238
Mg23	0.076456	2.402073	0.825839
Mg24	-3.957600	-0.232972	1.695336
Mg25	-3.101754	2.335700	0.351757
Mg26	-6.921501	-1.176146	1.641647
Mg27	1.194653	2.355259	-2.164254
Mg28	1.586412	5.009017	-0.472361
Mg29	-4.856174	-2.463239	-0.433069
Mg30	-7.270686	-0.585217	-1.243771
Mg31	-6.239594	1.624403	0.626430

@mg31-isomer37 bp86/6-31G(d) Etot=-6202.940633 Eb=-15.79

Mg1	-0.032652	-0.638364	-1.070415
Mg2	-0.752536	-0.285174	2.023284
Mg3	-1.397383	2.703271	-0.024973
Mg4	1.908345	-2.049056	2.338775
Mg5	1.952001	0.667575	0.803117
Mg6	4.393364	-0.126164	2.442349
Mg7	2.668862	0.059875	-2.362757
Mg8	-2.820364	0.057645	-0.070889
Mg9	1.297840	3.720311	0.707965
Mg10	-2.887679	-1.489661	-2.859967
Mg11	-2.929514	1.896810	2.568450
Mg12	-5.433188	0.228907	1.557610

Mg13	5.576914	0.224134	-1.651578
Mg14	0.824210	2.440974	-2.019873
Mg15	-0.726489	-3.386893	2.217533
Mg16	6.752629	-1.094405	0.782912
Mg17	2.695665	-2.931057	-2.677390
Mg18	-1.827192	1.266087	-2.870302
Mg19	3.763866	2.826847	2.139334
Mg20	-4.986868	0.985341	-1.913855
Mg21	1.192031	-3.632941	-0.153654
Mg22	-2.158092	-3.219647	-0.488836
Mg23	-3.547507	-2.241909	2.033231
Mg24	-3.588279	3.633309	-2.304122
Mg25	-3.802412	-0.346467	4.244654
Mg26	-4.575683	3.006877	0.371848
Mg27	-0.320766	-3.049514	-2.913562
Mg28	6.260735	1.901089	0.758661
Mg29	3.801348	2.667307	-0.960158
Mg30	3.799041	-1.903001	-0.026756
Mg31	-5.100248	-1.892106	-0.620636

@mg31-isomer38 bp86/6-31G(d) Etot=-6202.936445 Eb=-15.70

Mg1	-3.321853	-0.588144	0.086504
Mg2	-4.622258	0.945540	2.490847
Mg3	0.557104	2.171422	2.429689
Mg4	-2.445680	2.674344	1.196556
Mg5	-4.532413	-2.064092	2.666494
Mg6	-1.690909	0.159865	2.873932
Mg7	4.898037	2.041805	0.092098
Mg8	0.003884	-4.528765	0.819065
Mg9	0.932070	-1.426658	2.411822
Mg10	2.232071	0.610048	0.370757
Mg11	4.224891	-0.933858	1.758125
Mg12	4.474023	-0.505537	-1.467568
Mg13	3.620819	2.751353	2.632705
Mg14	4.770775	-3.580332	-0.987595
Mg15	-0.574825	-1.231877	-0.340648
Mg16	0.918941	3.506691	-2.829200
Mg17	2.110251	-2.456762	-0.214426
Mg18	-0.673539	4.904892	-0.571672
Mg19	-0.223176	-3.719653	-2.148583
Mg20	-1.757579	-2.850280	2.559442
Mg21	-2.804792	-3.701500	-0.088850
Mg22	-4.013188	0.566752	-3.142360
Mg23	-2.699758	-2.039908	-2.572655
Mg24	-1.013615	0.461483	-3.259451
Mg25	2.173548	3.732604	0.024111
Mg26	1.918909	0.611160	-2.702500
Mg27	-2.511541	2.905356	-2.005024
Mg28	2.639095	-2.332993	-3.173346
Mg29	-0.241966	1.708387	-0.535064
Mg30	-4.930824	1.807241	-0.460474
Mg31	2.583498	0.401414	4.087269

@mg31-isomer39 bp86/6-31G(d) Etot=-6202.935763 Eb=-15.69

Mg1	-4.049613	-0.200402	-0.413263
Mg2	-2.044068	1.160798	1.429408
Mg3	0.647148	-0.674534	2.257526
Mg4	-2.098380	-0.583449	-2.552111
Mg5	0.164070	0.465736	-0.548893
Mg6	-5.651653	0.191737	2.228235
Mg7	-1.565391	-1.909343	0.583679
Mg8	1.448236	-3.018152	-0.067404
Mg9	0.292870	3.093291	1.491280
Mg10	3.019182	-2.772614	2.545357

Mg11	2.847462	-0.446687	4.422945
Mg12	-6.511846	-1.963872	-0.128219
Mg13	2.509099	3.083170	-0.489369
Mg14	4.726851	-2.836060	0.127682
Mg15	-4.733880	2.813713	1.088750
Mg16	-1.056764	-3.761641	-1.851572
Mg17	3.517682	-2.360989	-2.509851
Mg18	2.419480	0.885575	-2.673560
Mg19	0.754283	-1.581746	-2.726561
Mg20	4.838255	2.670193	-2.362667
Mg21	2.883616	-0.285193	0.127258
Mg22	-6.760050	1.266481	-0.434089
Mg23	5.398164	-0.232900	-1.550885
Mg24	-0.325057	2.984173	-1.971377
Mg25	-3.339445	2.249305	-1.938982
Mg26	2.790516	1.848035	2.403616
Mg27	5.085378	-0.497190	2.206142
Mg28	-3.911923	-3.207810	-1.184259
Mg29	-4.305219	-2.539382	1.855160
Mg30	5.243096	2.049987	0.533063
Mg31	-2.232096	4.109769	0.102962

@mg31-isomer40 bp86/6-31G(d) Etot=-6202.894190 Eb=-14.85

Mg1	-1.335101	-0.543002	-0.015646
Mg2	-1.220093	-3.573442	-0.517390
Mg3	-1.735006	2.274704	1.002673
Mg4	3.621656	-2.459672	-0.765809
Mg5	3.041222	-0.241403	1.481181
Mg6	0.985241	1.355681	-0.154931
Mg7	-4.006672	0.938535	-0.932446
Mg8	-1.595579	-2.656594	2.387752
Mg9	3.275678	0.393330	-1.935417
Mg10	5.736098	-1.730537	1.365139
Mg11	-7.571269	2.436949	0.472645
Mg12	3.901239	2.486063	0.262353
Mg13	0.159909	-0.020773	2.534754
Mg14	-6.132679	-0.250469	1.377977
Mg15	6.058704	-0.589983	-1.338501
Mg16	1.243778	-2.609022	1.213888
Mg17	5.568510	1.181171	2.480139
Mg18	0.802703	-1.471290	-1.867265
Mg19	7.985080	0.230816	0.907616
Mg20	-6.855687	1.452519	-2.221136
Mg21	6.924807	3.041773	0.380495
Mg22	-5.935871	-1.315030	-1.605513
Mg23	-4.797183	2.503606	1.688788
Mg24	1.462841	-4.583421	-1.196574
Mg25	-5.204519	3.758375	-1.109073
Mg26	8.474577	1.596666	-1.766602
Mg27	-3.919955	-2.221898	0.467152
Mg28	-2.723013	-1.388326	-2.432645
Mg29	5.581629	2.308642	-2.264997
Mg30	-3.200019	-0.005022	2.465976
Mg31	-8.591024	-0.298948	-0.364583

@mg32-isomer01 bp86/6-31G(d) Etot=-6403.141877 Eb=-17.88

Mg1	0.209846	-0.000254	-2.687619
Mg2	-3.770700	0.000472	0.149048
Mg3	-3.326796	-2.764868	1.616062
Mg4	3.420660	-2.468158	-0.740871
Mg5	0.705356	-4.034020	-0.773814
Mg6	1.707658	-0.000060	0.139969
Mg7	-2.741518	0.000031	-2.759558
Mg8	1.662132	-2.732685	1.779102

Mg9	-0.821191	-4.402728	2.023848
Mg10	-1.281266	2.843982	-2.897122
Mg11	-2.235483	4.758693	-0.569517
Mg12	-3.876171	-2.526484	-1.445443
Mg13	4.355023	-1.468827	2.016124
Mg14	1.931002	0.000119	3.323962
Mg15	-1.282078	-2.844500	-2.896727
Mg16	-0.931719	1.499565	-0.009445
Mg17	-0.931913	-1.499555	-0.009605
Mg18	4.355451	1.468075	2.015853
Mg19	1.662903	2.732691	1.778751
Mg20	-3.875550	2.527117	-1.445925
Mg21	5.265410	-0.000735	-0.457514
Mg22	-0.717642	1.549124	3.244450
Mg23	3.330632	-0.000699	-2.750243
Mg24	1.729701	2.547968	-3.247881
Mg25	-3.326242	2.766213	1.615571
Mg26	-3.299402	0.000890	3.053051
Mg27	-0.820083	4.403364	2.023059
Mg28	-2.236745	-4.758356	-0.568571
Mg29	0.706354	4.033267	-0.774468
Mg30	-0.718054	-1.547846	3.244215
Mg31	3.421523	2.467252	-0.741306
Mg32	1.728901	-2.549050	-3.247436

@mg32-isomer02 bp86/6-31G(d) Etot=-6403.140134 Eb=-17.84

Mg1	-1.482545	-0.943071	0.132767
Mg2	-3.277763	1.280508	-1.635931
Mg3	-4.477772	-2.003291	1.904878
Mg4	2.186734	-3.760252	-2.128219
Mg5	0.499904	-2.618465	2.666830
Mg6	-0.499867	-2.618541	-2.666824
Mg7	4.972481	-1.059300	0.778714
Mg8	-1.527779	3.255442	-3.012026
Mg9	-2.416322	3.692999	0.012199
Mg10	2.416175	3.693017	-0.012241
Mg11	3.224412	-1.456937	3.095610
Mg12	3.696902	1.001249	-1.288916
Mg13	-0.121533	5.040949	1.464705
Mg14	-3.696899	1.001126	1.288897
Mg15	0.641466	0.336314	2.743667
Mg16	3.277813	1.280627	1.635949
Mg17	-0.641421	0.336236	-2.743667
Mg18	-4.972452	-1.059474	-0.778696
Mg19	1.510130	2.483331	-2.761758
Mg20	-3.224350	-1.457000	-3.095583
Mg21	-0.000125	1.727792	0.000005
Mg22	1.482515	-0.942919	-0.132782
Mg23	1.527675	3.255527	3.011935
Mg24	0.000069	-3.881374	-0.000003
Mg25	0.121296	5.040868	-1.464663
Mg26	-2.186596	-3.760397	2.128261
Mg27	3.088393	-3.474818	0.768747
Mg28	-2.066650	-0.697693	3.271370
Mg29	2.066728	-0.697638	-3.271354
Mg30	-1.510231	2.483291	2.761779
Mg31	4.477931	-2.003134	-1.904905
Mg32	-3.088318	-3.474972	-0.768742

@mg32-isomer03 bp86/6-31G(d) Etot=-6403.139312 Eb=-17.83

Mg1	1.194916	1.180683	0.851295
Mg2	1.702994	-1.722916	2.393741
Mg3	-1.722475	-1.702416	-2.394442
Mg4	1.087917	1.074840	3.768298

Mg5	4.030132	-1.684418	0.313902
Mg6	-3.925285	-0.393374	2.478577
Mg7	1.181149	-1.194262	-0.851220
Mg8	1.075785	-1.086843	-3.768325
Mg9	-1.194962	-1.181207	0.850489
Mg10	3.329695	3.291588	2.196110
Mg11	-3.329246	-3.292400	2.194034
Mg12	-1.684345	-4.029971	-0.314755
Mg13	-1.703390	1.721469	2.394723
Mg14	0.393098	-3.923980	-2.479985
Mg15	1.685092	4.029673	-0.313924
Mg16	1.640443	-4.048403	0.313154
Mg17	3.920768	-0.435282	-2.478711
Mg18	3.925117	0.391844	2.479221
Mg19	4.048798	1.639406	-0.313505
Mg20	1.722101	1.703924	-2.393988
Mg21	-1.088831	-1.077363	3.767534
Mg22	-0.435903	-3.921086	2.477800
Mg23	-1.639307	4.048638	0.314649
Mg24	-1.181300	1.194847	-0.850549
Mg25	0.436573	3.919663	2.479224
Mg26	3.292518	-3.328413	-2.196295
Mg27	-0.392646	3.925390	-2.478374
Mg28	-4.029601	1.684351	0.314922
Mg29	-4.048866	-1.639630	-0.314312
Mg30	-3.292715	3.329445	-2.193940
Mg31	-1.076971	1.089458	-3.767404
Mg32	-3.921249	0.436746	-2.477945

@mg32-isomer04 bp86/6-31G(d) Etot=-6403.138468 Eb=-17.81

Mg1	-2.175340	-0.187670	3.866483
Mg2	-3.452188	1.510970	-1.622584
Mg3	-2.037758	4.263768	-1.929338
Mg4	0.437179	0.542066	2.672866
Mg5	1.215009	3.412359	1.723018
Mg6	1.761644	-0.278777	-0.108331
Mg7	-3.403563	0.568233	1.275196
Mg8	3.354166	2.369759	-0.188403
Mg9	0.934199	3.867018	-1.405209
Mg10	-3.180101	-2.501974	2.025851
Mg11	-3.791144	-4.503825	-0.196954
Mg12	-3.562526	3.552964	0.604140
Mg13	4.861647	0.208451	-1.808759
Mg14	3.099258	-1.711319	-3.171375
Mg15	-1.675806	2.750842	2.854612
Mg16	-1.004732	-1.298432	0.067737
Mg17	-0.700212	1.668986	-0.069785
Mg18	3.997527	-2.389014	-0.287359
Mg19	1.168789	-3.306936	-1.385255
Mg20	-3.994931	-1.562524	-0.848876
Mg21	5.089399	0.043342	1.151469
Mg22	0.213994	-0.901568	-2.926610
Mg23	2.900598	-1.388066	2.772894
Mg24	-0.200170	-2.418488	3.029606
Mg25	-2.647546	-0.716602	-3.448261
Mg26	-0.799139	1.875650	-3.292464
Mg27	-1.812076	-3.424443	-2.242245
Mg28	-1.051558	5.042941	0.798054
Mg29	-0.977649	-4.360970	0.663904
Mg30	2.251635	1.410174	-2.913468
Mg31	1.884851	-3.797313	1.423439
Mg32	3.296543	1.660401	2.916005

@mg32-isomer05 bp86/6-31G(d) Etot=-6403.138020 Eb=-17.80

Mg1	-2.800727	1.499617	1.716382
Mg2	-4.706002	-0.897350	1.697174
Mg3	-2.471932	3.511769	-0.611199
Mg4	-1.423561	4.013353	2.332473
Mg5	-4.019613	0.748988	-0.901280
Mg6	0.000013	5.275834	-0.062735
Mg7	-4.722177	-2.276596	-0.867768
Mg8	-2.481518	1.945730	-3.242211
Mg9	1.423575	4.013343	2.332474
Mg10	-2.454967	-0.878051	3.571874
Mg11	0.000011	3.664657	-2.570423
Mg12	-2.705710	-1.157198	-2.949010
Mg13	-0.000006	1.769954	0.103883
Mg14	-2.831647	-3.335876	1.553350
Mg15	-1.495016	-0.935289	0.046245
Mg16	-0.000002	0.953468	3.048900
Mg17	2.471941	3.511749	-0.611194
Mg18	-2.447617	-3.913392	-1.487680
Mg19	0.000010	0.384361	-2.666475
Mg20	-0.000006	-2.264325	2.722855
Mg21	2.800725	1.499600	1.716381
Mg22	2.481544	1.945722	-3.242213
Mg23	-0.000001	-2.587807	-2.566362
Mg24	1.495003	-0.935287	0.046239
Mg25	-0.000010	-3.847414	0.273602
Mg26	2.454953	-0.878058	3.571884
Mg27	2.705718	-1.157212	-2.949009
Mg28	4.019622	0.748969	-0.901275
Mg29	2.831623	-3.335873	1.553353
Mg30	4.706001	-0.897367	1.697192
Mg31	2.447602	-3.913403	-1.487675
Mg32	4.722170	-2.276619	-0.867752

@mg32-isomer06 bp86/6-31G(d) Etot=-6403.137447 Eb=-17.79

Mg1	1.901436	1.419167	-3.223980
Mg2	-1.213153	1.305706	-3.396908
Mg3	-0.172645	-1.738010	0.539179
Mg4	0.347580	-1.029090	-2.278447
Mg5	-3.102032	-2.035786	-0.600184
Mg6	-2.335722	-1.579405	-3.449923
Mg7	4.480092	-0.284065	1.578971
Mg8	-0.237549	-0.294000	3.292115
Mg9	3.165484	-1.425600	-3.288087
Mg10	-4.750958	-0.019482	0.873157
Mg11	3.205068	3.474455	-1.397506
Mg12	2.241249	-1.993382	2.672763
Mg13	-2.928539	1.486442	2.691780
Mg14	2.903657	-2.057555	-0.277729
Mg15	-0.215189	2.636337	3.120540
Mg16	-0.275290	-3.529180	3.240163
Mg17	-2.765931	-1.749828	2.436990
Mg18	1.099458	-4.512288	0.628969
Mg19	1.604187	3.867359	1.154696
Mg20	4.273602	0.662738	-1.290836
Mg21	-1.677868	3.893985	0.845592
Mg22	2.451847	1.251962	3.174094
Mg23	-1.537152	0.845361	-0.088318
Mg24	-2.817544	3.548155	-2.003598
Mg25	1.477368	0.807208	0.171597
Mg26	1.801262	-3.985041	-2.356408
Mg27	-4.476231	2.851823	0.297089
Mg28	-3.974350	0.693193	-1.997486
Mg29	-1.094642	-3.957243	-1.816859
Mg30	0.172269	3.239229	-1.481307

Mg31	4.389250	2.655035	1.188601
Mg32	-1.939016	-4.448200	1.041282

@mg32-isomer07 bp86/6-31G(d) Etot=-6403.137303 Eb=-17.79

Mg1	0.439754	1.862921	0.072288
Mg2	-2.790977	2.323255	-0.092622
Mg3	1.436421	-2.053136	-3.101706
Mg4	-1.504136	-0.534829	0.110218
Mg5	-4.610015	-0.134769	-0.434883
Mg6	-0.346763	-3.501940	-0.767135
Mg7	0.368052	-0.883720	2.667299
Mg8	3.041008	0.781986	-2.249292
Mg9	-4.375266	-2.001493	1.978152
Mg10	-1.125024	3.763278	-2.082174
Mg11	-3.349134	-3.043631	-0.657542
Mg12	-0.993484	1.894540	2.797880
Mg13	-2.958855	1.052226	-2.815110
Mg14	1.176053	5.274040	-0.546442
Mg15	4.360462	0.069455	0.442613
Mg16	2.420137	1.374409	2.548786
Mg17	-3.915423	1.051996	2.320578
Mg18	3.270380	3.000083	-0.003402
Mg19	1.535307	-1.055401	-0.146400
Mg20	4.275225	-1.950999	-1.928933
Mg21	-1.229417	4.517166	1.071817
Mg22	1.410000	4.191623	2.255373
Mg23	-4.602573	-1.625923	-3.038273
Mg24	-2.275903	-0.875440	3.792149
Mg25	0.027598	0.698715	-2.680012
Mg26	-1.561616	-3.237293	2.009139
Mg27	-1.605631	-1.806890	-2.939374
Mg28	3.299966	-1.501346	2.915094
Mg29	1.538041	-3.718817	1.690450
Mg30	1.728119	3.422503	-2.733885
Mg31	2.507183	-4.212088	-1.249332
Mg32	4.410510	-3.140480	0.794684

@mg32-isomer08 bp86/6-31G(d) Etot=-6403.137034 Eb=-17.78

Mg1	3.717017	-1.164317	0.762864
Mg2	-1.392921	-2.416768	-2.551918
Mg3	-4.217490	-1.737341	1.727920
Mg4	1.444321	-2.874852	-3.304878
Mg5	0.948639	3.660666	2.281360
Mg6	-2.020056	-3.295367	0.216747
Mg7	2.892145	1.171539	2.537993
Mg8	3.313903	-0.644978	-2.167383
Mg9	-0.071900	0.760290	2.917880
Mg10	0.463198	-0.027288	-2.823038
Mg11	0.046007	-4.445463	2.145518
Mg12	-1.343917	-1.914736	2.900190
Mg13	-0.567368	4.504660	-0.151403
Mg14	-5.245211	1.130595	-2.104111
Mg15	2.797904	-4.070410	1.414660
Mg16	2.312362	4.284261	-0.852575
Mg17	-0.303391	2.898725	-2.718999
Mg18	-2.019709	2.823567	1.828857
Mg19	-2.862377	2.764384	-1.089560
Mg20	3.811324	4.071710	1.740207
Mg21	0.564001	-4.590120	-0.950508
Mg22	3.498816	-3.583932	-1.377111
Mg23	1.717430	-1.705036	3.049325
Mg24	4.066515	1.741729	-0.261257
Mg25	2.656807	2.225257	-2.974082
Mg26	-2.425781	0.489060	-3.120986

Mg27	-4.647544	1.119006	0.834925
Mg28	-3.138909	0.513208	3.367115
Mg29	0.949599	1.438195	-0.019735
Mg30	-4.038761	-1.491880	-1.296976
Mg31	-1.676309	0.008727	0.072789
Mg32	0.771657	-1.643095	-0.033832

@mg32-isomer09 bp86/6-31G(d) Etot=-6403.136916 Eb=-17.78

Mg1	-2.233316	-1.009341	3.105871
Mg2	-4.551846	-2.245814	1.617755
Mg3	3.332295	-3.558034	1.840984
Mg4	-1.889075	-3.449525	0.974282
Mg5	0.465138	-2.671267	2.779878
Mg6	3.077853	-1.027045	3.288651
Mg7	-4.072569	0.757559	1.205850
Mg8	-3.659242	-2.375412	-1.365766
Mg9	-1.769007	2.190026	2.608004
Mg10	4.438308	-0.924894	0.504120
Mg11	-5.997225	-0.793119	-0.581299
Mg12	0.942082	-4.073361	0.039114
Mg13	0.480967	0.335699	2.798757
Mg14	-3.687311	0.696923	-1.962637
Mg15	3.733331	-3.528198	-1.128979
Mg16	-1.221845	-3.848222	-2.029750
Mg17	1.447495	-0.968176	-0.018046
Mg18	-1.492730	-0.452796	0.046985
Mg19	1.121949	3.333856	3.101493
Mg20	3.142350	1.626671	1.798040
Mg21	3.938194	-0.987309	-2.614376
Mg22	-1.318448	-0.968352	-3.080909
Mg23	-2.492686	2.943031	-0.283271
Mg24	-0.675150	4.844161	1.395688
Mg25	1.353229	-2.612828	-2.864882
Mg26	0.404649	1.857486	-0.053045
Mg27	2.183643	4.288653	0.255145
Mg28	3.446736	1.621905	-1.111109
Mg29	-1.172851	2.186727	-2.953978
Mg30	1.293341	0.472290	-2.992308
Mg31	-0.378597	4.853135	-1.527309
Mg32	1.810335	3.485572	-2.792952

@mg32-isomer10 bp86/6-31G(d) Etot=-6403.136539 Eb=-17.77

Mg1	-0.699457	1.552608	0.315847
Mg2	-1.041380	-1.413933	-0.074932
Mg3	-3.142222	-0.470475	-2.497063
Mg4	-0.036697	3.779035	-2.265643
Mg5	1.512412	2.207530	2.458969
Mg6	2.914046	-2.649300	1.626950
Mg7	-0.247492	0.529139	-2.536537
Mg8	-2.251890	-1.685701	2.953207
Mg9	-0.004472	4.504437	0.987207
Mg10	-0.793536	-2.533484	-3.033072
Mg11	-4.110518	-1.290597	0.387433
Mg12	-3.429979	-3.380246	-1.746405
Mg13	2.110435	-1.167994	-3.211662
Mg14	-3.046030	-4.074049	1.214665
Mg15	1.869131	-0.139671	-0.041515
Mg16	4.323307	1.938597	1.264327
Mg17	2.180842	2.917774	-0.514724
Mg18	3.456237	-0.127286	3.219511
Mg19	-0.077040	-3.776568	1.846692
Mg20	-1.086273	-4.874129	-0.888850
Mg21	4.160722	-2.246266	-1.260874
Mg22	2.258461	1.901623	-3.383236

Mg23	-3.736652	1.699456	-0.331187
Mg24	-2.506376	4.531092	-0.781470
Mg25	5.339573	-0.822487	0.987736
Mg26	-1.161771	1.360373	3.557525
Mg27	-2.634750	3.635515	2.072575
Mg28	1.362337	-3.190366	-0.914767
Mg29	-2.602064	2.520445	-3.026249
Mg30	0.601786	-0.847355	2.656962
Mg31	4.413389	0.785954	-1.594548
Mg32	-3.894078	0.826328	2.553124

@mg32-isomer11 bp86/6-31G(d) Etot=-6403.135866 Eb=-17.76

Mg1	0.014557	1.838923	-0.035323
Mg2	-1.811468	4.556462	1.254664
Mg3	1.610608	-0.703583	-0.087466
Mg4	-1.412386	-0.846775	0.083840
Mg5	2.335337	2.068305	2.359350
Mg6	-0.459499	-0.898440	-2.948385
Mg7	-2.672827	1.785530	2.322146
Mg8	-2.969399	2.436246	-0.652352
Mg9	3.156885	2.297056	-0.560480
Mg10	-1.062111	4.762914	-1.560533
Mg11	-0.128220	-2.630655	3.371864
Mg12	-1.329818	-3.912435	0.914852
Mg13	4.510996	0.400677	1.289054
Mg14	1.213141	4.573310	0.668940
Mg15	4.569818	-2.536596	1.194843
Mg16	-4.416197	-0.044370	0.517053
Mg17	1.849843	1.017511	-2.950896
Mg18	1.734757	-3.623166	1.222436
Mg19	2.318020	-1.938534	-3.453632
Mg20	2.549613	-1.101853	3.036718
Mg21	4.347194	-0.600191	-1.584474
Mg22	-3.254993	-0.014769	-2.381212
Mg23	-2.542132	-3.104273	-1.817905
Mg24	0.443949	-3.454258	-1.526250
Mg25	-0.116661	0.293634	2.811113
Mg26	1.572085	3.973183	-2.458062
Mg27	-1.035501	2.102000	-3.085297
Mg28	-5.326550	-2.111231	-1.646733
Mg29	-2.857104	-1.309832	2.890136
Mg30	-4.193315	-3.098481	0.883587
Mg31	3.508240	-3.528672	-1.323768
Mg32	-0.146860	3.352361	3.252171

@mg32-isomer12 bp86/6-31G(d) Etot=-6403.135132 Eb=-17.74

Mg1	-0.401012	-0.250636	2.522242
Mg2	-1.440323	-3.159362	2.990113
Mg3	1.784998	-0.380673	0.034000
Mg4	-2.556974	1.527470	3.508118
Mg5	-3.021024	1.132380	-2.284068
Mg6	-0.447644	1.692854	-0.101573
Mg7	0.672067	4.642002	-1.767671
Mg8	0.400269	2.579308	3.000606
Mg9	1.838245	1.979565	-2.431443
Mg10	-3.496224	-3.825339	0.975785
Mg11	-1.222405	-1.264381	-0.187288
Mg12	2.530089	0.326494	3.067340
Mg13	2.483666	2.651383	0.585286
Mg14	-2.464155	4.067781	2.021125
Mg15	-2.685757	-4.049206	-1.817138
Mg16	-0.944012	2.884654	-3.447597
Mg17	-3.523904	-1.095754	2.227495
Mg18	0.214950	-3.055714	-2.514254

Mg19	-0.367697	-4.237506	0.255696
Mg20	0.181450	4.810802	1.063195
Mg21	4.841397	0.642570	1.257140
Mg22	-0.170412	-0.070381	-2.858333
Mg23	5.041599	-1.686119	-0.804100
Mg24	1.379920	-2.679729	2.280749
Mg25	-4.222509	-1.363547	-0.817179
Mg26	4.272303	-2.171614	1.986832
Mg27	4.470100	1.085726	-1.603134
Mg28	-2.302622	4.042477	-1.004261
Mg29	-3.487369	1.463691	0.590157
Mg30	-2.643441	-1.635617	-3.439381
Mg31	2.536806	-3.367124	-0.468522
Mg32	2.749623	-1.236455	-2.819938

@mg32-isomer13 bp86/6-31G(d) Etot=-6403.135098 Eb=-17.74

Mg1	4.140579	-0.054573	1.441093
Mg2	1.604105	0.977638	2.929362
Mg3	3.415037	3.054415	1.825530
Mg4	-0.520506	-3.171037	-0.973696
Mg5	2.648705	-1.951589	3.339136
Mg6	4.093454	-3.171981	1.153899
Mg7	-4.326463	0.888997	-0.874662
Mg8	0.352409	1.802747	0.082807
Mg9	-1.952172	2.523582	-2.275661
Mg10	-3.160587	0.037110	-3.488908
Mg11	-0.276468	-1.464042	2.838370
Mg12	2.361128	4.684253	-0.383979
Mg13	3.279561	1.653659	-0.925497
Mg14	-4.961217	-1.534093	1.060893
Mg15	-1.548353	-2.478138	-3.712564
Mg16	0.509401	4.049925	2.049922
Mg17	1.047209	-3.953128	1.602116
Mg18	1.403554	-1.021966	0.206840
Mg19	-4.366302	1.223771	2.129850
Mg20	-3.181286	-1.160547	3.435826
Mg21	3.930594	-1.371752	-1.418873
Mg22	1.124091	3.020289	-2.690711
Mg23	-0.173476	0.043619	-2.422722
Mg24	2.598676	0.439198	-3.618330
Mg25	-3.541188	-2.266920	-1.456313
Mg26	-0.515086	4.866144	-0.812620
Mg27	2.450589	-4.195742	-1.068266
Mg28	-1.760654	-0.350746	0.258085
Mg29	-1.372360	1.385955	2.915094
Mg30	-2.378610	-3.244501	1.366422
Mg31	-2.456153	3.041919	0.656591
Mg32	1.531790	-2.302468	-3.169035

@mg32-isomer14 bp86/6-31G(d) Etot=-6403.134976 Eb=-17.74

Mg1	-3.644141	2.001983	0.947341
Mg2	-2.451640	4.120655	-1.087690
Mg3	-2.822832	4.726423	1.954591
Mg4	-3.689074	1.574206	-2.052945
Mg5	-0.079390	4.350722	0.946482
Mg6	-3.965899	-0.799563	-0.186399
Mg7	-2.848589	-0.487319	2.681875
Mg8	0.249490	4.085370	-2.236423
Mg9	-1.397684	2.243679	2.996588
Mg10	-0.697687	1.416585	-0.132501
Mg11	-3.657001	-3.295461	1.580397
Mg12	-1.055996	1.586473	-3.372801
Mg13	-2.548007	-1.091999	-2.963269
Mg14	-3.424438	-3.601128	-1.363436

Mg15	2.302374	3.011235	-0.284530
Mg16	1.571594	2.151552	2.548991
Mg17	-0.935381	-1.535511	0.018672
Mg18	0.157611	-0.428323	2.877869
Mg19	-1.316635	-3.107557	3.231188
Mg20	1.929381	1.531842	-2.965285
Mg21	1.872434	-0.192825	0.050310
Mg22	0.465639	-1.033485	-2.867742
Mg23	-0.940993	-3.784844	-2.806184
Mg24	-1.079698	-4.601352	0.386531
Mg25	4.371531	1.803502	1.540577
Mg26	4.560818	1.390375	-1.496586
Mg27	1.273285	-3.095736	1.863950
Mg28	3.309425	-0.758471	2.728184
Mg29	1.460577	-3.355544	-1.165042
Mg30	3.602495	-1.311141	-2.260890
Mg31	5.569706	-0.618168	0.392653
Mg32	3.858725	-2.896177	0.495523

@mg32-isomer15 bp86/6-31G(d) Etot=-6403.134531 Eb=-17.73

Mg1	-4.772225	1.527207	1.297252
Mg2	-2.892814	3.829638	1.253469
Mg3	-2.678510	1.779880	3.415551
Mg4	-0.143192	3.133404	2.366370
Mg5	-3.131576	-1.006602	2.360319
Mg6	-4.129550	-0.607655	-0.682710
Mg7	-3.577402	2.540124	-1.416030
Mg8	-0.431550	3.737337	-0.564267
Mg9	-0.203515	0.099725	3.034520
Mg10	2.410655	1.907060	3.187748
Mg11	-0.735570	-2.960607	2.982816
Mg12	-2.438026	-2.995809	0.218377
Mg13	-1.529920	0.844646	0.303346
Mg14	2.456524	3.785500	0.785804
Mg15	2.061818	3.260509	-2.253942
Mg16	-3.134885	-2.577950	-2.814878
Mg17	2.492153	-1.075878	2.786542
Mg18	-3.311109	0.412440	-3.464961
Mg19	-0.927359	2.248574	-3.077123
Mg20	0.417023	-1.810847	0.372225
Mg21	1.381209	0.957582	-0.154954
Mg22	2.079249	-4.017422	2.192237
Mg23	-0.328977	-5.109407	0.835952
Mg24	4.338261	0.965217	1.043301
Mg25	-0.492924	-3.928179	-2.047852
Mg26	-0.746164	-0.716839	-2.226974
Mg27	4.798727	3.181083	-0.990108
Mg28	1.502550	0.638591	-3.689295
Mg29	3.572184	-1.910613	0.127500
Mg30	2.040816	-2.041524	-2.506739
Mg31	2.118878	-4.508210	-0.752387
Mg32	3.935218	0.419024	-1.921110

@mg32-isomer16 bp86/6-31G(d) Etot=-6403.134081 Eb=-17.72

Mg1	-5.704429	-1.923975	-0.825856
Mg2	2.689459	0.820715	3.520768
Mg3	-3.010247	-0.985616	3.185049
Mg4	2.667347	-1.101996	-3.669315
Mg5	2.521319	3.822186	-1.922264
Mg6	-3.083936	-2.136055	-2.378184
Mg7	-1.320756	4.510885	1.162914
Mg8	1.455778	5.045364	0.558670
Mg9	-4.604448	0.295802	1.046635
Mg10	0.334597	1.677939	-0.062037

Mg11	1.238234	-1.237785	0.064465
Mg12	-3.516674	-2.902570	0.831274
Mg13	-1.750691	-0.480939	-0.008571
Mg14	3.924319	-3.525707	0.855974
Mg15	1.241898	-4.552407	1.020493
Mg16	2.119864	-2.186560	2.961187
Mg17	-0.468044	4.013501	-1.887274
Mg18	4.058784	-0.454059	1.167398
Mg19	-0.938099	-3.511089	-0.784702
Mg20	4.497318	-1.950663	-1.559356
Mg21	-2.882176	2.554459	-0.413923
Mg22	1.958662	-3.576235	-1.877705
Mg23	3.257324	0.881281	-1.429828
Mg24	3.141871	2.564499	1.039809
Mg25	0.685973	3.075311	2.858738
Mg26	-0.142062	-1.249101	-2.777235
Mg27	-2.312342	1.979074	2.533910
Mg28	-1.785093	1.253895	-2.912398
Mg29	-0.847575	-2.898792	2.303844
Mg30	-0.028601	0.027149	2.766988
Mg31	1.111056	1.601219	-3.407118
Mg32	-4.508632	0.550270	-1.962348

@mg32-isomer17 bp86/6-31G(d) Etot=-6403.134011 Eb=-17.72

Mg1	4.785629	0.171137	1.249328
Mg2	4.975518	-2.574170	0.262121
Mg3	4.488259	-0.410517	-1.773075
Mg4	2.062540	4.364620	1.015940
Mg5	2.490999	1.670157	2.450321
Mg6	2.983827	-1.675940	2.758606
Mg7	3.219632	2.100247	-0.529943
Mg8	-0.170541	3.275566	2.750952
Mg9	-0.598998	5.258431	0.389868
Mg10	2.607154	-4.062582	0.853232
Mg11	1.763763	-0.833989	0.005871
Mg12	2.905370	-2.888674	-2.117657
Mg13	2.090008	0.927180	-3.002217
Mg14	0.083170	0.005193	2.700784
Mg15	1.135211	3.874454	-2.028873
Mg16	0.022715	1.725453	-0.098534
Mg17	0.169902	-2.981167	2.165575
Mg18	-0.782855	1.584379	-3.378000
Mg19	-2.646767	3.090300	0.929570
Mg20	-2.445815	1.364083	3.476866
Mg21	-1.838834	4.030860	-1.990794
Mg22	0.234362	-3.636438	-0.863187
Mg23	0.145843	-1.341087	-2.914880
Mg24	-1.352991	-0.933540	-0.066415
Mg25	-2.413348	-1.670542	3.028835
Mg26	-4.038037	0.299529	1.186264
Mg27	-2.261276	-3.350994	-2.440846
Mg28	-4.920384	-2.609333	1.641642
Mg29	-2.413315	-3.805286	0.660682
Mg30	-3.150299	1.341349	-1.478316
Mg31	-2.783536	-0.688931	-3.649005
Mg32	-4.346905	-1.619751	-1.194715

@mg32-isomer18 bp86/6-31G(d) Etot=-6403.133889 Eb=-17.72

Mg1	-0.337397	-3.933661	-2.579077
Mg2	5.352346	-0.752294	2.052004
Mg3	4.105587	1.887921	-2.045522
Mg4	-1.874888	1.369108	-3.156241
Mg5	-0.741697	4.093985	-2.250920
Mg6	-1.018927	1.310140	-0.059966

Mg7	2.135657	-2.763229	-1.364308
Mg8	-0.831967	4.367972	0.817722
Mg9	1.796013	3.453954	-0.598415
Mg10	0.288046	-4.570701	0.412351
Mg11	-2.381357	-4.103870	1.947201
Mg12	3.071983	-0.620701	-3.356428
Mg13	-3.602964	4.140474	1.919055
Mg14	-1.591729	2.155310	3.007123
Mg15	0.137785	-0.879264	-2.870904
Mg16	-0.682055	-1.711131	0.043817
Mg17	1.723540	0.270836	-0.251415
Mg18	-3.926965	1.122676	1.347415
Mg19	-2.405604	-1.063858	2.839337
Mg20	0.123452	-3.056776	3.099531
Mg21	-3.291229	3.345893	-0.970846
Mg22	1.336823	2.726251	2.238062
Mg23	-4.115472	0.429719	-1.499020
Mg24	-2.656646	-4.549483	-0.940875
Mg25	3.055485	0.489105	3.404040
Mg26	1.198326	1.903960	-3.136390
Mg27	-3.815922	-1.945473	0.304273
Mg28	2.579821	-2.151082	1.523700
Mg29	4.127866	1.940259	0.968011
Mg30	0.355935	-0.120623	2.542975
Mg31	4.573513	-0.870461	-0.768002
Mg32	-2.687358	-1.914958	-2.618289

@mg32-isomer19 bp86/6-31G(d) Etot=-6403.133762 Eb=-17.72

Mg1	-2.570604	-0.745549	-2.477236
Mg2	-3.851265	-2.659221	-0.605073
Mg3	-1.455724	-3.741194	-2.019135
Mg4	-3.806115	1.993890	-2.359911
Mg5	-0.862524	1.736708	-3.315736
Mg6	-2.311767	-4.744287	0.831496
Mg7	0.390424	-0.942234	-2.571382
Mg8	-4.178002	0.253762	0.101188
Mg9	1.454403	-3.924189	-2.643344
Mg10	2.235241	1.382106	-3.091135
Mg11	-2.120170	4.316658	-1.756884
Mg12	-3.149611	-1.745076	2.186417
Mg13	-0.687979	-1.663477	0.195645
Mg14	0.628679	-4.470738	0.354307
Mg15	-1.276184	1.279878	-0.143471
Mg16	3.268992	-1.504094	-3.255859
Mg17	-4.009698	3.332967	0.347451
Mg18	0.688092	3.408677	-1.298898
Mg19	-2.972927	1.547843	2.588500
Mg20	-0.836030	-3.550968	3.022705
Mg21	1.582223	0.498459	0.142798
Mg22	2.713698	-2.343329	-0.372161
Mg23	4.570056	0.157309	-1.093959
Mg24	-1.189838	4.184524	1.156744
Mg25	3.636805	2.996415	-1.001913
Mg26	4.574694	1.928945	1.614893
Mg27	4.366018	-0.951009	1.763041
Mg28	1.836111	3.326434	1.496869
Mg29	-0.232177	2.527675	3.453410
Mg30	1.789148	-2.277346	2.501766
Mg31	-0.516492	-0.357592	2.977414
Mg32	2.292523	0.748054	3.271454

@mg32-isomer20 bp86/6-31G(d) Etot=-6403.131684 Eb=-17.68

Mg1	5.040098	-1.873904	-0.915098
Mg2	4.271588	0.849022	-1.661005

Mg3	4.007732	0.988845	1.339048
Mg4	3.986358	-2.003603	1.853005
Mg5	2.700397	3.133973	-0.360918
Mg6	2.716936	-1.531169	-2.889427
Mg7	2.566566	-3.581696	-0.404235
Mg8	1.456033	1.335087	-2.572803
Mg9	1.677837	2.922764	2.586878
Mg10	1.696688	-0.648214	-0.059978
Mg11	1.829089	-0.127541	3.196698
Mg12	0.441482	4.222246	-2.148426
Mg13	0.565003	5.130981	0.682460
Mg14	1.377040	-3.193053	2.524597
Mg15	-0.302482	-0.808258	-3.818043
Mg16	0.381149	-3.460672	-2.640863
Mg17	-0.012964	1.851146	0.280408
Mg18	-0.530608	-3.572962	0.178912
Mg19	-1.446935	2.018133	-3.009018
Mg20	-1.428367	3.971821	2.520417
Mg21	-0.716668	-0.959857	1.814704
Mg22	-1.246469	-0.508659	-0.980048
Mg23	-0.911646	1.255190	3.686741
Mg24	-2.089572	4.085785	-0.452788
Mg25	-2.723410	-3.133006	-2.036401
Mg26	-1.614832	-3.551749	3.151178
Mg27	-3.434306	-0.435281	-3.224583
Mg28	-3.556010	-3.604928	0.891871
Mg29	-3.975843	1.880207	-1.413198
Mg30	-4.266420	-0.937312	-0.243398
Mg31	-3.541873	-1.177022	2.780763
Mg32	-2.915594	1.463686	1.342549

@mg32-isomer21 bp86/6-31G(d) Etot=-6403.131641 Eb=-17.67

Mg1	5.736599	-1.092384	1.101613
Mg2	3.527943	-2.687825	-0.250964
Mg3	3.205848	-0.912299	2.610619
Mg4	1.190368	-3.107143	1.640114
Mg5	5.016482	-0.474284	-1.691966
Mg6	-1.155957	-4.865839	0.794856
Mg7	0.820181	-3.719225	-1.341533
Mg8	-1.628137	-3.012915	3.062466
Mg9	4.210043	1.478514	0.745506
Mg10	2.286335	-1.403783	-2.865233
Mg11	0.113050	-0.555396	2.759561
Mg12	1.669290	-0.154895	-0.000544
Mg13	1.815563	1.920023	2.836149
Mg14	-2.163219	-4.418482	-1.846576
Mg15	3.200942	1.755707	-2.183076
Mg16	-1.119659	-1.518800	-0.114372
Mg17	-3.675216	-2.994055	0.847845
Mg18	-0.789550	-1.908787	-3.241572
Mg19	-2.951028	-0.285159	2.810974
Mg20	-1.135558	1.870889	3.894449
Mg21	0.252203	0.926875	-2.576968
Mg22	1.718266	3.225905	0.159228
Mg23	-0.919386	1.431611	0.350721
Mg24	-0.270627	4.193652	2.361235
Mg25	-3.865486	-2.113269	-2.069044
Mg26	-3.906774	0.112033	0.072389
Mg27	-2.662924	0.525151	-2.656235
Mg28	-3.103278	2.975071	1.984719
Mg29	1.102787	3.944200	-2.644758
Mg30	-1.158264	4.574892	-0.433934
Mg31	-3.635731	2.951789	-0.968968
Mg32	-1.725109	3.338229	-3.146700

@mg32-isomer22 bp86/6-31G(d) Etot=-6403.129309 Eb=-17.63

Mg1	2.934672	-0.690592	-2.811666
Mg2	4.032441	1.730494	-0.979552
Mg3	0.981822	-1.572751	-0.107291
Mg4	3.204962	-3.582243	-1.956248
Mg5	4.050092	-1.302671	-0.020237
Mg6	0.781518	-4.898381	-0.657137
Mg7	4.038322	0.909133	1.961398
Mg8	2.960632	-4.028102	1.097129
Mg9	0.427354	-2.714704	-2.856988
Mg10	2.347477	2.328777	-3.351151
Mg11	0.011608	-3.655637	2.106067
Mg12	2.498672	-1.496122	2.764763
Mg13	-1.711169	0.095828	-0.021649
Mg14	2.528940	4.482496	-1.256590
Mg15	1.143742	1.378098	0.290597
Mg16	0.120095	0.373295	-2.592161
Mg17	-1.781258	-3.207521	-0.411818
Mg18	3.150458	3.704032	1.497179
Mg19	-0.342194	-0.654584	2.607708
Mg20	-0.205799	3.314433	-1.903780
Mg21	-2.357399	-1.447925	-2.767067
Mg22	-2.876343	-2.226065	2.307867
Mg23	1.568771	1.504061	3.418229
Mg24	-1.375262	2.165052	2.702060
Mg25	0.227207	4.286906	0.995005
Mg26	-5.036975	-0.211778	-3.120752
Mg27	-2.732105	-0.096523	4.531890
Mg28	-4.338155	-1.490222	-0.295942
Mg29	-2.549866	3.112630	0.126179
Mg30	-4.979863	1.493496	-0.684682
Mg31	-2.676850	1.675122	-2.639027
Mg32	-4.045547	0.721968	2.027666

@mg32-isomer23 bp86/6-31G(d) Etot=-6403.128717 Eb=-17.62

Mg1	-2.535847	4.505503	-0.881786
Mg2	-3.539032	3.570372	1.676339
Mg3	-0.567874	3.986370	1.556248
Mg4	2.290320	3.207336	0.609809
Mg5	0.236970	3.564121	-1.489064
Mg6	-1.886169	1.458857	3.271864
Mg7	-2.052322	2.595458	-3.172275
Mg8	4.206157	1.119430	1.882594
Mg9	5.130297	2.672576	-0.458596
Mg10	-4.325804	0.703654	1.676280
Mg11	-4.020705	1.739738	-1.084336
Mg12	2.775075	2.092483	-2.297718
Mg13	1.169015	1.743317	2.953436
Mg14	-1.203160	1.240769	0.205640
Mg15	2.732420	-0.963967	3.465760
Mg16	0.168005	0.574429	-2.574051
Mg17	1.700805	0.108560	0.188085
Mg18	-0.120277	-0.977714	2.782487
Mg19	-2.899969	-1.810754	2.390750
Mg20	-3.787332	-1.351224	-0.500798
Mg21	-2.540647	-0.506532	-3.078916
Mg22	4.563874	-0.171259	-1.228162
Mg23	-0.665334	-1.655725	-0.264655
Mg24	4.357284	-1.864818	1.146352
Mg25	2.649198	-0.739032	-3.527122
Mg26	1.676983	-3.198212	1.544572
Mg27	0.165002	-2.449935	-3.282704
Mg28	-0.884645	-4.180170	2.581519

Mg29	-2.460013	-3.544365	-2.458488
Mg30	2.469151	-2.665828	-1.235309
Mg31	-2.779500	-4.193069	0.401713
Mg32	-0.021928	-4.610366	-0.799468

@mg32-isomer24 bp86/6-31G(d) Etot=-6403.126744 Eb=-17.58

Mg1	-3.294176	3.540431	0.244274
Mg2	-4.308295	0.308096	0.774784
Mg3	3.226248	-3.005327	-0.382746
Mg4	-2.856721	-2.415806	1.280639
Mg5	4.778646	2.585051	0.811440
Mg6	1.048845	-3.665921	-2.305131
Mg7	1.796477	0.763920	-0.106600
Mg8	0.569071	0.440266	2.741862
Mg9	-1.600980	-4.256648	-0.946348
Mg10	4.615760	-0.400627	0.272911
Mg11	-1.210066	2.922857	2.502590
Mg12	-2.066696	3.465803	-2.548992
Mg13	2.647643	3.824884	-0.889290
Mg14	4.251588	1.661092	-2.081660
Mg15	-1.297455	0.971547	-0.097135
Mg16	-2.958002	-1.298383	-1.458522
Mg17	-1.569074	-2.800824	-3.642841
Mg18	-2.318621	-0.005985	3.057302
Mg19	-0.424701	-2.479519	3.205603
Mg20	0.720152	2.260572	-2.709123
Mg21	-4.195693	2.462829	2.866438
Mg22	-0.220745	3.901146	-0.169918
Mg23	3.151314	-1.085349	-2.623030
Mg24	0.251095	-0.679337	-2.506725
Mg25	-1.543343	-5.050773	2.030670
Mg26	-4.296201	1.605679	-1.913815
Mg27	0.017530	-1.715463	0.256518
Mg28	3.673155	0.877783	2.909206
Mg29	2.482433	-1.914675	2.259033
Mg30	1.059616	-4.600217	0.843025
Mg31	-2.028645	0.594641	-3.672809
Mg32	1.899841	3.188257	1.998391

@mg32-isomer25 bp86/6-31G(d) Etot=-6403.125758 Eb=-17.56

Mg1	-0.463786	1.583546	-0.011693
Mg2	0.864377	3.159927	-2.544974
Mg3	-1.966609	5.255562	1.388661
Mg4	-2.804949	-3.406260	-1.635028
Mg5	-2.561576	0.302632	2.157168
Mg6	-2.107728	-1.143844	-3.602118
Mg7	-0.246260	-4.395247	0.197835
Mg8	3.118011	1.230928	-3.262796
Mg9	3.085774	2.447770	-0.500448
Mg10	4.436448	-2.119216	1.468007
Mg11	-1.553898	-2.740721	2.758518
Mg12	2.418188	-3.049247	-0.697844
Mg13	4.805106	0.921856	1.545402
Mg14	0.811633	4.344287	0.536104
Mg15	0.189950	-0.087363	3.052010
Mg16	1.503318	-2.792988	2.260644
Mg17	0.459444	0.020156	-2.534578
Mg18	-1.554777	4.611022	-1.560128
Mg19	2.708183	-1.787253	-3.390356
Mg20	-1.991494	1.945184	-2.977694
Mg21	1.885773	-0.228422	0.385774
Mg22	-0.828445	-1.432635	0.016598
Mg23	3.121832	-0.481621	3.536705
Mg24	-3.405155	-0.030250	-1.184579

Mg25	4.490025	-0.558058	-1.204606
Mg26	-3.283857	2.790084	0.173970
Mg27	-4.013796	-2.131709	0.911449
Mg28	-0.939111	2.876917	2.825888
Mg29	0.041562	-3.148354	-2.704447
Mg30	2.132715	2.244230	2.440926
Mg31	-3.021774	-4.879871	1.105021
Mg32	-5.329124	0.678958	1.050609

@mg32-isomer26 bp86/6-31G(d) Etot=-6403.119814 Eb=-17.44

Mg1	-1.629400	0.874752	0.275851
Mg2	3.156493	2.710513	-2.613076
Mg3	0.038473	-0.679179	-1.618276
Mg4	0.390209	3.129948	-1.570889
Mg5	-0.925068	-3.844805	3.147722
Mg6	-1.887166	1.523013	-2.933978
Mg7	0.052032	-1.591118	1.270996
Mg8	-1.126516	-3.560660	-2.004775
Mg9	1.649203	0.916578	0.358100
Mg10	3.174706	-0.567691	-2.278251
Mg11	-0.179744	-4.909960	0.543822
Mg12	2.360619	-0.641707	3.191643
Mg13	-2.701851	-3.056659	0.632117
Mg14	2.098553	-3.662187	2.072241
Mg15	2.167781	2.583775	3.248205
Mg16	4.542498	1.311126	2.241647
Mg17	-0.227575	0.832956	3.281991
Mg18	-1.457453	-1.352068	-4.247140
Mg19	1.935831	-3.235200	-0.981987
Mg20	1.010581	1.060462	-3.836672
Mg21	-2.504928	-1.211049	3.039689
Mg22	-4.503738	1.554175	-1.539866
Mg23	4.809117	1.358952	-0.644377
Mg24	-2.505812	3.699857	-0.638989
Mg25	3.780737	-1.362346	0.641194
Mg26	2.944644	3.621783	0.360217
Mg27	-4.459440	-0.219726	0.970249
Mg28	1.288562	-2.447146	-3.850451
Mg29	-3.200171	-1.199112	-1.744129
Mg30	-2.936537	1.997872	2.808051
Mg31	-0.164354	3.402305	1.412350
Mg32	-4.990288	2.962546	1.006771

@mg32-isomer27 bp86/6-31G(d) Etot=-6403.118235 Eb=-17.41

Mg1	1.635403	-0.743567	-0.006231
Mg2	-2.962641	-1.031373	-3.714278
Mg3	-0.016413	1.637996	-0.728404
Mg4	-0.245007	-1.944931	-2.810842
Mg5	1.098227	1.807359	4.478233
Mg6	1.996161	0.091447	-3.188752
Mg7	-0.215718	0.491823	2.145808
Mg8	1.260931	4.432092	-0.279396
Mg9	-1.604927	-0.974835	-0.132334
Mg10	-3.068000	1.630619	-1.783075
Mg11	0.015535	3.744409	2.340764
Mg12	-2.595354	-1.179691	3.118085
Mg13	2.587670	2.254367	1.811609
Mg14	-2.366563	2.101341	3.385619
Mg15	-2.245671	-3.950352	1.592736
Mg16	-4.562527	-2.322733	1.112535
Mg17	0.122721	-2.480277	2.591892
Mg18	1.390665	3.197156	-3.096765
Mg19	-2.349216	3.475588	0.589633
Mg20	-0.809060	1.020693	-3.678689

Mg21	2.520492	-0.595608	3.214191
Mg22	4.610182	-0.578944	-1.965669
Mg23	-4.730798	-0.873156	-1.428424
Mg24	2.612850	-2.892168	-1.923655
Mg25	-3.840117	0.757453	1.072523
Mg26	-2.887399	-3.322098	-1.463457
Mg27	4.508158	-0.168516	1.017334
Mg28	-1.226216	4.255368	-2.107028
Mg29	3.250461	1.997344	-1.044992
Mg30	2.800282	-3.240319	1.374551
Mg31	0.115710	-3.672709	-0.271827
Mg32	5.200180	-2.923780	-0.221696

@mg32-isomer28 bp86/6-31G(d) Etot=-6403.105166 Eb=-17.16

Mg1	-4.094930	1.396795	3.211990
Mg2	4.836156	-1.404281	0.087702
Mg3	-2.907417	3.739435	1.563364
Mg4	-2.369223	-4.414218	-2.471990
Mg5	0.689603	-0.080644	-2.876224
Mg6	2.192528	0.312556	-0.130403
Mg7	-1.118756	4.450188	-1.307816
Mg8	-0.624941	-4.661114	-0.104785
Mg9	-3.091327	0.455731	0.560385
Mg10	3.309205	-2.383690	2.648716
Mg11	0.348301	-3.355522	2.525366
Mg12	-1.930642	-1.423353	-2.811217
Mg13	0.836339	2.952885	-3.103772
Mg14	2.133547	-3.028397	-0.002761
Mg15	-4.373505	-0.000153	-2.038415
Mg16	-3.710362	2.935481	-1.133804
Mg17	0.938682	-0.387288	2.675489
Mg18	0.545091	-3.209472	-2.606984
Mg19	-3.308225	-2.576785	-0.183102
Mg20	-0.477067	1.626606	-0.068485
Mg21	5.001456	1.744297	-0.153546
Mg22	4.246111	0.513162	2.474089
Mg23	-1.033402	1.815853	3.036511
Mg24	-2.505762	-4.223511	2.226837
Mg25	3.237479	-1.619609	-2.455248
Mg26	1.932154	2.383386	2.329410
Mg27	-1.859262	1.619457	-3.064510
Mg28	2.125534	3.433292	-0.470934
Mg29	-0.431497	-1.363164	0.008123
Mg30	3.557898	1.488215	-2.749611
Mg31	-0.056113	4.458885	1.526044
Mg32	-2.037653	-1.195023	2.859582

@mg32-isomer29 bp86/6-31G(d) Etot=-6403.102406 Eb=-17.10

Mg1	-2.369773	0.215015	0.067726
Mg2	0.362687	-1.694960	-2.556937
Mg3	-1.011647	-2.715021	0.417712
Mg4	0.064364	2.599322	0.631026
Mg5	-3.023982	-1.579326	2.533926
Mg6	1.642956	1.110640	3.043699
Mg7	0.043141	-1.577780	3.085535
Mg8	2.647263	0.388396	-2.301621
Mg9	0.927360	-0.352057	0.282016
Mg10	3.052017	-1.677789	3.469906
Mg11	-3.944569	-2.643066	-0.310706
Mg12	3.284046	-2.569447	-1.810987
Mg13	-3.549705	2.161163	-2.175231
Mg14	-5.345632	-0.341162	-1.650938
Mg15	-0.447199	1.267825	-2.289731
Mg16	-4.294853	1.268498	2.732245

Mg17	1.059133	-4.449001	-1.403185
Mg18	3.160006	2.173491	0.594095
Mg19	4.684826	0.962285	2.977826
Mg20	-5.585696	1.979625	0.184555
Mg21	-2.632446	-0.825415	-2.847913
Mg22	-5.789389	-0.872079	1.252153
Mg23	4.022732	-0.929539	0.625449
Mg24	-1.336900	1.155130	2.917110
Mg25	-2.909320	3.231219	0.782400
Mg26	4.838665	2.502310	-1.920739
Mg27	1.817709	3.329764	-1.884388
Mg28	-1.383941	4.128578	-1.727279
Mg29	2.068742	-3.281000	1.145291
Mg30	6.258723	1.250906	0.430682
Mg31	-1.967860	-3.697542	-2.332268
Mg32	5.658542	-0.518983	-1.961431

@mg32-isomer30 bp86/6-31G(d) Etot=-6403.079481 Eb=-16.65

Mg1	-1.114337	1.927544	-0.012086
Mg2	2.080154	2.153385	2.027663
Mg3	-4.997437	1.340319	0.206082
Mg4	-0.672761	0.876528	3.100580
Mg5	0.605428	-0.323232	0.309828
Mg6	-3.311622	3.808184	-0.597425
Mg7	-5.405338	-0.751634	-1.998258
Mg8	-2.891385	-1.719409	-3.315290
Mg9	-3.114632	2.550515	2.239501
Mg10	-2.571764	-0.632887	-0.112869
Mg11	-5.567921	-1.535016	0.906616
Mg12	1.800115	-3.141417	0.931043
Mg13	-0.324967	3.838396	2.235829
Mg14	-0.735603	-2.042099	2.421954
Mg15	-3.296298	-3.329141	1.572061
Mg16	3.682619	0.032397	0.444567
Mg17	-0.490014	2.833249	-2.804386
Mg18	2.156624	1.353212	-1.959870
Mg19	6.468196	1.501646	-0.910058
Mg20	4.396378	-3.247278	-0.678877
Mg21	4.525939	-2.322576	2.159290
Mg22	-4.132911	-3.363611	-1.221634
Mg23	-3.488053	-0.393474	2.833307
Mg24	2.011582	-0.735934	3.080865
Mg25	-0.457103	-0.218845	-2.620871
Mg26	6.601761	-1.376548	0.029839
Mg27	4.156177	3.108687	-0.234504
Mg28	-0.872218	-2.958882	-0.767791
Mg29	2.007682	-1.866073	-1.940356
Mg30	-3.156611	1.376873	-2.499772
Mg31	1.298842	3.853650	-0.435798
Mg32	4.809481	-0.596529	-2.389177

@mg32-isomer31 bp86/6-31G(d) Etot=-6403.077442 Eb=-16.61

Mg1	1.413972	2.355359	1.441753
Mg2	-0.736399	0.193070	0.006066
Mg3	1.139922	2.188051	-1.742578
Mg4	0.308731	-2.493928	1.628250
Mg5	0.867517	-0.342723	-3.329628
Mg6	-2.832257	2.567516	-0.078232
Mg7	-4.201219	1.041331	2.156604
Mg8	2.264506	-0.371410	-0.015518
Mg9	-1.751048	1.472175	-2.773425
Mg10	-2.336915	-2.545623	0.004341
Mg11	-6.764635	0.350064	0.940270
Mg12	-0.822726	4.503258	1.100185

Mg13	0.480108	-2.647791	-1.371134
Mg14	3.311027	-2.024475	-2.511200
Mg15	0.854930	0.026722	3.249669
Mg16	-2.075367	-0.985765	2.801064
Mg17	2.869467	-2.211338	3.264282
Mg18	-4.470854	-3.016028	-2.148659
Mg19	3.935267	0.770548	2.331440
Mg20	5.387882	0.113662	-0.437969
Mg21	5.377175	-1.852973	1.863773
Mg22	3.973270	2.704594	-0.292800
Mg23	5.619695	-2.876713	-0.918817
Mg24	-4.920290	-1.924077	1.594691
Mg25	1.829972	4.792435	-0.364929
Mg26	-1.439950	2.052459	2.746422
Mg27	-1.088751	4.306348	-1.931587
Mg28	-6.866055	-2.030703	-0.857998
Mg29	3.648058	0.961892	-2.825431
Mg30	-1.922510	-1.533348	-2.921805
Mg31	-4.005568	-0.078910	-1.022325
Mg32	2.953045	-3.463679	0.415225

@mg32-isomer32 bp86/6-31G(d) Etot=-6403.075753 Eb=-16.58

Mg1	-1.682080	-0.685992	-0.031707
Mg2	0.237044	-3.662174	-0.216617
Mg3	-1.848815	3.988670	2.073010
Mg4	2.795399	2.631254	0.910654
Mg5	-2.638490	1.239160	2.403015
Mg6	0.473517	1.883022	2.935157
Mg7	-3.240687	-0.943139	-3.076733
Mg8	2.574346	1.640508	-1.885101
Mg9	-3.070199	2.309348	-0.386260
Mg10	3.665309	1.692610	3.578949
Mg11	1.344204	-0.660346	-0.092879
Mg12	-1.442954	4.846369	-0.865089
Mg13	-3.990698	1.868408	-3.193148
Mg14	-2.015222	-3.644481	1.813432
Mg15	2.502600	-2.835197	-2.166812
Mg16	-4.573531	-0.376628	-0.270784
Mg17	2.399707	-0.822443	2.867453
Mg18	3.172443	-3.109375	0.945337
Mg19	-0.068530	2.024768	-0.114660
Mg20	0.798105	4.964377	1.357331
Mg21	5.297260	-2.567032	-0.963123
Mg22	0.990507	-3.640856	2.827847
Mg23	1.658101	-0.285210	-3.986310
Mg24	-2.776531	-3.349559	-1.230635
Mg25	-0.926955	1.179760	-2.815721
Mg26	4.346525	-0.547464	-2.847013
Mg27	-3.739867	-1.429923	2.716533
Mg28	4.248850	0.025672	0.411191
Mg29	-0.396724	-1.880160	-2.626529
Mg30	-0.593023	-1.028725	2.780152
Mg31	1.388500	4.441514	-1.603924
Mg32	-4.888111	-3.266734	0.752982

@mg32-isomer33 bp86/6-31G(d) Etot=-6403.054873 Eb=-16.17

Mg1	-0.350213	2.168401	-1.535973
Mg2	-0.941602	2.353893	2.436661
Mg3	1.792438	2.851650	1.263367
Mg4	-3.364635	3.863771	1.423142
Mg5	1.808117	4.224208	-1.534969
Mg6	4.033878	2.473229	-0.689126
Mg7	-4.728653	1.778191	-0.259018
Mg8	2.251361	1.480494	-3.003280

Mg9	1.332326	0.370980	3.025746
Mg10	-2.901328	3.831352	-1.616835
Mg11	4.965642	-0.030347	-1.884848
Mg12	-2.960726	0.856426	-2.466794
Mg13	-4.492569	-1.217163	-0.590948
Mg14	-1.569222	0.095173	0.341252
Mg15	2.594027	-1.559570	-2.930429
Mg16	-0.261398	-0.628475	-2.735883
Mg17	4.043863	-2.492321	-0.439711
Mg18	1.731967	0.071337	-0.228114
Mg19	7.076711	-1.603826	-0.240157
Mg20	-0.223079	-2.178206	2.078932
Mg21	0.972935	-2.826948	-0.671463
Mg22	5.870564	-2.199401	2.385573
Mg23	-2.850916	-2.092034	-3.265723
Mg24	-4.555261	-4.176564	-2.079795
Mg25	-0.623954	4.631610	0.338588
Mg26	2.790388	-2.175551	2.230318
Mg27	-3.401613	-1.945780	2.301198
Mg28	4.194508	0.400152	1.509540
Mg29	-3.833341	1.080028	2.502657
Mg30	-1.997398	-3.040970	-0.385272
Mg31	-4.835383	-4.154587	0.801085
Mg32	-1.567435	-0.209151	3.920276

@mg32-isomer34 bp86/6-31G(d) Etot=-6403.038870 Eb=-15.86

Mg1	-0.163443	0.535643	0.294325
Mg2	-1.451570	-0.069272	-2.875451
Mg3	0.299214	2.671802	-2.130250
Mg4	-0.778372	-2.999386	1.352927
Mg5	2.794617	0.293823	-0.554391
Mg6	6.050668	-0.828956	-0.355021
Mg7	0.707455	-2.038147	-1.295275
Mg8	0.012881	3.661352	0.778592
Mg9	1.940143	1.739674	2.214182
Mg10	-2.669630	-1.015411	-0.170081
Mg11	-5.503782	-2.353373	-0.006334
Mg12	-2.799482	4.244180	1.815384
Mg13	-3.384473	-4.473226	0.208892
Mg14	1.974098	-4.134243	0.695430
Mg15	-3.121023	1.091658	1.859063
Mg16	1.861465	-1.329228	1.898526
Mg17	-2.614015	2.050576	-1.005906
Mg18	4.631361	-2.732292	1.539168
Mg19	4.598899	0.316723	1.994150
Mg20	-1.880837	5.009383	-1.216786
Mg21	3.357876	2.412444	-2.773189
Mg22	-2.114668	-3.096595	-2.357048
Mg23	5.529300	2.114796	-0.429686
Mg24	-3.555685	-2.277906	2.433625
Mg25	-4.457469	-0.933893	-2.561590
Mg26	-0.842212	-0.591864	3.193368
Mg27	-0.634235	-5.120309	-0.837222
Mg28	-4.869166	4.300521	-0.333181
Mg29	-0.865643	2.414957	3.348130
Mg30	3.697336	-2.542218	-1.288803
Mg31	2.835963	3.548469	-0.106814
Mg32	1.414427	0.130317	-3.328734

@mg32-isomer35 bp86/6-31G(d) Etot=-6403.021653 Eb=-15.52

Mg1	-0.183006	-0.518616	0.077084
Mg2	1.640386	-0.922297	-2.394516
Mg3	-2.501279	-1.550105	-1.826197
Mg4	2.720600	0.871027	0.478919

Mg5	-2.022015	1.883987	-0.663486
Mg6	-3.300483	5.135945	-0.229330
Mg7	1.063717	2.081312	-1.674571
Mg8	-2.721818	-2.470792	1.105421
Mg9	-2.401710	0.382091	2.095834
Mg10	2.658048	-2.252500	0.328350
Mg11	5.864299	-2.436456	0.593997
Mg12	-1.590520	-5.345083	1.131605
Mg13	5.853532	0.463962	-0.138273
Mg14	1.971367	4.234609	0.625235
Mg15	0.295203	-3.186653	1.940859
Mg16	-0.008402	2.188352	1.626964
Mg17	-0.027329	-3.345135	-1.072982
Mg18	-0.811315	5.202571	1.713565
Mg19	-3.129147	3.310937	2.066565
Mg20	-2.836530	-4.546378	-1.606425
Mg21	-4.027077	0.909580	-2.722395
Mg22	4.037349	1.041286	-2.592828
Mg23	-5.129231	2.788681	-0.439642
Mg24	4.471502	-0.554424	2.474443
Mg25	4.545282	-1.864843	-2.018437
Mg26	1.214300	-0.337259	2.953358
Mg27	4.512684	3.176672	-0.615675
Mg28	-2.847097	-7.538666	-0.643490
Mg29	-1.354461	-1.704396	3.897656
Mg30	-0.456624	4.563760	-1.208794
Mg31	-4.547374	-0.167112	0.037152
Mg32	-0.952854	0.505943	-3.299968