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Electronic Supplementary Information

For

Density Functional Theory and Atoms-in Molecule Study on the Role of Two-electron Stabilizing Interactions in Retro Diels-Alder Reaction of Cycloadducts Derived from Substituted Cyclopentadiene and p-Benzoquinone

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Table of Contents

	Details	Page Number
Table S1	Comparison of key structural parameters obtained at the B3LYP/6-31G* level for the cycloadducts and the corresponding saturated bicyclic compounds (with hydrogenated C_3-C_4 Bond).	S3
Table S2	Summary of Natural Bond Orbital (NBO) analyses of cycloadducts performed at the B3LYP/6-311+G**//B3LYP/6-31G* level of theory. The second order perturbation energies reported in kcal mol^{-1}.	S4
Table S3	Summary of Atoms in Molecule (AIM) analyses performed with wave functions generated at the B3LYP/6-311+G**//B3LYP/6-31G* level of theory for the cycloadducts as well as the corresponding saturated analogue (hydrogenated C_3-C_4 bond).	S5
Table S4	Properties of bond critical points (BCP) for the C_1-C_5 bond for the transition states computed at the AIM/B3LYP/6-311+G**//B3LYP/6-31G* level.	S6
Table S5	Marcus Type Analysis Based on the Energetics of retro Diels-Alder reaction of C_7 substituted cycloadducts at the B3LYP/6-311+G**//B3LYP/6-31G* level of theory	S7

Figure S1	Correlation between intrinsic free energies of activation (kcal mol^{-1}) and electron density $\rho(r_c)$ at bond critical points for **1** to **19** at the B3LYP/6-311+G**//B3LYP/6-31G* level.	S8
Figure S2	Correlation between computed intrinsic activation barrier (kcal mol^{-1}) and (i) bond length (**S2.1**) (ii) occupancies of C_1-C_5 bond (**S2.2**)	S8
Table S6	The B3LYP/6-31G* optimized geometries (in Cartesian coordinates), total electronic energies (in hartree/particle), and number of imaginary frequencies for cycloadducts and the corresponding transition states for cycloreversion reaction.	S9
Table S7	The B3LYP/6-31G* optimized geometries (in Cartesian coordinates), total electronic energies (in hartree/particle), and number of imaginary frequencies of substituted cyclopentadienes and quinone.	S21
Table S8	The B3LYP/6-31G* optimized geometries (in Cartesian coordinates), total electronic energies (in hartree/particle), of different rotamers of the substituent attached to the C7 position of the cycloadduct.	S26

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Table S1. Comparison of key structural parameters obtained at the B3LYP/6-31G* level for the cycloadducts formed and the corresponding saturated bycyclic compounds (with hydrogenated C_3-C_4 Bond).

	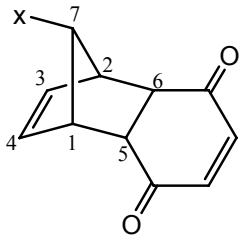			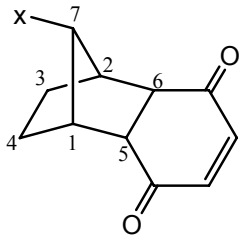		
Substituents	C_3-C_4	C_1-C_5	C_7-X	C_3-C_4	C_1-C_5	C_7-X
-$SiMe_3$ (**1**)	1.341	1.587	1.916	1.560	1.564	1.916
-GeH_3 (**2**)	1.340	1.586	1.957	1.561	1.562	1.957
-BH_2 (**3**)	1.344	1.582	1.572	1.564	1.560	1.561
-PH_2 (**4**)	1.340	1.585	1.888	1.560	1.561	1.888
-CMe_3 (**5**)	1.340	1.584	1.555	1.559	1.563	1.562
-CHO (**6**)	1.340	1.581	1.513	1.561	1.559	1.510
-H (**7**)	1.341	1.583	1.094	1.563	1.561	1.096
-C_2H_5 (**8**)	1.340	1.583	1.538	1.562	1.560	1.534
-Me (**9**)	1.340	1.581	1.526	1.262	1.559	1.530
-SH (**10**)	1.341	1.581	1.833	1.561	1.560	1.844
-COMe (**11**)	1.341	1.579	1.528	1.561	1.560	1.524
-COOH (**12**)	1.341	1.579	1.515	1.562	1.559	1.512
-Cl (**13**)	1.339	1.581	1.810	1.562	1.560	1.817
-NH_2 (**14**)	1.342	1.577	1.450	1.564	1.557	1.458
-CN (**15**)	1.340	1.577	1.463	1.562	1.557	1.462
-OMe (**16**)	1.339	1.578	1.402	1.562	1.556	1.411
-NO_2 (**17**)	1.340	1.577	1.510	1.564	1.558	1.512
-OH (**18**)	1.344	1.575	1.403	1.562	1.556	1.417
-F (**19**)	1.340	1.577	1.380	1.563	1.556	1.390

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Table S2. Summary of Natural Bond Orbital (NBO) analyses of cycloadducts performed at the B3LYP/6-311+G**//B3LYP/6-31G* level of theory.[a] The second order perturbation energies are reported in kcal mol^{-1}.

Substituents	σ (C_7-X) → σ^*(C_1-C_5)	σ (C_1-C_5) → σ^*(C_7-X)	π(C_3-C_4) → σ^*(C_1-C_5)	σ (C_1-C_5) → π^*(C_3-C_4)	Occupancy of σ^*(C_1-C_5)	Occupancy of σ(C_1-C_5)
-$SiMe_3$(**1**)	1.72	2.57	3.25	2.79	0.03582	1.9415
-GeH_3 (**2**)	1.83	3.90	3.23	2.76	0.03547	1.9410
-BH_2 (**3**)	1.62	2.78	3.14	2.69	0.03368	1.9440
-PH_2 (**4**)	1.72	4.11	3.26	2.72	0.03348	1.9401
-CMe_3 (**5**)	0.74	3.60	3.26	2.86	0.03080	1.9412
-CHO (**6**)	1.03	2.98	3.21	2.66	0.03126	1.9440
-H (**7**)	1.81	2.32	3.30	2.65	0.03270	1.9444
-C_2H_5 (**8**)	1.00	3.12	3.20	2.70	0.03011	1.9429
-Me (**9**)	1.03	3.36	3.20	2.69	0.03032	1.9431
-SH (**10**)	1.23	4.99	3.22	2.70	0.03181	1.9382
-COMe (**11**)	1.05	2.94	3.04	2.65	0.02914	1.9445
-COOH (**12**)	1.13	2.77	3.11	2.59	0.02940	1.9453
-Cl (**13**)	1.10	5.53	3.33	2.60	0.03105	1.9377
-NH_2 (**14**)	0.87	3.45	3.16	2.68	0.02800	1.9434
-CN (**15**)	0.96	3.07	3.19	2.52	0.02974	1.9464
-OMe (**16**)	0.75	3.65	3.25	2.59	0.02763	1.9433
-NO_2 (**17**)	0.76	4.62	3.26	2.50	0.02957	1.9440
-OH (**18**)	0.61	3.82	3.22	2.63	0.02878	1.9428
-F (**19**)	0.62	4.19	3.34	2.52	0.02871	1.9428

[a] Second order perturbation energies for various delocalizations are represented as "donor → acceptor" in this table

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Table S3. Summary of Atoms in Molecule (AIM) analyses performed with wave functions generated at the B3LYP/6-311+G**//B3LYP/6-31G* level of theory for the cycloadducts as well as the corresponding saturated analogue (hydrogenated C_3-C_4 bond).

Substituents	C_3-C_4 unsaturated cycloadduct				C_3-C_4 saturated compound			
	$\rho(r_c)$[a]	$\nabla^2(r_c)$ [a]	$H(r_c)$[a]	Wiberg BI[b]	$\rho(r_c)$[a]	$\nabla^2(r_c)$ [a]	$H(r_c)$[a]	Wiberg BI[b]
-$SiMe_3$ (**1**)	0.2144	0.1008	-3.135	0.9383	0.2269	0.1158	-3.356	0.9661
-GeH_3 (**2**)	0.2152	0.1018	-3.141	0.9383	0.2276	0.1166	-3.3619	0.9652
-BH_2 (**3**)	0.2170	0.1041	-2.734	0.9439	0.2286	0.1172	-2.919	0.9693
-PH_2 (**4**)	0.2160	0.1028	-2.879	0.9396	0.2280	0.1172	-3.078	0.9667
-CMe_3 (**5**)	0.2159	0.1027	-3.087	0.9429	0.2272	0.1164	-3.286	0.9705
-CHO (**6**)	0.2175	0.1045	-2.862	0.9460	0.2292	0.1173	-3.058	0.9721
-H (**7**)	0.2164	0.1034	-2.631	0.9446	0.2282	0.1176	-2.814	0.9701
-C_2H_5 (**8**)	0.2171	0.1042	-2.875	0.9444	0.2287	0.1183	-3.068	0.9706
-Me (**9**)	0.2172	0.1044	-2.776	0.9455	0.2288	0.1184	-2.9646	0.9709
-SH (**10**)	0.2172	0.1042	-2.9012	0.9397	0.2281	0.1174	-3.087	0.9671
-COMe (**11**)	0.2186	0.1058	-2.992	0.9483	0.2290	0.1186	-3.174	0.9720
-COOH (**12**)	0.2190	0.1064	-3.006	0.9490	0.2292	0.1189	-3.1813	0.9721
-Cl (**13**)	0.2172	0.1043	-2.909	0.9396	0.2284	0.1179	-3.098	0.9636
-NH_2 (**14**)	0.2189	0.1065	-2.805	0.9484	0.2298	0.1194	-2.984	0.9729
-CN (**15**)	0.2199	0.1075	-2.865	0.9504	0.2306	0.1206	-3.043	0.9730
-OMe (**16**)	0.2189	0.1068	-2.918	0.9485	0.2296	0.1191	-3.112	0.9752
-NO_2 (**17**)	0.2195	0.1071	-3.027	0.9477	0.2298	0.1197	-3.207	0.9700
-OH (**18**)	0.2194	0.1069	-2.818	0.9480	0.2298	0.1194	-2.991	0.9701
-F (**19**)	0.2189	0.1063	-2.817	0.9473	0.2300	0.1199	-3.000	0.9711

*[a] $\rho(r_c)$, $\nabla^2(r_c)$ and H are respectively the electron density, Laplacian of electron density and the total energy density at the BCP. [b] Wiberg Bond index computed at the B3LYP//6-311+G**/6-31G* level of theory*

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Table S4. Properties of bond critical points (BCP) for the C_1-C_5 bond for the transition states computed at the AIM/B3LYP/6-311+G**//B3LYP/6-31G* level

Substituents	$\rho(r_c)^a$	$\nabla^2(r_c)^a$	H^a
-$SiMe_3$ (**1**)	0.06395	-0.00851	-0.8777
-GeH_3 (**2**)	0.06235	-0.00897	-0.8521
-BH_2 (**3**)	0.06148	-0.00931	-0.7202
-PH_2 (**4**)	0.06030	-0.00940	-0.7474
-CMe_3 (**5**)	0.05863	-0.00945	-0.7815
-CHO (**6**)	0.05953	-0.00959	-0.7275
-H (**7**)	0.05735	-0.00995	-0.6437
-C_2H_5 (**8**)	0.05807	-0.00961	-0.7155
-Me (**9**)	0.05606	-0.00100	-0.6621
-SH (**10**)	0.05624	-0.01010	-0.6961
-COMe (**11**)	0.05409	-0.01033	-0.6958
-COOH (**12**)	0.05579	-0.01012	-0.7099
-Cl (**13**)	0.05428	-0.01049	-0.6725
-NH_2 (**14**)	0.05407	-0.01033	-0.6392
-CN (**15**)	0.05533	-0.01011	-0.6653
-OMe (**16**)	0.05225	-0.01067	-0.6429
-NO_2 (**17**)	0.05378	-0.01041	-0.6856
-OH (**18**)	0.05205	-0.01082	-0.6157
-F (**19**)	0.05105	-0.01097	-0.6047

[a] *$\rho(r_c)$, $\nabla^2(r_c)$ and H are respectively the electron density, Laplacian of electron density and the total energy density at the BCP.*

Table S5. Marcus Type Analysis Based on the Energetics of retro Diels-Alder reaction of C_7 substituted cycloadducts at the B3LYP/6-311+G**//B3LYP/6-31G* level of theory[a]

Substituents	$\Delta G^{\dagger}_{298}$	$\Delta G^{\dagger}_{\text{intrinsic}}$	ΔG_{298}
-$SiMe_3$ (**1**)	20.28	27.42	-15.36
-GeH_3 (**2**)	21.19	27.57	-13.60
-BH_2 (**3**)	23.41	28.47	-10.62
-PH_2 (**4**)	23.58	28.51	-10.34
-CMe_3 (**5**)	23.77	29.19	-11.40
-CHO (**6**)	24.40	28.97	-9.55
-H (**8**)	24.69	28.44	-7.77
-C_2H_5 (**7**)	25.62	27.96	-4.79
-Me (**9**)	25.84	29.53	-7.64
-SH (**10**)	26.15	29.43	-6.77
-COMe (**11**)	26.59	30.94	-9.03
-COOH (**12**)	27.53	30.99	-7.14
-Cl (**13**)	27.41	30.28	-5.89
-NH_2 (**14**)	28.57	29.62	-2.39
-CN (**15**)	28.76	31.95	-6.55
-OMe (**16**)	29.42	31.01	-3.24
-NO_2 (**17**)	29.65	32.29	-5.41
-OH (**18**)	29.98	30.49	-1.08
-F (**19**)	29.98	31.27	-2.62

[a] T. H. Lowry and K. S. Richardson 'Mechanism and Theory in Organic Chemistry' 3rd Ed. Harper Collins Publishers, New York, 1987. (pape 225)

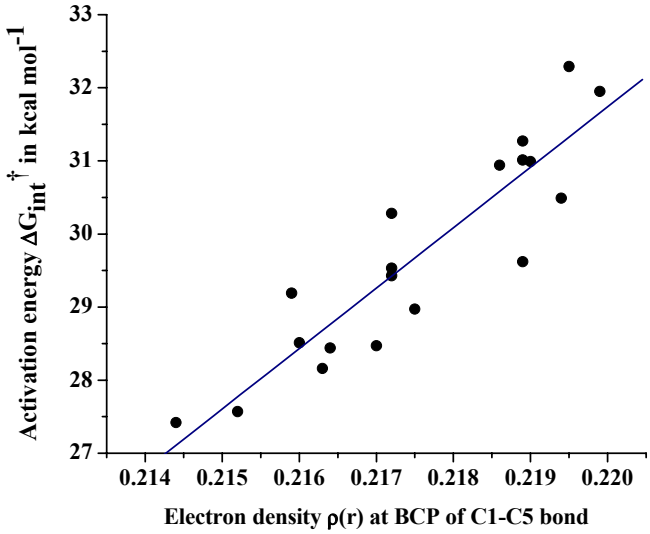
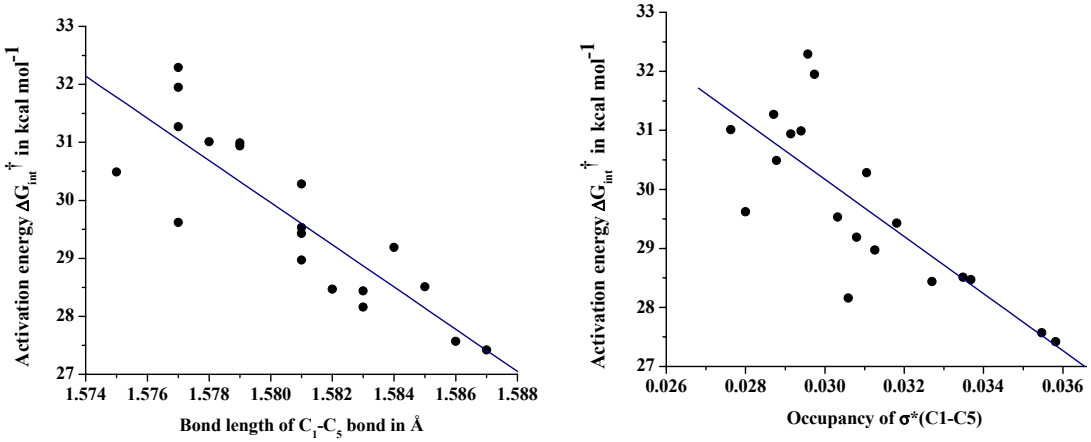


Figure S1. Correlation between intrinsic free energies of activation (kcal mol^{-1}) and electron density $\rho(r_c)$ at bond critical points for **1** to **19** at the B3LYP/6-311+G**//B3LYP/6-31G* level.



S2.1 **S2.2**

Figure S2. Correlation between computed intrinsic activation barrier (kcal mol^{-1}) and (i) bond length (**S2.1**) (ii) occupancies of C_1-C_5 bond (**S2.2**)

Table S6. The B3LYP/6-31G* optimized geometries (in Cartesian coordinates), total electronic energies (in hartree/particle), and number of imaginary frequencies (in cm^{-1}) for cycloadducts and the corresponding transition states for cycloreversion reaction. The values in parenthesis implies single-point energies evaluated at the B3LYP/6-311+G**//B3LYP/6-31G* level.

1 Et = -984.2451822 (-984.4654879) Nimag = 0				**1**† Et = -984.2060574 (-984.4295805) Nimag = 1 (-469.51)			
6	-.990784	.000013	-.556512	6	-0.987906	-0.000033	-0.494010
6	-.057447	1.126687	-.028058	6	-0.238833	1.142736	0.136146
6	.174460	.670112	1.404179	6	0.188897	0.693605	1.413308
6	.174462	-.670409	1.404071	6	0.188844	-0.694089	1.413187
6	-.057453	-1.126759	-.028236	6	-0.238965	-1.142972	0.135972
6	1.270380	-.779300	-.825907	14	-2.885415	0.000023	-0.070554
6	2.487972	-1.485379	-.255023	6	-3.627537	1.547323	-0.871319
6	3.621832	-.672573	.248145	6	-3.245502	-0.000173	1.783549
6	3.621827	.672580	.248188	6	-3.627676	-1.547029	-0.871674
6	2.487956	1.485404	-.254919	6	1.501923	-0.710024	-1.050518
6	1.270362	.779349	-.825818	6	2.546208	-1.460967	-0.318313
14	-2.843814	.000038	-.070903	6	3.424547	-0.672197	0.589021
1	-.993813	.000117	-1.659152	6	3.424475	0.672392	0.589057
1	-.364345	2.164300	-.165565	6	2.546056	1.461103	-0.318246
1	.409985	1.330492	2.232451	6	1.501792	0.710083	-1.050425
1	.409974	-1.330927	2.232237	1	-0.962708	0.000063	-1.589071
1	-.364352	-2.164357	-.165892	1	-0.422267	2.186535	-0.098426
1	1.156239	-1.160131	-1.847741	1	0.583508	1.329930	2.197708
8	2.540563	-2.706568	-.205314	1	0.583407	-1.330583	2.197473
1	4.463944	-1.244209	.631736	1	-0.422445	-2.186716	-0.098810
1	4.463936	1.244198	.631813	1	-3.414257	1.592279	-1.946085
8	2.540537	2.706591	-.205146	1	-3.239226	2.465820	-0.415745
1	1.156159	1.160291	-1.847604	1	-4.717977	1.557953	-0.752689
6	-3.619736	-1.546061	-.849201	1	-2.832241	0.883404	2.281253
6	-3.199320	-.003202	1.788337	1	-2.832457	-0.883986	2.281015
6	-3.618494	1.549407	-.843904	1	-4.330485	-0.000075	1.948525
1	-4.283680	-.003288	1.958881	1	-3.238391	-2.465699	-0.417278
1	-2.782811	-.886885	2.283888	1	-3.415597	-1.591021	-1.946719
1	-2.782348	.878331	2.287277	1	-4.717973	-1.558294	-0.751803
1	-4.703037	-1.568458	-.678386	1	1.110366	-1.242835	-1.912509
1	-3.456913	-1.581269	-1.933327	8	2.701116	-2.673127	-0.438505
1	-3.202523	-2.466058	-.421987	1	4.100520	-1.253042	1.212068
1	-4.701457	1.573171	-.671134	1	4.100387	1.253278	1.212132
1	-3.198995	2.467590	-.415020	8	2.700830	2.673280	-0.438411
1	-3.457472	1.587168	-1.928211	1	1.110146	1.242898	-1.912377

2 Et = -2651.750423 (-2653.9341535) Nimag = 0				**2**† Et =-2651.709212 (-2653.89691) Nimag = 1(-469.30)			
6	-0.132165	0.670224	1.380891	6	-1.226994	-0.001261	-0.553617
6	-0.327306	1.128059	-0.057206	6	-0.511522	1.144892	0.103436
6	1.017182	0.780080	-0.822447	6	-0.121477	0.694090	1.390216
6	1.017186	-0.780098	-0.822427	6	-0.121713	-0.694994	1.390898
6	-0.327311	-1.128069	-0.057195	6	-0.512554	-1.146947	0.104987
6	-0.132170	-0.670216	1.380899	6	1.263059	-0.709052	-1.048914
6	2.222122	1.485803	-0.222288	6	2.286120	-1.460636	-0.285488
6	3.352133	0.672636	0.287867	6	3.138952	-0.671492	0.644923
6	3.352142	-0.672605	0.287874	6	3.138325	0.673205	0.645087
6	2.222107	-1.485793	-0.222197	6	2.284469	1.461566	-0.284929
6	-1.235907	-0.000009	-0.609797	6	1.261630	0.708968	-1.048267
8	2.265481	-2.706088	-0.156936	1	-1.205096	-0.002066	-1.645668
8	2.265409	2.706095	-0.156902	1	-0.704752	2.185575	-0.136546
32	-3.105168	-0.000004	-0.028248	1	0.241489	1.331452	2.188353
1	-1.246096	-0.000015	-1.708664	1	0.241070	-1.331678	2.189660
1	-0.645408	2.161118	-0.201668	1	-0.705073	-2.187837	-0.134599
1	0.078381	1.332141	2.214014	1	0.889707	-1.243813	-1.917729
1	0.078374	-1.332123	2.214029	8	2.442559	-2.672190	-0.402246
1	-0.645419	-2.161128	-0.201647	1	3.798003	-1.251915	1.286070
1	0.929430	-1.159414	-1.847494	1	3.796829	1.254147	1.286323
1	4.189534	-1.243951	0.681897	8	2.439599	2.673206	-0.401934
1	4.189513	1.243997	0.681893	1	0.888674	1.243439	-1.917472
1	0.929384	1.159372	-1.847518	32	-3.144148	0.000101	-0.041068
1	-3.809503	-1.251464	-0.608318	1	-3.315588	0.000352	1.488961
1	-3.288454	0.000137	1.502801	1	-3.820607	-1.253157	-0.644715
1	-3.809555	1.251319	-0.608549	1	-3.818955	1.254112	-0.645015

3 Et = -601.0034415(-601.165081) Nimag = 0				**3**† Et = -600.9612899 (-601.1255111) Nimag = 1(-483.23)			
6	1.088201	-0.671562	1.349858	6	-2.153327	-.138778	-.626126
6	1.238846	-1.129772	-0.096015	6	-1.511112	1.046927	.072285
6	-0.117759	-0.780214	-0.830498	6	-1.134000	.591741	1.366296
6	-0.117593	0.779937	-0.830799	6	-1.039431	-.790741	1.339922
6	1.239169	1.129511	-0.096640	6	-1.362184	-1.240281	.032340
6	1.088386	0.672116	1.349504	6	.386186	-.696127	-1.053934
6	-1.311699	-1.485761	-0.209241	6	1.438545	-1.396011	-.276489
6	-2.429719	-0.672354	0.326633	6	2.228814	-.569395	.676081
6	-2.429565	0.672925	0.326436	6	2.154566	.773263	.685020
6	-1.311248	1.485924	-0.209446	6	1.276573	1.521139	-.255584
6	2.160521	-0.000410	-0.629411	6	.316864	.720616	-1.049793
8	-1.356223	2.706528	-0.146770	5	-3.648924	-.004139	-.119623
8	-1.357226	-2.706358	-0.146800	1	-2.091049	-.102931	-1.715617
5	3.636771	-0.000492	-0.087660	1	-1.745178	2.081946	-.155951

1	2.212758	-0.000690	-1.735185	1	-.828946	1.235300	2.184109
1	1.554098	-2.162455	-0.247507	1	-.665074	-1.418110	2.140803
1	0.892978	-1.329706	2.190294	1	-1.482389	-2.289653	-.219190
1	0.893298	1.330771	2.189569	1	.072974	-1.239507	-1.941202
1	1.554727	2.162019	-0.248669	8	1.662056	-2.595761	-.398904
1	-0.050202	1.158184	-1.858061	1	2.905016	-1.118146	1.327121
1	-3.258667	1.244473	0.737434	1	2.766983	1.384229	1.343759
1	-3.258964	-1.243589	0.737776	8	1.362922	2.741517	-.355639
1	-0.050128	-1.158888	-1.857584	1	-.069645	1.241382	-1.920991
1	4.224456	1.028116	0.088006	1	-4.443017	.555410	-.817961
1	4.224155	-1.029178	0.088500	1	-3.983843	-.409392	.949462

4 Et =-917.5145057 (-917.6999361) Nimag = 0				**4**† Et = -917.4697174 (-917.658433) Nimag = 1(-451.25)			
6	-1.776682	-0.008789	-0.596146	6	-1.770824	-0.002901	-0.528499
6	-0.870381	1.121254	-0.037898	6	-1.050472	1.146283	0.136492
6	-0.664171	0.654287	1.395416	6	-0.655058	0.694392	1.413775
6	-0.659489	-0.685972	1.388886	6	-0.656191	-0.699211	1.414727
6	-0.859654	-1.138240	-0.050744	6	-1.054422	-1.152238	0.139368
6	0.476923	-0.778292	-0.819180	6	0.721283	-0.707087	-1.059504
6	1.688889	-1.478784	-0.225790	6	1.742393	-1.459697	-0.294868
6	2.822838	-0.660359	0.266444	6	2.593411	-0.669950	0.636285
6	2.815630	0.684931	0.269902	6	2.591520	0.674993	0.636901
6	1.674011	1.493697	-0.220659	6	1.737858	1.462555	-0.293366
6	0.468522	0.782890	-0.813845	6	0.716920	0.707168	-1.057146
15	-3.590146	-0.103832	-0.101749	15	-3.610321	0.001117	0.012692
1	-1.784995	-0.011464	-1.694934	1	-1.730095	-0.004397	-1.617276
1	-1.193199	2.153215	-0.177319	1	-1.235969	2.187650	-0.105730
1	-0.458986	1.311774	2.233409	1	-0.293067	1.328599	2.214929
1	-0.448832	-1.351133	2.219434	1	-0.295040	-1.332901	2.216681
1	-1.172195	-2.171556	-0.202915	1	-1.238257	-2.193638	-0.103671
1	0.389165	-1.153481	-1.846001	1	0.330993	-1.245902	-1.918178
8	1.735274	-2.698420	-0.154207	8	1.899500	-2.670813	-0.413621
1	3.669234	-1.227943	0.646410	1	3.253376	-1.249653	1.277078
1	3.655977	1.259614	0.652647	1	3.249805	1.256144	1.278102
8	1.709281	2.713794	-0.147717	8	1.890784	2.674025	-0.412171
1	0.372351	1.164235	-1.837592	1	0.326532	1.245224	-1.916304
1	-3.475856	0.369698	1.233396	1	-4.015362	1.030919	-0.889069
1	-3.955533	1.171785	-0.623223	1	-4.018887	-1.030325	-0.885585

5 Et = -732.8242492 (-733.0231861) Nimag = 0				**5**† Et = -732.7783793 (-732.9805611) Nimag = 1(-440.44)			
6	-.945454	-.780785	-.796388	6	-1.295422	-.000064	-.387897
6	.350654	-1.127573	.045795	6	-.522560	1.148476	.244852
6	1.291538	.000021	-.475777	6	-.046560	.698591	1.488253
6	.350633	1.127629	.045747	6	-.046734	-.699940	1.487873

6	-.945457	.780784	-.796423	6	-.522866	-1.149075	.244290
6	.063717	.669851	1.466028	6	-2.853963	.000024	-.116307
6	.063699	-.669745	1.466056	6	-3.243021	-.001422	1.372032
6	-2.182335	-1.486066	-.266186	6	-3.452352	-1.251886	-.792182
6	-3.340856	-.672644	.175210	6	-3.451827	1.253586	-.789569
6	-3.340836	.672598	.175257	6	1.187811	-.706692	-1.053955
6	-2.182342	1.486041	-.266172	6	2.242553	-1.460983	-.341485
8	-2.231463	2.706561	-.203553	6	3.133325	-.672255	.552817
8	-2.231416	-2.706586	-.203545	6	3.133068	.672900	.552908
6	2.804788	-.000028	-.114422	6	2.241998	1.461390	-.341307
1	1.268645	.000029	-1.575709	6	1.187399	.706782	-1.053712
1	.661649	-2.164801	-.080835	1	-1.212357	.000251	-1.477869
1	-.194526	-1.330879	2.286857	1	-.700889	2.192998	.013595
1	-.194481	1.331017	2.286807	1	.376876	1.329635	2.262116
1	.661664	2.164841	-.080942	1	.376573	-1.331507	2.261374
1	-.801928	1.159492	-1.815589	1	-.701260	-2.193445	.012426
1	-4.201208	1.243826	.516653	1	-2.864049	.881564	1.895914
1	-4.201255	-1.243864	.516551	1	-2.865313	-.886188	1.893833
1	-.801836	-1.159540	-1.815524	1	-4.336056	-.000749	1.462707
6	3.442465	1.252829	-.755784	1	-3.100341	-2.175880	-.320586
6	3.144109	-.000228	1.389113	1	-4.545931	-1.238210	-.715208
6	3.442458	-1.252635	-.756091	1	-3.195389	-1.295982	-1.857781
1	4.528964	-1.247997	-.609075	1	-3.193265	1.300817	-1.854647
1	3.053374	-2.176415	-.313104	1	-3.100881	2.176360	-.314803
1	3.253320	-1.291216	-1.836093	1	-4.545514	1.239263	-.714282
1	4.234721	-.000280	1.512106	1	.746980	-1.246616	-1.886903
1	2.749886	.882042	1.903110	8	2.396048	-2.672309	-.468949
1	2.749772	-.882593	1.902855	1	3.820539	-1.252417	1.164068
1	4.528989	1.248067	-.608926	1	3.820060	1.253248	1.164230
1	3.253138	1.291739	-1.835736	8	2.395061	2.672766	-.468713
1	3.053453	2.176444	-.312408	1	.746254	1.246617	-1.886554

6 Et = -688.8884332 (-689.0807532) Nimag = 0				**6**† Et = -688.8424493 (-689.0378774) Nimag = 1(-451.21)			
6	0.635472	-0.670027	1.485071	6	-1.851443	-0.000284	-0.390784
6	0.909837	-1.130081	0.060062	6	-1.089415	1.151540	0.232175
6	-0.377837	-0.779813	-0.788044	6	-0.646901	0.697968	1.492562
6	-0.377829	0.779811	-0.788044	6	-0.647323	-0.698275	1.492863
6	0.909850	1.130067	0.060062	6	-1.090442	-1.152180	0.232918
6	0.635490	0.670016	1.485073	6	0.617252	-0.706113	-1.055554
6	-1.618954	-1.485975	-0.263406	6	1.672577	-1.460867	-0.337414
6	-2.794587	-0.672707	0.129020	6	2.568240	-0.672215	0.551309
6	-2.794579	0.672731	0.129022	6	2.568001	0.672848	0.551352
6	-1.618941	1.485987	-0.263414	6	1.671973	1.461127	-0.337279
6	1.855846	-0.000013	-0.446641	6	0.616571	0.705912	-1.055161
8	-1.652471	2.703883	-0.166883	6	-3.297586	0.000518	0.144439

8	-1.652504	-2.703872	-0.166894	1	-1.913978	-0.000519	-1.478828
6	3.251599	-0.000011	0.137503	1	-1.291702	2.191718	-0.000995
8	4.250460	0.000010	-0.550854	1	-0.245711	1.329646	2.277271
1	1.964925	-0.000010	-1.536464	1	-0.246505	-1.329882	2.277816
1	1.236637	-2.162119	-0.069218	1	-1.292548	-2.192397	-0.000147
1	0.382782	-1.332086	2.306248	1	0.179379	-1.245638	-1.890498
1	0.382816	1.332079	2.306251	8	1.817568	-2.672403	-0.460089
1	1.236663	2.162100	-0.069220	1	3.256866	-1.252589	1.160482
1	-0.227320	1.157416	-1.806562	1	3.256426	1.253459	1.160525
1	-3.664339	1.243736	0.445581	8	1.816325	2.672695	-0.460031
1	-3.664354	-1.243702	0.445577	1	0.178610	1.245282	-1.890163
1	-0.227334	-1.157420	-1.806562	8	-4.264292	-0.000321	-0.579080
1	3.323447	-0.000069	1.243829	1	-3.386672	0.001279	1.249568

7 Et = -575.57696 (-575.7339514) Nimag = 0				**7**† Et = -575.529184 (-575.6901174) Nimag = 1(-439.42)			
6	2.391678	-.000223	-.652924	6	2.385943	-.007161	-.659164
6	1.495100	-1.129374	-.095085	6	1.700272	-1.158147	.042641
6	1.347257	-.670560	1.348578	6	1.374541	-.701341	1.331609
6	1.347425	.670513	1.348519	6	1.380832	.698130	1.331008
6	1.495314	1.129150	-.095192	6	1.712759	1.150679	.042659
6	.137407	.779934	-.830166	6	-.138606	.705047	-1.077717
6	-1.054374	1.486200	-.206689	6	-1.109050	1.463226	-.256900
6	-2.174245	.672792	.325075	6	-1.908832	.676778	.721614
6	-2.174339	-.672493	.325089	6	-1.911753	-.668160	.722213
6	-1.054648	-1.486071	-.206792	6	-1.115353	-1.458493	-.255761
6	.137292	-.779980	-.830159	6	-.139655	-.704920	-1.075673
1	3.390930	-.000297	-.207602	1	3.450833	-.013301	-.373178
1	2.474276	-.000284	-1.746665	1	2.331935	-.006782	-1.749232
1	1.805853	-2.162876	-.250662	1	1.862842	-2.200390	-.210067
1	1.169149	-1.330750	2.190972	1	1.044413	-1.329024	2.151986
1	1.169467	1.330824	2.190849	1	1.055963	1.329558	2.150638
1	1.806253	2.162579	-.250879	1	1.881757	2.191145	-.212856
1	.203537	1.157613	-1.857799	1	.223437	1.245629	-1.947383
8	-1.098389	2.706669	-.141320	8	-1.268766	2.675157	-.366819
1	-3.004395	1.244083	.734282	1	-2.529244	1.258976	1.398717
1	-3.004563	-1.243658	.734321	1	-2.534711	-1.247165	1.399707
8	-1.098756	-2.706528	-.141250	8	-1.280436	-2.669534	-.365965
1	.203452	-1.157692	-1.857776	1	.219805	-1.247463	-1.945233

8 Et = -654.2037292 (-654.3817009) Nimag = 0				**8**† Et =-654.155253 (-654.3366516) Nimag = 1(-439.42)			
6	1.755195	-.346844	-.451230	6	1.767160	-0.327588	-0.344881
6	.649948	-1.333597	.020305	6	0.831188	-1.383953	0.218827
6	.439893	-.879628	1.457431	6	0.410591	-0.928975	1.479448

6	.639003	.445393	1.494429	6	0.609087	0.455653	1.545799
6	.984122	.896049	.082846	6	1.160754	0.891739	0.330550
6	-.344380	.766431	-.765945	6	-0.585343	0.747244	-1.021310
6	-1.466076	1.631859	-.216841	6	-1.531191	1.614257	-0.285591
6	-2.736684	.987399	.193509	6	-2.541407	0.924405	0.562701
6	-2.936569	-.342260	.152442	6	-2.730752	-0.406093	0.505914
6	-1.907218	-1.305953	-.306592	6	-1.943299	-1.275701	-0.409904
6	-.574757	-.776777	-.810388	6	-0.782164	-0.648010	-1.080282
1	1.807217	-.322571	-1.549835	1	1.750020	-0.270571	-1.436766
1	.817407	-2.400485	-.136076	1	0.882339	-2.432112	-0.058802
1	.093507	-1.518761	2.262914	1	-0.100738	-1.529274	2.223947
1	.489733	1.112661	2.336888	1	0.274882	1.102375	2.349715
1	1.449790	1.877106	-.016760	1	1.489949	1.908840	0.146973
1	-.141651	1.146869	-1.774520	1	-0.048225	1.253348	-1.818045
8	-1.332527	2.843257	-.114099	8	-1.508222	2.839309	-0.361639
1	-3.505539	1.670018	.548409	1	-3.150387	1.571101	1.189821
1	-3.875214	-.788960	.472575	1	-3.503231	-0.907924	1.083704
8	-2.136796	-2.506907	-.278991	8	-2.261508	-2.447256	-0.590516
1	-.480507	-1.142609	-1.840095	1	-0.402723	-1.212610	-1.927007
6	3.167683	-.590980	.088081	6	3.242150	-0.583403	0.077652
1	3.147980	-.632928	1.182503	1	3.302635	-0.641414	1.169804
1	3.497338	-1.581737	-.254708	1	3.537519	-1.567697	-0.308703
6	4.181935	.463020	-.373045	6	4.213280	0.477379	-0.451392
1	5.188596	.221405	-.014211	1	5.244858	0.225765	-0.181498
1	4.225698	.524672	-1.467675	1	4.165920	0.554292	-1.544537
1	3.927672	1.459860	.005296	1	3.994696	1.467736	-0.036546

9 Et = -614.8907833 (-615.0581986) Nimag = 0				**9**† Et = -614.8419005 (-615.0127482) Nimag = 1(-434.76)			
6	-.164427	-.780808	-.815123	6	-2.099703	-0.002459	-0.536122
6	1.174410	-1.127683	-.048838	6	-1.369117	1.149366	0.134992
6	2.090287	-.000142	-.603801	6	-0.974222	0.700030	1.405266
6	1.174609	1.127648	-.049059	6	-0.975208	-0.700794	1.407368
6	-.164387	.780735	-.815139	6	-1.372828	-1.153418	0.139724
6	.980120	.670399	1.389015	6	-3.613687	0.000643	-0.210740
6	.979541	-.670066	1.389088	6	0.424642	-0.705293	-1.069559
6	-1.371939	-1.486294	-.220964	6	1.431336	-1.460063	-0.291069
6	-2.506793	-.672571	.277640	6	2.264537	-0.670958	0.656798
6	-2.506726	.672692	.277677	6	2.263205	0.674114	0.657321
6	-1.371840	1.486325	-.220997	6	1.428306	1.461631	-0.290056
8	-1.416791	2.706665	-.153896	6	0.421214	0.704954	-1.067718
8	-1.416951	-2.706626	-.153768	1	-1.996064	-0.004907	-1.623936
6	3.543990	-.000219	-.136607	1	-1.549492	2.191533	-0.108999
1	2.076046	-.000222	-1.702892	1	-0.607681	1.331369	2.207232
1	1.490164	-2.161903	-.194633	1	-0.609345	-1.330210	2.211166

1	.778798	-1.330735	2.225999	1	-1.551903	-2.196060	-0.102963
1	.779842	1.331320	2.225836	1	-4.093538	0.884912	-0.644316
1	1.490488	2.161788	-.195155	1	-3.790401	0.003815	0.868121
1	-.075606	1.157431	-1.841464	1	-4.096159	-0.884529	-0.639520
1	-3.348583	1.243890	.662475	1	0.025745	-1.247576	-1.921846
1	-3.348704	-1.243703	.662416	8	1.593778	-2.670884	-0.410449
1	-.075581	-1.157578	-1.841419	1	2.913091	-1.250886	1.309064
1	4.069886	.884016	-.515696	1	2.910550	1.255000	1.309930
1	3.622325	-.000223	.954201	8	1.587584	2.672686	-0.409574
1	4.069790	-.884506	-.515705	1	0.023454	1.246610	-1.920990

10 Et = -973.759503 (-973.9460691) Nimag = 0				**10**† Et =-973.7095899(-973.8998407) Nimag = 1(-435.96)			
6	0.681678	-0.670746	1.388589	6	-1.774383	-0.000139	-0.501584
6	0.875960	-1.132968	-0.047896	6	-1.063468	1.156712	0.170852
6	-0.461286	-0.781509	-0.815575	6	-0.650082	0.701330	1.431823
6	-0.461253	0.781480	-0.815626	6	-0.650059	-0.701610	1.431820
6	0.875938	1.132910	-0.047842	6	-1.063694	-1.157003	0.170988
6	0.681606	0.670596	1.388614	6	0.712196	-0.705568	-1.068657
6	-1.669143	-1.486811	-0.218681	6	1.728414	-1.461756	-0.300317
6	-2.811135	-0.672673	0.260818	6	2.572626	-0.672492	0.636481
6	-2.811107	0.672810	0.260779	6	2.572454	0.672934	0.636486
6	-1.669159	1.486878	-0.218946	6	1.728031	1.461957	-0.300302
6	1.777080	-0.000006	-0.606131	6	0.711860	0.705473	-1.068587
8	-1.705141	2.705934	-0.136194	16	-3.615079	-0.000065	-.203296
8	-1.705406	-2.705886	-0.136347	1	-1.721430	-0.000169	-1.590086
16	3.547657	0.000000	-0.133262	1	-1.259667	2.193204	-0.078151
1	1.806158	0.000022	-1.701441	1	-0.276854	1.331291	2.231230
1	1.203345	-2.161015	-0.197964	1	-0.276780	-1.331560	2.231216
1	0.482885	-1.331646	2.225314	1	-1.259719	-2.193478	-0.078177
1	0.482762	1.331441	2.225370	1	0.303283	-1.248642	-1.915943
1	1.203320	2.160968	-0.197839	8	1.886734	-2.671942	-0.423190
1	-0.373421	1.158754	-1.841712	1	3.229685	-1.252120	1.280323
1	-3.657572	1.243566	0.635646	1	3.229366	1.252737	1.280322
1	-3.657635	-1.243373	0.635689	8	1.885981	2.672172	-0.423201
1	-0.373569	-1.158836	-1.841654	1	0.303239	1.248282	-1.916204
1	3.350508	-0.000035	1.202510	1	-3.554956	0.000620	1.145310

11 Et = -728.2134853 (-728.4159983) Nimag = 0				**11**† Et = -728.1631777 (-728.3687799) Nimag = 1(-433.71)			
6	0.448158	-0.769621	1.342176	6	1.563112	-0.073030	-0.457419
6	0.596041	-1.186212	-0.115396	6	0.752214	-1.242913	0.049880
6	-0.733228	-0.750660	-0.849467	6	0.354349	-0.917008	1.358165
6	-0.664399	0.808954	-0.796889	6	0.430325	0.469863	1.521615
6	0.691179	1.074091	-0.031139	6	0.885846	1.044078	0.324195
6	0.503222	0.568801	1.393575	6	-0.897729	0.829431	-0.992933

6	-1.965663	-1.419552	-0.261629	6	-1.887568	1.548126	-0.163963
6	-3.062777	-0.571083	0.263406	6	-2.789138	0.707572	0.670571
6	-3.003600	0.772332	0.306406	6	-2.852648	-0.628626	0.528890
6	-1.832071	1.548872	-0.163170	6	-2.027050	-1.353835	-0.474233
6	1.549186	-0.080338	-0.623119	6	-0.953560	-0.573229	-1.136498
8	-1.809639	2.765376	-0.041200	6	3.064892	-0.154259	-0.047008
8	-2.060983	-2.637471	-0.223288	1	1.534602	0.072546	-1.540493
6	2.991522	-0.203790	-0.133409	1	0.900805	-2.259425	-0.297480
6	3.850391	1.045847	-0.203277	1	-0.060543	-1.615119	2.076108
8	3.435097	-1.265076	0.260173	1	0.072233	1.024949	2.381412
1	1.587416	-0.024097	-1.722765	1	1.126518	2.094780	0.203312
1	0.882339	-2.219939	-0.299093	1	-0.442372	1.437697	-1.769181
1	0.241241	-1.454746	2.156842	8	-1.982678	2.772296	-0.152843
1	0.343175	1.205897	2.256777	1	-3.429363	1.248232	1.363471
1	1.047212	2.098110	-0.146820	1	-3.547618	-1.240836	1.098441
1	-0.570297	1.216219	-1.811264	8	-2.241293	-2.533779	-0.730604
1	-3.818291	1.367288	0.712854	1	-0.564958	-1.039684	-2.037514
1	-3.927979	-1.116283	0.633613	8	3.478634	-0.919802	0.794580
1	-0.677801	-1.094390	-1.889692	6	3.981917	0.789522	-0.805578
1	4.900886	0.779593	-0.069585	1	4.967215	0.800669	-0.335695
1	3.713640	1.577635	-1.152408	1	4.085249	0.447139	-1.843667
1	3.554896	1.736224	0.597649	1	3.571160	1.805189	-0.841888

12 Et = -764.1400915 (-764.3625643) Nimag = 0				**12**† Et = -764.0885005 (-764.3140489) Nimag = 1(-433.36)			
6	0.489528	-0.731727	1.339216	6	1.564270	-0.064492	-0.488028
6	0.630528	-1.163977	-0.115018	6	0.789374	-1.236877	0.073321
6	-0.711886	-0.762785	-0.843130	6	0.398335	-0.875387	1.370676
6	-0.674355	0.799032	-0.807163	6	0.457991	0.519077	1.493871
6	0.683309	1.100913	-0.060263	6	0.887075	1.067548	0.276305
6	0.519998	0.608206	1.372023	6	-0.902078	0.801641	-1.006513
6	-1.924420	-1.452466	-0.237584	6	-1.890937	1.528303	-0.178828
6	-3.038985	-0.622483	0.278718	6	-2.771844	0.696476	0.685328
6	-3.006823	0.722187	0.309024	6	-2.824305	-0.642825	0.570707
6	-1.852229	1.519202	-0.169280	6	-2.005963	-1.380349	-0.429266
6	1.552354	-0.042912	-0.646804	6	-0.953246	-0.602082	-1.125212
8	-1.853943	2.736076	-0.052582	6	3.051875	-0.117864	-0.113620
8	-1.988031	-2.671620	-0.178654	1	1.520279	0.049719	-1.572952
6	2.978770	-0.128292	-0.142494	1	0.942650	-2.259063	-0.253050
8	3.595058	1.079378	-0.179266	1	-0.001671	-1.556355	2.113158
8	3.542984	-1.139437	0.208846	1	0.102907	1.091792	2.343256
1	1.594418	-0.005862	-1.744777	1	1.128862	2.112202	0.118713
1	0.936370	-2.193707	-0.291272	1	-0.462659	1.398780	-1.800480
1	0.304462	-1.410830	2.164023	8	-1.998839	2.750468	-0.194077
1	0.360668	1.254003	2.228593	1	-3.407819	1.244839	1.376030
1	1.033767	2.123140	-0.192949	1	-3.505447	-1.249973	1.161959

1	-0.600591	1.197020	-1.826883	8	-2.211235	-2.567605	-0.657607
1	-3.832336	1.304116	0.712457	1	-0.563210	-1.085955	-2.016228
1	-3.891850	-1.181728	0.656488	8	3.709437	0.906726	-0.713035
1	-0.658143	-1.115804	-1.880439	8	3.600440	-0.930939	0.589917
1	4.509946	0.925091	0.124537	1	4.644404	0.825802	-0.444446

13 Et = -1035.170332 (-1035.355123) Nimag = 0				**13**† Et = -1035.118538 (-1035.3068541) Nimag = 1(-418.34)			
6	-1.658277	1.487408	-.213065	6	-1.750644	.000140	-.511388
6	-.452735	.782111	-.816838	6	-1.070123	1.160696	.184009
6	-.452747	-.782126	-.816818	6	-.670899	.702259	1.442853
6	-1.658276	-1.487386	-.212977	6	-.670971	-.703253	1.442458
6	-2.805065	-.672735	.253354	6	-1.070291	-1.160915	.183371
6	-2.805058	.672784	.253332	6	.709756	-.704398	-1.080615
6	.885075	1.133382	-.049896	6	1.717318	-1.461935	-.30036
6	1.762001	-.000005	-.622786	6	2.550902	-.672704	.645344
6	.885079	-1.133400	-.049904	6	2.550840	.672961	.645341
6	.699594	.669584	1.386865	6	1.717071	1.462155	-.300259
6	.699608	-.669617	1.386862	6	.709588	.704511	-1.080516
17	3.481174	-.000005	-.057198	17	-3.557336	.000103	-.137589
8	-1.687800	-2.705198	-.118628	1	-1.712939	.000480	-1.596507
8	-1.687706	2.705212	-.118581	1	-1.266707	2.195430	-.069994
1	1.816300	-.000001	-1.713553	1	-.314058	1.330906	2.250427
1	1.217622	-2.158839	-.205379	1	-.314179	-1.332404	2.249664
1	.515449	-1.332978	2.224243	1	-1.266916	-2.195464	-.071330
1	.515426	1.332937	2.224251	1	.298961	-1.249730	-1.925561
1	1.217618	2.158823	-.205358	8	1.876025	-2.671337	-.424141
1	-.372616	1.158066	-1.844144	1	3.201463	-1.252086	1.295847
1	-3.654110	1.243282	.622650	1	3.201395	1.252393	1.295804
1	-3.654125	-1.243212	.622684	8	1.875693	2.671570	-.424013
1	-.372668	-1.158107	-1.844119	1	.298671	1.249749	-1.925479

14 Et = -630.9205428 (-631.101355) Nimag = 0				**14**† Et = -630.8671985 (-631.0513755) Nimag = 1(-418.15)			
6	1.377796	-1.483467	-0.208790	6	2.104605	-0.011058	-0.539761
6	0.161341	-0.793465	-0.802560	6	1.375693	-1.167088	0.137587
6	0.149720	0.769314	-0.825996	6	0.988219	-0.721770	1.404135
6	1.345800	1.489933	-0.223983	6	0.992335	0.687542	1.417954
6	2.489920	0.690285	0.275894	6	1.383231	1.148265	0.158122
6	2.503376	-0.654922	0.285321	6	-0.420697	0.707049	-1.080752
6	-1.166720	-1.140377	-0.025531	6	-1.409023	1.469471	-0.286112
6	-2.098712	-0.024785	-0.612943	6	-2.233892	0.683550	0.670917
6	-1.196858	1.121619	-0.083790	6	-2.242483	-0.661843	0.667334
6	-0.994530	-0.643748	1.399833	6	-1.427504	-1.452908	-0.293763
6	-1.017436	0.698079	1.367622	6	-0.427149	-0.699237	-1.084004
7	-3.479330	0.065106	-0.177573	7	3.552107	-0.097655	-0.276361

8	1.374247	2.710193	-0.153558	1	1.992430	0.000059	-1.625274
8	1.436782	-2.703060	-0.138535	1	1.560336	-2.203881	-0.120483
1	-2.102849	-0.057372	-1.710066	1	0.624817	-1.354755	2.206330
1	-1.536782	2.141914	-0.260177	1	0.641352	1.307086	2.235985
1	-0.839058	1.380587	2.192001	1	1.560648	2.191984	-0.082668
1	-0.800850	-1.277606	2.259103	1	-0.008792	1.252345	-1.924945
1	-1.473399	-2.180512	-0.150250	8	-1.563309	2.681536	-0.402463
1	0.067237	-1.184404	-1.823239	1	-2.870261	1.265767	1.333037
1	3.352094	-1.214741	0.671795	1	-2.886418	-1.239513	1.326089
1	3.326737	1.272323	0.655427	8	-1.597934	-2.661595	-0.417204
1	0.075477	1.129778	-1.859351	1	-0.024229	-1.244967	-1.932126
1	-4.002008	-0.744874	-0.506435	1	3.718825	-0.055915	0.728431
1	-3.521708	0.051301	0.840479	1	4.016482	0.714002	-0.682454

15 Et = -667.8126125 (-667.9940374) Nimag = 0				**15**† Et = -667.7591846 (-667.9437432) Nimag = 1(-435.70)			
6	0.841249	-0.670159	1.344329	6	-1.881836	-0.001016	-0.566644
6	0.976229	-1.134687	-0.099453	6	-1.177053	1.161553	0.130142
6	-0.377337	-0.780815	-0.827023	6	-0.809150	0.700468	1.399851
6	-0.377031	0.780787	-0.826989	6	-0.808929	-0.702570	1.399708
6	0.976668	1.134059	-0.099419	6	-1.176990	-1.163550	0.130091
6	0.841372	0.669558	1.344332	6	0.631617	-0.703486	-1.078189
6	-1.567834	-1.485639	-0.192104	6	1.628965	-1.460312	-0.281933
6	-2.712756	-0.672375	0.280803	6	2.454282	-0.671574	0.671534
6	-2.712488	0.673198	0.280848	6	2.453442	0.673831	0.671634
6	-1.567258	1.486044	-0.192043	6	1.627113	1.461561	-0.281742
6	1.871013	-0.000508	-0.683822	6	0.630456	0.703516	-1.077866
8	-1.583650	2.702288	-0.078138	6	-3.321585	-0.000884	-0.245844
8	-1.584607	-2.701866	-0.078062	1	-1.787824	-0.000915	-1.654848
6	3.256753	-0.000545	-0.212879	1	-1.368907	2.198202	-0.121579
7	4.367774	0.000545	0.123733	1	-0.457150	1.328704	2.210000
1	1.880148	-0.000534	-1.780912	1	-0.456708	-1.330854	2.209729
1	1.301026	-2.162129	-0.259308	1	-1.368246	-2.200218	-0.121972
1	0.679964	-1.333642	2.186293	1	0.240439	-1.249350	-1.932245
1	0.680250	1.333079	2.186301	8	1.782838	-2.670715	-0.398037
1	1.301934	2.161357	-0.259239	1	3.096193	-1.251297	1.330182
1	-0.325155	1.156726	-1.856291	1	3.094614	1.254286	1.330356
1	-3.555941	1.244202	0.661792	8	1.779260	2.672157	-0.397828
1	-3.556434	-1.243069	0.661714	1	0.238773	1.248953	-1.931967
1	-0.325638	-1.156692	-1.856359	7	-4.461423	0.000819	-0.025027

16 Et = -690.0906904 (-690.2829441) Nimag = 0				**16**† Et = -690.035742 (-690.231504) Nimag = 1(-411.48)			
6	-0.530917	-0.775582	-0.812538	6	1.778399	-0.273321	-0.323210
6	0.713320	-1.305047	-0.000392	6	0.887626	-1.360079	0.269305
6	1.769357	-0.281357	-0.473387	6	0.458516	-0.903464	1.513011

6	0.978097	0.941861	0.086569	6	0.621446	0.496661	1.573946
6	-0.339999	0.775584	-0.765061	6	1.154905	0.946598	0.368504
6	0.671353	0.459738	1.494432	6	-0.579277	0.740900	-1.048465
6	0.518382	-0.869967	1.444623	6	-1.532787	1.592603	-0.303171
6	-1.841659	-1.339007	-0.286372	6	-2.512288	0.883425	0.563538
6	-2.897390	-0.400708	0.164049	6	-2.671855	-0.451756	0.514446
6	-2.735064	0.934391	0.197010	6	-1.880179	-1.306964	-0.410376
6	-1.483988	1.612462	-0.216880	6	-0.745299	-0.652489	-1.100571
8	-1.382880	2.827240	-0.120977	8	3.111841	-0.529749	0.106284
8	-2.032164	-2.545532	-0.238763	1	1.765474	-0.218458	-1.418151
8	3.026418	-0.547377	0.088942	1	0.974698	-2.403461	-0.011262
1	1.855108	-0.237782	-1.573235	1	-0.027525	-1.510120	2.269015
1	0.930236	-2.358890	-0.174177	1	0.280902	1.130288	2.385515
1	0.222496	-1.533280	2.249970	1	1.455182	1.970607	0.176531
1	0.530115	1.109804	2.351143	1	-0.036191	1.257151	-1.834802
1	1.417928	1.934969	-0.010308	8	-1.538794	2.816593	-0.390637
1	-0.148727	1.160195	-1.774562	1	-3.128163	1.518250	1.195915
1	-3.523348	1.596891	0.547260	1	-3.425457	-0.967931	1.104267
1	-3.823098	-0.871270	0.487487	8	-2.175351	-2.484422	-0.587689
1	-0.449448	-1.132369	-1.846708	1	-0.333974	-1.222568	-1.928395
6	4.035514	0.360828	-0.309356	6	4.067658	0.343445	-0.469306
1	4.975063	-0.007412	0.109908	1	5.048738	-0.009735	-0.142597
1	4.128288	0.408547	-1.406374	1	4.027378	0.320099	-1.569975
1	3.852352	1.376770	0.069803	1	3.936201	1.383148	-0.135638

17 Et = -780.0716469 (-780.2929738) Nimag = 0				**17**† Et = -780.0166751(-780.2410079) Nimag = 1(-422.59)			
6	0.544003	-0.670258	1.352157	6	-1.548499	-0.034037	-0.503901
6	0.683673	-1.136818	-0.092121	6	-0.885406	1.098932	0.264427
6	-0.667005	-0.782152	-0.825840	6	-0.487544	0.556475	1.490586
6	-0.666996	0.782202	-0.825800	6	-0.453823	-0.845642	1.387447
6	0.683696	1.136810	-0.092081	6	-0.837141	-1.221286	0.096858
6	0.544014	0.670205	1.352182	6	0.928527	-0.608786	-1.135545
6	-1.860557	-1.486894	-0.196031	6	1.955440	-1.403749	-0.417809
6	-3.010341	-0.672837	0.263226	6	2.773368	-0.674650	0.587700
6	-3.010329	0.672852	0.263271	6	2.744073	0.666532	0.694327
6	-1.860532	1.486920	-0.195933	6	1.890458	1.509290	-0.185077
6	1.553308	-0.000008	-0.659901	6	0.896006	0.794386	-1.021801
8	-1.875947	2.702311	-0.076007	7	-3.057171	-0.012647	-0.168666
8	-1.875977	-2.702289	-0.076148	1	-1.540113	0.057958	-1.587266
7	2.971053	-0.000015	-0.139117	1	-1.124158	2.140260	0.085766
8	3.505346	-1.091318	0.027923	1	-0.143016	1.132099	2.341927
8	3.505492	1.091289	0.027467	1	-0.085742	-1.522404	2.149676
1	1.656022	0.000023	-1.750332	1	-1.004065	-2.241041	-0.227609
1	1.020797	-2.157949	-0.254354	1	0.528671	-1.094380	-2.021314
1	0.388768	-1.334440	2.194471	8	2.138685	-2.595307	-0.637812

1	0.388785	1.334359	2.194518	1	3.436929	-1.289868	1.190310
1	1.020854	2.157932	-0.254291	1	3.382458	1.206680	1.389067
1	-0.612621	1.156438	-1.855815	8	2.018712	2.727832	-0.210161
1	-3.858129	1.243224	0.635462	1	0.469911	1.396044	-1.819899
1	-3.858151	-1.243219	0.635378	8	-3.520259	-0.863207	0.576974
1	-0.612614	-1.156330	-1.855875	8	-3.683817	0.890481	-0.711910

18 Et = -650.7870691 (-650.9764136) Nimag = 0				**18**† Et = -650.7310391 (-650.9240606) Nimag = 1 (-401.37)			
6	1.035397	-0.672023	1.371830	6	-2.096566	-0.000307	-0.553839
6	1.189737	-1.134038	-0.069533	6	-1.386641	1.161968	0.145515
6	-0.151740	-0.781799	-0.816319	6	-1.013966	0.706965	1.409237
6	-0.151737	0.781795	-0.816318	6	-1.014603	-0.708164	1.409360
6	1.189746	1.134037	-0.069545	6	-1.388232	-1.163093	0.146051
6	1.035415	0.672044	1.371824	6	0.426718	-0.701761	-1.092067
6	-1.354300	-1.486971	-0.208636	6	1.410358	-1.461014	-0.285817
6	-2.493098	-0.672705	0.278496	6	2.217946	-0.672489	0.683227
6	-2.493093	0.672710	0.278501	6	2.217612	0.673120	0.683474
6	-1.354294	1.486972	-0.208636	6	1.409665	1.461458	-0.285370
6	2.097730	-0.000007	-0.629512	6	0.425838	0.701901	-1.091451
8	-1.390465	2.705915	-0.123757	8	-3.503892	0.000740	-0.324248
8	-1.390473	-2.705914	-0.123749	1	-2.002026	-0.000584	-1.638769
8	3.432824	-0.000013	-0.197231	1	-1.566175	2.200559	-0.109678
1	2.142799	-0.000012	-1.723723	1	-0.669959	1.330480	2.227198
1	1.516350	-2.162309	-0.225280	1	-0.671066	-1.331852	2.227394
1	0.863463	-1.329075	2.218031	1	-1.567855	-2.201598	-0.109383
1	0.863497	1.329108	2.218019	1	0.018240	-1.249505	-1.936295
1	1.516360	2.162306	-0.225314	8	1.573269	-2.670829	-0.405297
1	-0.077001	1.156563	-1.844628	1	2.850630	-1.252243	1.350911
1	-3.337351	1.243508	0.658466	1	2.850007	1.252981	1.351339
1	-3.337359	-1.243500	0.658458	8	1.572011	2.671307	-0.404843
1	-0.077002	-1.156567	-1.844628	1	0.017512	1.249580	-1.935804
1	3.412579	-0.000009	0.775595	1	-3.639190	0.000931	0.638267

19 Et = 674.8056756 (-675.0000583) Nimag = 0				**19**† Et = -674.7493579 (-674.9477873) Nimag = (-393.4697)			
6	0.140923	0.782449	-0.816662	6	-2.072668	-.001194	-.550203
6	-1.197143	1.133028	-0.058730	6	-1.390897	1.163617	.158174
6	-2.080509	-0.000049	-0.620596	6	-1.027673	.707569	1.420828
6	-1.197134	-1.133120	-0.058728	6	-1.028662	-.707013	1.422363
6	0.140977	-0.782517	-0.816575	6	-1.393496	-1.165380	.161320
6	-1.034154	-0.669985	1.381357	6	.421624	-.701575	-1.099496
6	-1.034104	0.669882	1.381350	6	1.400584	-1.461328	-.287629
6	1.344100	1.487497	-0.209714	6	2.202490	-.672589	.685622
6	2.486567	0.672857	0.267191	6	2.202171	.673185	.685937
6	2.486613	-0.672634	0.267265	6	1.399612	1.461709	-.286809

6	1.344127	-1.487400	-0.209382	6	.420070	.701580	-1.098358
8	1.376981	-2.705709	-0.119735	9	-3.439445	.000881	-.248701
8	1.376566	2.705780	-0.119567	1	-1.997740	-.002713	-1.637980
9	-3.364495	-0.000055	-0.113299	1	-1.572776	2.200422	-.100292
1	-2.158155	-0.000051	-1.714979	1	-.694164	1.332289	2.241855
1	-1.529183	2.159153	-0.216149	1	-.695755	-1.330357	2.244689
1	-0.866489	1.332040	2.223514	1	-1.575023	-2.202554	-.095814
1	-0.866570	-1.332148	2.223523	1	.013823	-1.250382	-1.943570
1	-1.529151	-2.159249	0.216166	8	1.563419	-2.670813	-.407264
1	0.066948	-1.156538	-1.845351	1	2.831878	-1.252116	1.356528
1	3.333222	-1.243086	0.642321	1	2.831320	1.252779	1.357004
1	3.333126	1.243407	0.642212	8	1.561783	2.671170	-.406714
1	0.066760	1.156358	-1.845468	1	.012907	1.250365	-1.942787

Table S6. The B3LYP/6-31G* optimized geometries (in Cartesian coordinates), total electronic energies (in hartree/particle), and number of imaginary frequencies of substituted cyclopentadienes and quinone. The values in parenthesis implies single-point energies evaluated at the B3LYP/6-311+G**//B3LYP/6-31G* level. (**n**') indicate substituted cyclopentadiene.

1' Et =-602.7811806(-602.899291) Nimag = 0				**2'** Et = -2270.284222 (-2272.3669232) Nimag = 0			
6	-0.608435	-0.000116	-0.889142	6	-2.164874	0.728183	-0.386977
6	-1.434434	1.172213	-0.467830	6	-1.126807	1.174074	0.366969
6	-2.528765	0.728395	0.202434	6	-0.345927	-0.000014	0.853663
6	-2.528728	-0.728349	0.202693	6	-1.126820	-1.174081	0.366941
6	-1.434395	-1.172357	-0.467428	6	-2.164904	-0.728160	-0.386964
1	-0.335585	-0.000244	-1.954805	32	1.365119	-0.000001	-0.152437
14	1.082369	-0.000105	0.059650	1	-0.081819	-0.000030	1.917375
1	-1.161726	-2.206048	-0.648769	1	-0.857485	2.205258	0.565682
1	-3.292200	-1.346306	0.664416	1	-2.884361	1.345806	-0.914097
1	-1.161802	2.205832	-0.649612	1	-0.857511	-2.205273	0.565630
1	-3.292337	1.346483	0.663823	1	-2.884410	-1.345762	-0.914082
6	2.056065	-1.539591	-0.463876	1	2.196383	1.252750	0.219497
6	2.051444	1.545220	-0.455181	1	2.196592	-1.252512	0.219840
6	0.804986	-0.005403	1.927695	1	1.064780	-0.000230	-1.663659
1	1.763679	0.005184	2.460677				
1	0.232100	0.871623	2.246611				
1	0.252279	-0.895670	2.245487				
1	3.049844	-1.548641	0.000908				
1	1.545191	-2.462439	-0.165766				
1	2.201387	-1.575197	-1.550468				
1	3.047046	1.552182	0.005725				
1	2.192383	1.589953	-1.542011				
1	1.540148	2.464686	-0.147499				

3' Et = -219.5324457 (-219.5925372) Nimag = 0			
6	-.134194	1.180499	.154501
6	.778748	-.000123	.349830
6	-.134495	-1.180554	.154453
6	-1.369548	-.732631	-.160443
6	-1.369370	.732905	-.160382
1	1.178280	-.000412	1.394295
5	2.166915	-.000054	-.379733
1	.190710	2.211656	.232469
1	-2.236477	1.346955	-.381105
1	.190031	-2.211806	.232676
1	-2.236812	-1.346501	-.381068
1	2.726149	-1.031175	-.613682
1	2.726700	1.030977	-.612674

4' Et = -536.0439888 (-536.1270914) Nimag = 0			
6	.235276	.000000	.678611
1	.521655	.000002	1.736977
6	-.612281	-1.177376	.288913
1	-.316355	-2.209185	.440262
6	-1.749966	-.731556	-.290732
1	-2.546480	-1.346794	-.696079
6	-.612281	1.177376	.288910
1	-.316354	2.209186	.440257
6	-1.749969	.731555	-.290729
1	-2.546485	1.346792	-.696073
15	1.810103	.000000	-.394140
1	2.493904	1.032097	.318458
1	2.493905	-1.032094	.318462

5' Et = -351.353873 (-351.4507471) Nimag = 0			
6	-1.162748	-1.177462	-.290453
6	-.268460	.000032	-.616797
6	-1.162686	1.177511	-.290067
6	-2.366388	.734465	.124825
6	-2.366230	-.734462	.125124
6	1.154087	-.000043	.040965
6	1.043710	-.003044	1.577032
6	1.931142	-1.248933	-.420204
6	1.929124	1.251911	-.415456
1	-.101274	.000296	-1.709772
1	-.866703	-2.213103	-.409847
1	-3.215759	-1.348976	.406238
1	-.866482	2.213118	-.409323
1	-3.216034	1.348917	.405728
1	2.040808	.001547	2.034365
1	.502745	.878460	1.937403
1	.512217	-.891376	1.934721
1	2.951667	-1.233330	-.018519
1	1.457084	-2.174321	-.075961
1	2.005665	-1.293439	-1.514098
1	2.952037	1.232748	-.020059
1	1.997091	1.304748	-1.509407
1	1.457634	2.174864	-.061282

6' Et = -307.4164566(-307.506418) Nimag = 0			
6	.578767	-1.180505	.267727
6	-.307901	-.000211	.579388
6	.578352	1.180426	.267876
6	1.749931	.732835	-.236025
6	1.750235	-.732437	-.236003
1	-.734639	-.000366	1.588024
6	-1.467709	-.000176	-.427651
1	.266712	-2.211130	.387986
1	2.576436	-1.346107	-.579761
1	.265939	2.210928	.388252
1	2.575872	1.346856	-.579780
8	-2.638539	.000082	-.126320
1	-1.132055	-.000429	-1.486037

7' Et = -272.7236322 (-272.7996242) Nimag = 0			
6	-0.150478	0.000019	-0.851119
1	-0.063929	0.000038	-1.952152
6	0.625602	-1.177875	-0.309701
1	0.351783	-2.211140	-0.495139
6	1.679559	-0.735445	0.405770
1	2.423716	-1.348478	0.904647
6	0.625612	1.177887	-0.309659
1	0.351800	2.211160	-0.495058
6	1.679568	0.735422	0.405792
1	2.423731	1.348432	0.904689
6	-1.662811	0.000019	-0.514918
1	-2.116285	0.874668	-0.997477
1	-2.116297	-0.874595	-0.997526
6	-1.977064	-0.000023	0.999003
1	-2.557170	0.881696	1.290801
1	-2.557640	-0.881482	1.290653
1	-1.059630	-0.000318	1.595550

8' Et = -194.101061(-194.156098) Nimag = 0			
6	1.184388	.282257	.000000
6	.547814	-1.083887	.000000
6	-.793759	-.944831	.000000
6	-1.134665	.485268	.000000
6	.000000	1.214368	.000000
1	1.830476	.436458	.878061
1	1.830476	.436458	-.878061
1	.081157	2.295398	.000000
1	-2.148598	.872496	.000000
1	1.107848	-2.012098	.000000
1	-1.524025	-1.747769	.000000

9' Et = -233.4149779 (-233.480406) Nimag = 0			
6	0.210807	-1.178242	0.182623
6	-0.696614	-0.000053	0.452099
6	0.210757	1.178216	0.182827
6	1.432934	0.735416	-0.173972
6	1.433073	-0.735326	-0.173726
1	-0.976474	-0.000164	1.520018
6	-1.994904	-0.000006	-0.378385
1	-0.108896	-2.211105	0.270917
1	2.293380	-1.348205	-0.423882
1	-0.109017	2.211046	0.271243
1	2.293147	1.348372	-0.424258
1	-2.601201	-0.885468	-0.156242
1	-2.600378	0.886303	-0.157389
1	-1.766876	-0.000802	-1.449206

10' Et = -592.2821052 (-592.3666809) Nimag = 0			
6	-0.608196	1.193681	0.208489
6	0.253125	0.025775	0.613414
6	-0.597787	-1.170654	0.262718
6	-1.770379	-0.739413	-0.241103
6	-1.777718	0.731711	-0.275113
1	0.484972	0.043966	1.686281
16	1.867228	-0.082531	-0.302913
1	-0.297461	2.227010	0.307018
1	-2.603608	1.332086	-0.642018
1	-0.280343	-2.193960	0.422139
1	-2.593919	-1.364031	-0.570821
1	2.420440	1.028813	0.233574

11' Et = -346.7402073(-346.8406111) Nimag = 0			
6	-0.804187	-1.176151	0.401642
6	-0.003599	-0.413104	-0.632328
6	-0.895419	0.763575	-0.939668
6	-2.016084	0.685591	-0.190690
6	-1.958096	-0.519343	0.645118
1	0.187776	-1.029740	-1.520216
6	1.389908	-0.047828	-0.067336

12' Et = -382.6635037 (-382.7836801) Nimag = 0			
6	-.780606	-1.220468	.002760
6	-.021844	-.041453	.585153
6	-.981497	1.107826	.412579
6	-2.122664	.646485	-.133514
6	-1.997126	-.797013	-.389577
6	1.354635	.174791	-.026156
1	.151576	-.232774	1.658493

1	-0.461364	-2.099023	0.854404	1	-.372768	-2.221738	-.048419
1	-2.736602	-0.825954	1.336135	1	-2.777314	-1.412416	-.825357
1	-0.643974	1.534925	-1.658787	1	-.745411	2.127111	.690146
1	-2.843498	1.387737	-0.199095	1	-3.006003	1.233621	-.361569
8	2.378977	-0.649915	-0.432715	8	2.124038	-.936735	.108317
6	1.458201	1.067650	0.958677	8	1.758686	1.187175	-.548337
1	0.573037	1.078726	1.601271	1	2.982738	-.718338	-.300608
1	2.366741	0.956318	1.555062				
1	1.501728	2.033986	0.440466				

13' Et = -653.6919636 (-653.7744958) Nimag = 0				**14'** Et = -249.4349114(-249.5146512) Nimag = 0			
				6	-.190972	1.180770	.134830
6	1.776071	-0.739309	-0.239845	6	.719982	-.000003	.397333
6	0.590050	-1.187659	0.207047	6	-.191037	-1.180794	.135021
6	-0.259462	0.000000	0.583071	6	-1.429681	-.737010	-.145097
6	0.590050	1.187659	0.207047	6	-1.429765	.737006	-.144655
6	1.776071	0.739310	-0.239846	1	.945155	.000046	1.486919
17	-1.887798	0.000000	-0.252743	7	1.931726	-.000116	-.438888
1	-0.498126	0.000000	1.652855	1	.135291	2.212978	.203197
1	0.261624	-2.212356	0.324687	1	-2.304155	1.348919	-.342678
1	2.615385	-1.349906	-0.555222	1	.135239	-2.212995	.203417
1	0.261624	2.212356	0.324688	1	-2.304021	-1.348886	-.343437
1	2.615385	1.349906	-0.555223	1	2.500119	-.812381	-.199075
				1	2.499128	.813320	-.200716

15' Et = -286.3352393(-286.4144668) Nimag = 0				**16'** Et =-308.6074871 (-308.6980455) Nimag = 0			
7	-2.727916	.000463	-.504174	6	-.431319	1.147443	.105001
6	-1.674353	-.000898	-.016468	6	.231902	-.198381	.364523
6	-.344128	-.000581	.604082	6	-.890157	-1.181991	.116763
6	.513797	-1.190089	.203095	6	-2.025461	-.504984	-.123716
6	1.678537	-.734886	-.292868	6	-1.739435	.945430	-.129942
6	1.677872	.735951	-.292508	1	.488170	-.237653	1.444988
6	.512717	1.189879	.203652	8	1.382770	-.518509	-.398329
1	-.486476	-.000912	1.697678	1	.079448	2.100580	.171706
1	.193157	2.216491	.329613	1	-2.489518	1.712196	-.297069
1	2.502847	1.348527	-.639934	1	-.750543	-2.254729	.171557
1	2.504055	-1.346547	-.640616	1	-3.008302	-.933355	-.291086
1	.195174	-2.217053	.328574	6	2.531713	.217436	-.030477
				1	3.360197	-.171060	-.628669
				1	2.424097	1.293070	-.235859
				1	2.770827	.089315	1.038151

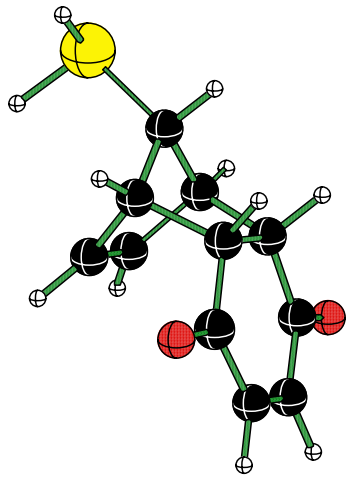
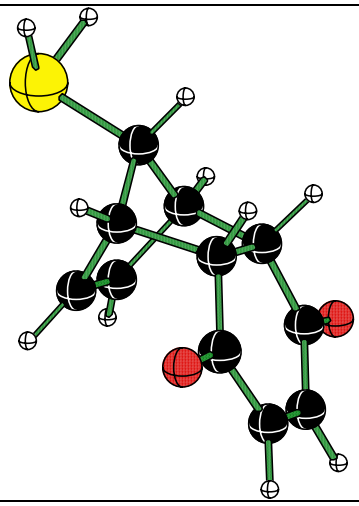
17' Et = -398.5924439(-398.7112019) Nimag = 0			
6	-0.770812	1.224114	0.023693
6	0.013057	0.057594	0.585533
6	-0.883402	-1.132022	0.370219
6	-2.049075	-0.691199	-0.134941
6	-1.978056	0.769233	-0.352719
1	0.222542	0.215091	1.652847
7	1.400842	-0.052809	-0.032143
1	-0.382052	2.232564	-0.012212
1	-2.786791	1.366279	-0.759826
1	-0.605571	-2.145572	0.624568
1	-2.918097	-1.299636	-0.360625
8	2.093552	0.957710	0.024481
8	1.740673	-1.128382	-0.508288

18' Et = -269.2986506(-269.3874521) Nimag = 0			
6	-0.162605	1.187855	0.109887
6	0.736211	-0.008211	0.375570
6	-0.181716	-1.182408	0.123398
6	-1.421685	-0.727766	-0.125553
6	-1.410494	0.750700	-0.132189
1	0.979959	-0.006093	1.457928
8	1.930666	-0.101830	-0.393936
1	0.172637	2.217799	0.171822
1	-2.287400	1.365833	-0.308250
1	0.152090	-2.211163	0.183020
1	-2.306942	-1.331140	-0.298161
1	2.486069	0.658374	-0.161544

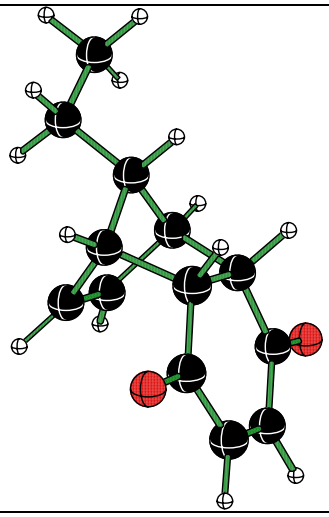
19' Et =-293.3210101 (-293.4142663) Nimag = 0			
6	-.153408	1.189213	.106332
6	.743851	-.000001	.371266
6	-.153408	-1.189213	.106329
6	-1.399280	-.741340	-.119693
6	-1.399278	.741340	-.119698
1	1.029835	-.000002	1.437327
9	1.925723	.000000	-.363309
1	.187614	2.215660	.163729
1	-2.283717	1.348817	-.281111
1	.187614	-2.215660	.163724
1	-2.283719	-1.348816	-.281105

Quinone(q) Et = -381.4516858(-381.5616335) Nimag = 0			
6	-1.268891	-.671764	.000000
6	.000000	-1.445180	.000000
6	1.268884	-.671724	.000000
6	1.268891	.671764	.000000
6	.000000	1.445180	.000000
6	-1.268885	.671724	.000000
8	.000000	-2.670345	.000000
8	.000001	2.670345	.000000
1	2.183088	-1.258551	.000000
1	2.183193	1.258439	.000000
1	-2.183089	1.258549	.000000
1	-2.183194	-1.258437	.000000

Table S8. The B3LYP/6-31G* optimized geometries (in Cartesian coordinates), total electronic energies (in hartree/particle), of different rotamers of the substituent attached to the C7 position of the cycloadduct. The values in parenthesis implies single-point energies evaluated at the B3LYP/6-311+G**//B3LYP/6-31G* level.

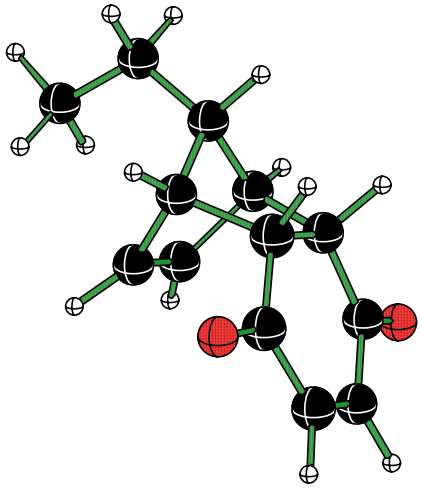
	
4 Et = -917.5145057 (-917.6999361) Nimag = 0 ΔE_{rel} = 0.0 kcal mol^{-1}	**4'** Et = -917.5141908 (-917.6996178) Nimag = 0 ΔE_{rel} = 0.19
6 -1.776682 -0.008789 -0.596146	6 -1.775037 0.000020 -0.601672
6 -0.870381 1.121254 -0.037898	6 -0.864497 1.128269 -0.043963
6 -0.664171 0.654287 1.395416	6 -0.663185 0.669824 1.392664
6 -0.659489 -0.685972 1.388886	6 -0.663207 -0.669914 1.392629
6 -0.859654 -1.138240 -0.050744	6 -0.864516 -1.128274 -0.044028
6 0.476923 -0.778292 -0.819180	6 0.472429 -0.779945 -0.818648
6 1.688889 -1.478784 -0.225790	6 1.680712 -1.486147 -0.224713
6 2.822838 -0.660359 0.266444	6 2.815814 -0.672662 0.273047
6 2.815630 0.684931 0.269902	6 2.815815 0.672657 0.273060
6 1.674011 1.493697 -0.220659	6 1.680734 1.486154 -0.224725
6 0.468522 0.782890 -0.813845	6 0.472429 0.779965 -0.818628
15 -3.590146 -0.103832 -0.101749	15 -3.546067 0.000016 0.053868
1 -1.784995 -0.011464 -1.694934	1 -1.787745 0.000053 -1.697633
1 -1.193199 2.153215 -0.177319	1 -1.178170 2.162638 -0.189578
1 -0.458986 1.311774 2.233409	1 -0.463065 1.331867 2.227962
1 -0.448832 -1.351133 2.219434	1 -0.463103 -1.332009 2.227889
1 -1.172195 -2.171556 -0.202915	1 -1.178204 -2.162629 -0.189702
1 0.389165 -1.153481 -1.846001	1 0.379999 -1.158596 -1.843651
8 1.735274 -2.698420 -0.154207	8 1.722913 -2.706191 -0.157365
1 3.669234 -1.227943 0.646410	1 3.657355 -1.243839 0.658340
1 3.655977 1.259614 0.652647	1 3.657358 1.243824 0.658365
8 1.709281 2.713794 -0.147717	8 1.722932 2.706197 -0.157347
1 0.372351 1.164235 -1.837592	1 0.379959 1.158646 -1.843614
1 -3.475856 0.369698 1.233396	1 -4.012536 1.031914 -0.814404

1	-3.955533	1.171785	-0.623223	1	-4.012545	-1.031842	-0.814446



8 Et = -654.2037292 (-654.3817009)
Nimag = 0 ΔE_{rel} = 0.0 kcal mol^{-1}

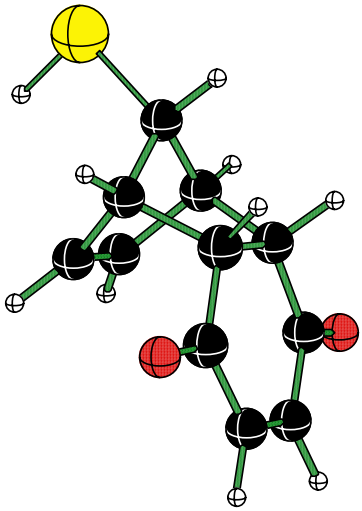
6	1.755195	-.346844	-.451230
6	.649948	-1.333597	.020305
6	.439893	-.879628	1.457431
6	.639003	.445393	1.494429
6	.984122	.896049	.082846
6	-.344380	.766431	-.765945
6	-1.466076	1.631859	-.216841
6	-2.736684	.987399	.193509
6	-2.936569	-.342260	.152442
6	-1.907218	-1.305953	-.306592
6	-.574757	-.776777	-.810388
1	1.807217	-.322571	-1.549835
1	.817407	-2.400485	-.136076
1	.093507	-1.518761	2.262914
1	.489733	1.112661	2.336888
1	1.449790	1.877106	-.016760
1	-.141651	1.146869	-1.774520
8	-1.332527	2.843257	-.114099
1	-3.505539	1.670018	.548409
1	-3.875214	-.788960	.472575
8	-2.136796	-2.506907	-.278991
1	-.480507	-1.142609	-1.840095
6	3.167683	-.590980	.088081
1	3.147980	-.632928	1.182503
1	3.497338	-1.581737	-.254708
6	4.181935	.463020	-.373045
1	5.188596	.221405	-.014211

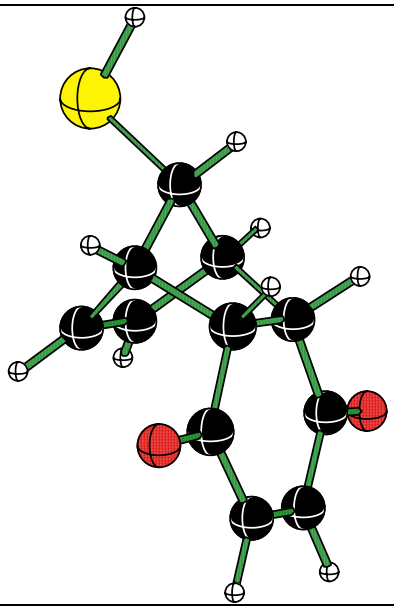


8' Et = -654.1987757 (-654.3765559)
Nimag = 0 ΔE_{rel} = 3.1

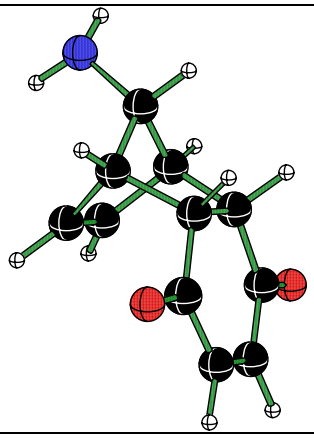
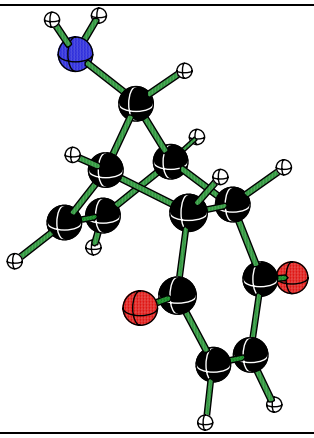
6	1.707518	-0.000338	-0.888865
6	0.848317	-1.138448	-0.235983
6	0.796680	-0.676942	1.211132
6	0.796850	0.676701	1.211061
6	0.848602	1.138050	-0.236099
6	-0.545993	0.775064	-0.845268
6	-1.664930	1.479519	-0.137974
6	-2.761976	0.668011	0.421849
6	-2.762147	-0.667429	0.421918
6	-1.665298	-1.479275	-0.137800
6	-0.546189	-0.775179	-0.845183
1	1.564616	-0.000388	-2.002678
1	1.164914	-2.180871	-0.411691
1	0.756568	-1.370976	2.047484
1	0.756920	1.370817	2.047354
1	1.165461	2.180374	-0.411914
1	-0.567047	1.133369	-1.912611
8	-1.688418	2.714035	-0.051574
1	-3.596691	1.246782	0.855565
1	-3.597014	-1.245942	0.855688
8	-1.689082	-2.713774	-0.051239
1	-0.567343	-1.133598	-1.912486
6	3.192451	-0.000550	-0.644373
1	3.620871	-0.905855	-1.157049
1	3.621364	0.903701	-1.158501
6	3.651273	0.000509	0.789087
1	4.768251	0.000493	0.827411

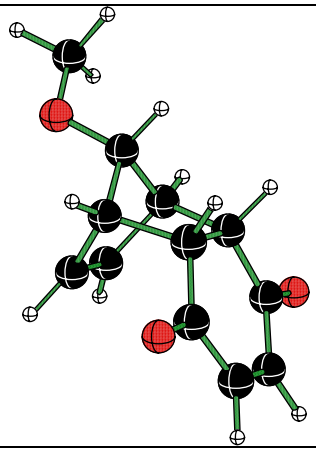
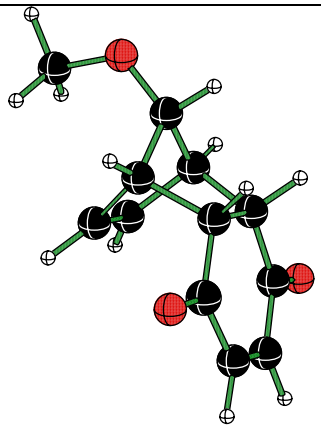
1	4.225698	.524672	-1.467675	1	3.279117	0.906572	1.326768
1	3.927672	1.459860	.005296	1	3.279062	-0.904714	1.328143



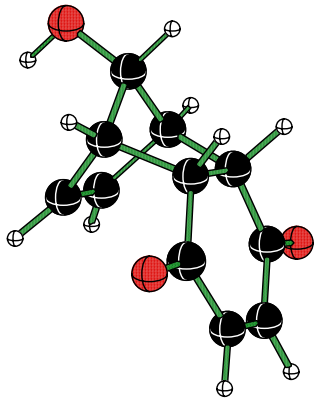
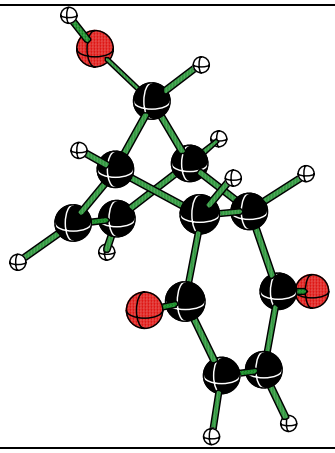


10 Et = -973.759503 (-973.9460691) Nimag = 0 ΔE_{rel} = 0.0				**10'** Et = -973.7576147 (-973.9444129) Nimag = 0 ΔE_{rel} = 1.18 kcal mol^{-1}			
6	0.681678	-0.670746	1.388589	6	0.700662	-0.670381	1.372411
6	0.875960	-1.132968	-0.047896	6	0.871779	-1.131530	-0.067980
6	-0.461286	-0.781509	-0.815575	6	-0.471059	-0.781431	-0.825160
6	-0.461253	0.781480	-0.815626	6	-0.471016	0.781243	-0.825346
6	0.875938	1.132910	-0.047842	6	0.871918	1.131485	-0.068391
6	0.681606	0.670596	1.388614	6	0.700818	0.670877	1.372188
6	-1.669143	-1.486811	-0.218681	6	-1.672866	-1.487203	-0.216651
6	-2.811135	-0.672673	0.260818	6	-2.798710	-0.672633	0.298972
6	-2.811107	0.672810	0.260779	6	-2.798654	0.672806	0.298871
6	-1.669159	1.486878	-0.218946	6	-1.672703	1.487206	-0.216790
6	1.777080	-0.000006	-0.606131	6	1.771238	-0.000151	-0.622116
8	-1.705141	2.705934	-0.136194	8	-1.716467	2.707174	-0.153597
8	-1.705406	-2.705886	-0.136347	8	-1.716821	-2.707167	-0.153467
16	3.547657	0.000000	-0.133262	16	3.497927	0.000008	0.041869
1	1.806158	0.000022	-1.701441	1	1.828973	-0.000315	-1.714612
1	1.203345	-2.161015	-0.197964	1	1.201039	-2.158588	-0.221016
1	0.482885	-1.331646	2.225314	1	0.518529	-1.331403	2.212512
1	0.482762	1.331441	2.225370	1	0.518808	1.332233	2.212052
1	1.203320	2.160968	-0.197839	1	1.201241	2.158465	-0.221804
1	-0.373421	1.158754	-1.841712	1	-0.392938	1.158785	-1.852113
1	-3.657572	1.243566	0.635646	1	-3.635527	1.243612	0.694727
1	-3.657635	-1.243373	0.635689	1	-3.635635	-1.243308	0.694906
1	-0.373569	-1.158836	-1.841654	1	-0.392822	-1.159227	-1.851821
1	3.350508	-0.000035	1.202510	1	4.099364	-0.002170	-1.166268

	
14 Et = -630.9205428 (-631.101355) Nimag = 0 ΔE_{rel} = 0.0	**14'** Et = -630.9159553 (-631.0975889) Nimag = 0 ΔE_{rel} = 2.87 kcal mol^{-1}
6 1.377796 -1.483467 -0.208790	6 -1.357752 1.486883 -0.221103
6 0.161341 -0.793465 -0.802560	6 -0.148610 0.781209 -0.811725
6 0.149720 0.769314 -0.825996	6 -0.148851 -0.781629 -0.811323
6 1.345800 1.489933 -0.223983	6 -1.358376 -1.486677 -0.220880
6 2.489920 0.690285 0.275894	6 -2.496950 -0.672251 0.267470
6 2.503376 -0.654922 0.285321	6 -2.496778 0.673016 0.267127
6 -1.166720 -1.140377 -0.025531	6 1.183404 1.126995 -0.037293
6 -2.098712 -0.024785 -0.612943	6 2.092745 -0.000533 -0.597066
6 -1.196858 1.121619 -0.083790	6 1.182937 -1.127332 -0.036415
6 -0.994530 -0.643748 1.399833	6 0.987861 0.669394 1.399697
6 -1.017436 0.698079 1.367622	6 0.987574 -0.668545 1.400178
7 -3.479330 0.065106 -0.177573	7 3.443121 -0.000636 -0.054443
8 1.374247 2.710193 -0.153558	8 -1.402915 -2.706821 -0.152105
8 1.436782 -2.703060 -0.138535	8 -1.401599 2.707034 -0.152167
1 -2.102849 -0.057372 -1.710066	1 2.066017 -0.000955 -1.702319
1 -1.536782 2.141914 -0.260177	1 1.503322 -2.160480 -0.183156
1 -0.839058 1.380587 2.192001	1 0.800466 -1.331481 2.237865
1 -0.800850 -1.277606 2.259103	1 0.801031 1.333028 2.236886
1 -1.473399 -2.180512 -0.150250	1 1.504062 2.159938 -0.184861
1 0.067237 -1.184404 -1.823239	1 -0.059582 1.155263 -1.839192
1 3.352094 -1.214741 0.671795	1 -3.341860 1.244182 0.644794
1 3.326737 1.272323 0.655427	1 -3.342182 -1.242999 0.645426
1 0.075477 1.129778 -1.859351	1 -0.059480 -1.156258 -1.838543
1 -4.002008 -0.744874 -0.506435	1 3.949758 -0.815325 -0.397331
1 -3.521708 0.051301 0.840479	1 3.949482 0.814661 -0.396281

	
16 Et = -690.0906904 (-690.2829441) Nimag = 0 ΔE_{rel} = 0.0	**16'** Et =-690.0862682(-690.2779367) Nimag = 0 ΔE_{rel} = 2.77 kcal mol^{-1}

6	-0.530917	-0.775582	-0.812538	6	-0.507820	-0.782487	-0.844210
6	0.713320	-1.305047	-0.000392	6	0.879177	-1.134816	-0.174208
6	1.769357	-0.281357	-0.473387	6	1.729009	-0.000144	-0.827496
6	0.978097	0.941861	0.086569	6	0.879330	1.134630	-0.174208
6	-0.339999	0.775584	-0.765061	6	-0.507738	0.782420	-0.844239
6	0.671353	0.459738	1.494432	6	0.792685	0.670935	1.267696
6	0.518382	-0.869967	1.444623	6	0.792603	-0.671111	1.267706
6	-1.841659	-1.339007	-0.286372	6	-1.669597	-1.486537	-0.160931
6	-2.897390	-0.400708	0.164049	6	-2.778075	-0.672492	0.391762
6	-2.735064	0.934391	0.197010	6	-2.778023	0.672801	0.391690
6	-1.483988	1.612462	-0.216880	6	-1.669415	1.486666	-0.160998
8	-1.382880	2.827240	-0.120977	8	-1.699400	2.705523	-0.071331
8	-2.032164	-2.545532	-0.238763	8	-1.699784	-2.705386	-0.071242
8	3.026418	-0.547377	0.088942	8	3.123622	-0.000251	-0.687464
1	1.855108	-0.237782	-1.573235	1	1.597692	-0.000129	-1.915599
1	0.930236	-2.358890	-0.174177	1	1.189669	-2.165197	-0.349554
1	0.222496	-1.533280	2.249970	1	0.662484	-1.330697	2.119323
1	0.530115	1.109804	2.351143	1	0.662674	1.330536	2.119317
1	1.417928	1.934969	-0.010308	1	1.189819	2.165006	-0.349560
1	-0.148727	1.160195	-1.774562	1	-0.499117	1.158636	-1.874508
1	-3.523348	1.596891	0.547260	1	-3.598098	1.243800	0.821120
1	-3.823098	-0.871270	0.487487	1	-3.598188	-1.243386	0.821259
1	-0.449448	-1.132369	-1.846708	1	-0.499293	-1.158724	-1.874473
6	4.035514	0.360828	-0.309356	6	3.730229	0.000166	0.593293
1	4.975063	-0.007412	0.109908	1	4.807365	0.000251	0.403205
1	4.128288	0.408547	-1.406374	1	3.467530	0.888991	1.182040
1	3.852352	1.376770	0.069803	1	3.467776	-0.888364	1.182587

	
18 Et = -650.7870691 (-650.9764136) Nimag = 0 ΔE_{rel} = 0.0	**18'** Et = -650.7820579 (-650.9723987) Nimag = 0 ΔE_{rel} = 3.14
6 1.035397 -0.672023 1.371830	6 1.003236 -.648439 1.403681
6 1.189737 -1.134038 -0.069533	6 1.179563 -1.135138 -.025373
6 -0.151740 -0.781799 -0.816319	6 -.147333 -.790023 -.805531
6 -0.151737 0.781795 -0.816318	6 -.140289 .774029 -.821816
6 1.189746 1.134037 -0.069545	6 1.200121 1.125229 -.067301
6 1.035415 0.672044 1.371824	6 1.019487 .690423 1.379800
6 -1.354300 -1.486971 -0.208636	6 -1.360652 -1.486065 -.211427
6 -2.493098 -0.672705 0.278496	6 -2.492777 -.662863 .275519
6 -2.493093 0.672710 0.278501	6 -2.484033 .682454 .269952
6 -1.354294 1.486972 -0.208636	6 -1.340709 1.488309 -.221365
6 2.097730 -0.000007 -0.629512	6 2.091101 -.015096 -.606535
8 -1.390465 2.705915 -0.123757	8 -1.373534 2.708037 -.147888
8 -1.390473 -2.705914 -0.123749	8 -1.410733 -2.705566 -.137822
8 3.432824 -0.000013 -0.197231	8 3.400421 .069958 -.092816
1 2.142799 -0.000012 -1.723723	1 2.108234 -.038629 -1.708570
1 1.516350 -2.162309 -0.225280	1 1.493394 -2.172392 -.159228
1 0.863463 -1.329075 2.218031	1 .819619 -1.292893 2.256532
1 0.863497 1.329108 2.218019	1 .848915 1.369834 2.207647
1 1.516360 2.162306 -0.225314	1 1.540371 2.146532 -.237766
1 -0.077001 1.156563 -1.844628	1 -.064857 1.137664 -1.854066
1 -3.337351 1.243508 0.658466	1 -3.324808 1.260125 .647259
1 -3.337359 -1.243500 0.658458	1 -3.341181 -1.226605 .656798
1 -0.077002 -1.156567 -1.844628	1 -.056708 -1.174678 -1.829033
1 3.412579 -0.000009 0.775595	1 3.881492 -.725302 -.368992