Supporting Information

First-Principles Anharmonic Quantum Calculations for Peptide Spectroscopy: VSCF Calculations and Comparison with Experiments

Tapta Kanchan Roy, [$±] *Rahul Sharma*[#] *and R. Benny Gerber**[$§]

[$]Institute of Chemistry, The Hebrew University of Jerusalem, 91904 (Israel)

[#]Department of Chemistry, Indian Institute of Technology, Roorkee, Uttarakhand 247667 (India)

[§]Department of Chemistry, University of California Irvine, CA 92697 (USA) and Department of Chemistry, University of Helsinki, PO Box 55, 00014 Helsinki (Finland)

[±]Department of Chemistry, Central University of Rajasthan, Rajasthan 305817, India

Contents:

Pair-wise coupling and VSCF-PT2 approximation

VSCF potential can be written as a sum of one-mode (diagonal approximation) and pair-wise coupling in terms of normal coordinate (Q),

$$V\left(Q_{1,\ldots,}Q_N\right) = \sum_{i=1}^{N} V_i^{diag}(Q_i) + \sum_{j}\sum_{i>j}^{N} V_{ij}^{2coup}(Q_i,Q_j) \quad . \qquad (1)$$

This type of potential needs multi-dimensional grid point calculations and the number of grid points increases rapidly with the dimensionality of the potential and the vibrational modes. If *NG* is the number of grid points along a normal mode and *NV* is the number of vibrational modes then the number of total grid points (*NP*) is

$$NP = [NV \times NG] + \frac{[NV(NV\text{ - }1) \times NG^2]}{2} \quad . \qquad (2)$$

The PT2 correction on to of VSCF is described by the following equation:

$$E_n^{PT2} = E_n^{VSCF} + \sum_{m \neq n} \frac{\left|\left\langle \prod_{j=1}^{N} \psi_j^{(n)}(Q_j) \middle| \Delta V \middle| \prod_{j=1}^{N} \psi_j^{(m)}(Q_j) \right\rangle\right|^2}{E_n^{(0)} - E_m^{(0)}}, \qquad (3)$$

where E_n^{PT2} is the correlation corrected energy of the state *n*.

Table S1. Comparisons of frequencies and intensities of experimental and computed vibrational frequencies and intensities of C5 conformer of NATA (local minima). % error is calculated for VSCF-PT2 against experimental frequencies.

Mode description	Exp. Freq.	Exp. intensity	HO (HF)	VSCF-PT2	Intensity	% error
NH_2 str	3538	1.0	3942	3537	0.80	0.03
Indole NH str	3523	0.85	3911	3568	1.0	1.28
φ-amide NH str.	3430	0.80	3869	3424	0.83	0.17
NH_2 str	3417	0.53	3802	3428	0.50	0.32
Pyrole CH str	--	--	3407	3127	0.02	--
Phenyl CH str.	3074	0.97	3367	3071	0.25	0.10
Phenyl CH str.	3059	0.57	3356	3054	0.14	0.16
Phenyl CH str.	--	--	3344	3050	0.13	--
Phenyl CH str.	--	--	3334	3041	0.01	--
Alkyl CH str.	3004	0.35	3293	3002	0.19	0.07
Alkyl CH str.	--	--	3287	2993	0.08	--
Alkyl CH str.	--	--	3269	2902	0.12	--
Alkyl CH str.	2956	0.24	3255	2966	0.11	0.51
Alkyl CH str.		--	3202	2917	0.12	--
Alkyl CH str.	2933	0.43	3201	2889	0.24	1.5
Avg. % error						**0.46**

Table S2: Comparisons frequencies and intensities of experimental and computed vibrational frequencies of C7 conformer of NATA (global minima).). % error is calculated for VSCF-PT2 against experimental frequencies.

Mode description	Exp. freq	Exp. Intensity	HO	VSCF-PT2	Intensity	% error
NH_2 str	3516	0.63	3921	3521	1.0	0.14
Indole NH str.	3521	0.74	3911	3573	0.94	1.47
φ-amide NH str.	3429	0.85	3861	3461	0.86	0.93
NH_2 str	3334	1.00	3773	3406	0.66	2.16
Pyrole CH str	--	--	3441	3064	0.02	--
Phenyl CH str.	3092	0.18	3366	3076	0.23	0.52
Phenyl CH str.	3072	0.36	3353	3082	0.35	0.33
Phenyl CH str.	3048	0.18	3341	3067	0.05	0.62
Phenyl CH str.	--	--	3332	3072	0.01	-
Alkyl CH str.	2999	0.19	3281	2975	0.12	0.80
Alkyl CH str.	2979	0.14	3310	2961	0.11	0.60
Alkyl CH str.	--		3278	2949	0.11	--
Alkyl CH str.	2938	0.51	3211	2915	0.22	0.78
Alkyl CH str.	2919	0.15	3237	2895	0.16	0.82
Alkyl CH str.	--	--	3199	2962	0.05	--
Avg. % error						**0.83**

Table S3: Comparisons of experimental and computed vibrational frequencies of global minima of AVPO. % error is calculated for VSCF-PT2 against experimental frequencies.

Mode description	Experiments	HO	PES except	% error
Phe NH str.	3451	3866	3423	0.81
Val NH str.	3441	3842	3411	0.87
Phenyl CH str.	3096	3370	3064	1.03
Phenyl CH str.	3076	3350	3048	0.91
Phenyl CH str.	3038	3359	3071	1.09
Phenyl CH str.	3006	3331	3040	1.13
Methyl CH str. of Val	2974	3256	2997	0.77
Methyl CH str. of Val	2965	3268	2974	0.30
Methyl CH str. of Val	2941	3259	2942	0.03
Phenyl CO str.	1765	1998	1789	1.36
Acetyl CO str.	1711	1950	1753	2.00
Val CO str.	1696	1913	1730	2.45
Avg. % error				**1.06**

Fig. S1. Spectra of AVPO (Black: experiment; Magenta: VSCF-PT2)

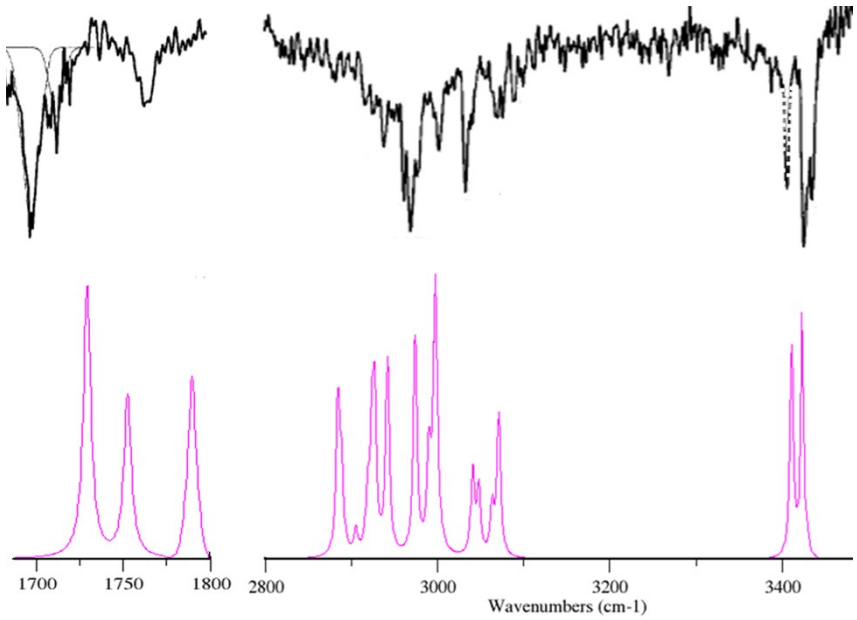

Table S4: Comparisons of computed vibrational harmonic frequencies by HF and MP2 of C7 conformer of NATA (using cc-pVDZ basis)

	MP2 (Harmonic)	HF (Harmonic)
1	3720	3921
2	3619	3911
3	3610	3861
4	3520	3773
5	3309	3441
6	3239	3366
7	3226	3353
8	3214	3341
9	3212	3310
10	3207	3332
11	3196	3278
12	3174	3281
13	3101	3199
14	3095	3237
15	3084	3211

Table S5: Comparisons of computed vibrational harmonic frequencies by HF and MP2 of C5 conformer of NATA (using cc-pVDZ basis)

	MP2 (Harmonic)	HF (Harmonic)
1	3726	3942
2	3680	3911
3	3612	3868
4	3573	3802
5	3278	3407
6	3239	3367
7	3227	3355
8	3215	3344
9	3209	3334
10	3217	3392
11	3194	3287
12	3099	3269
13	3149	3255
14	3096	3202
15	3080	3201

Table S6: Comparisons of computed vibrational harmonic frequencies by HF and MP2 of AVPO (using cc-pVDZ basis)

S. No.	MP2 (Harmonic)	HF (Harmonic)
1	3609	3866
2	3590	3842
3	3246	3370
4	3243	3350
5	3234	3337
6	3222	3332
7	3221	3359
8	3212	3317
9	3206	3340
10	3201	3318
11	3189	3268
12	3181	3268
13	3181	3278
14	3179	3226
15	3177	3262
16	3172	3259
17	3118	3256
18	3110	3249
19	3107	3245
20	3104	3224
21	3093	3194
22	3078	3186
23	3076	3179
24	3071	3172
25	1819	1998
26	1781	1950
27	1763	1913

RESULTS OF VIBRATIONAL SCF CALCULATION: (FREQUENCIES IN CM-1) for NATA-C7 (using HF/MP2 potential with cc-pVDZ basis)

HARMONIC	DIAGONAL	VSCF	PT2-VSCF
3920.57	3743.99	3533.98	3520.89
3910.98	3535.65	3562.47	3572.71
3861.17	3469.52	3452.83	3460.62
3772.64	3436.06	3426.71	3406.27
3440.59	3177.92	3157.81	3163.96
3366.02	3173.31	3109.76	3075.98
3353.46	3220.59	3094.68	3082.20
3341.02	3181.23	3078.51	3066.89
3332.14	3202.53	3081.40	3071.71
3310.27	3191.36	2988.99	2961.47
3280.62	3099.21	2986.22	2974.79
3277.59	3206.86	2988.11	2949.42
3236.96	2977.76	2909.16	2895.06
3211.36	3029.53	2939.89	2914.51
3198.93	3023.92	3003.48	2961.66
1943.15	1781.79	1775.32	1774.47
1908.03	1741.98	1738.23	1737.97
1813.63	1672.86	1654.08	1652.39
1767.98	1615.68	1598.02	1596.43
1763.40	1612.35	1581.31	1576.91
1729.27	1599.30	1580.90	1578.60
1695.21	1559.84	1527.24	1523.22
1645.08	1516.74	1499.62	1498.34
1605.10	1462.11	1445.77	1444.31
1587.36	1474.33	1510.58	1509.76
1584.90	1456.19	1440.69	1439.19
1573.28	1448.94	1434.91	1432.95
1567.10	1458.44	1502.50	1502.39
1545.73	1416.40	1390.47	1387.35
1517.18	1392.35	1414.62	1413.09
1497.32	1380.82	1403.46	1404.89
1477.68	1356.03	1340.56	1339.40
1453.64	1342.45	1325.94	1324.07
1415.25	1320.83	1305.85	1304.23
1398.21	1292.16	1274.03	1271.97
1385.93	1364.86	1351.91	1349.65
1379.79	1259.81	1251.04	1248.71
1371.93	1265.64	1256.25	1254.97
1332.35	1250.86	1237.87	1236.46
1327.72	1227.25	1256.08	1258.04
1229.52	1144.93	1132.11	1130.87
1228.87	1159.55	1194.57	1196.36
1226.43	1141.45	1132.58	1128.08
1217.06	1194.66	1190.41	1188.98
1183.89	1104.13	1097.21	1095.81
1171.85	1092.38	1127.89	1129.75
1150.83	1051.18	1088.85	1087.36
1106.29	1026.22	1047.09	1045.29
1104.84	1026.69	1022.74	1020.86
1083.90	969.22	964.24	960.29
1080.57	994.51	1010.28	1008.95
1071.75	995.54	988.29	986.44
1049.02	909.26	905.69	901.72
1028.34	953.23	952.62	950.49
981.66	832.33	817.24	811.30

948.08	834.29	833.33	829.64
946.36	881.41	879.36	878.33
908.26	842.17	844.69	842.80
855.17	838.70	838.48	837.68
830.14	755.44	756.61	751.22
819.22	761.29	759.92	758.45
802.24	749.55	752.51	750.28
784.53	734.73	739.76	738.62
740.84	690.82	691.74	690.99
697.08	650.85	695.85	693.36
684.33	702.58	725.19	711.79
679.03	636.79	663.97	655.72
640.67	580.99	598.95	596.88
631.74	542.20	548.79	548.08
602.65	555.03	560.26	559.71
596.52	547.19	564.02	562.96
564.57	523.71	536.87	533.33
533.78	648.90	658.74	633.58
499.10	459.38	462.29	461.22
484.45	513.84	541.92	523.05
472.66	413.53	427.02	425.38
441.91	462.47	481.97	467.26
418.47	536.39	538.19	525.84
374.82	388.94	378.72	371.10
372.03	353.81	385.12	382.83
324.61	322.02	319.96	316.48
308.91	289.63	305.00	304.33
243.62	224.55	249.04	247.15
218.65	208.63	232.88	232.27
167.36	151.77	160.86	160.64
162.17	157.89	176.68	175.82
124.76	129.03	133.77	132.41
97.11	107.96	90.69	88.93
88.49	103.75	73.54	65.18
58.77	82.09	125.67	116.55
54.78	91.19	100.24	98.35
45.27	51.25	-122.60	-135.58
30.69	38.61	40.09	39.53

RESULTS OF VIBRATIONAL SCF CALCULATION: (FREQUENCIES IN CM-1) for NATA-C5 (using HF/MP2 potential with cc-pVDZ basis)

HARMONIC	DIAGONAL	VSCF	PT2-VSCF
3941.78	3762.10	3550.71	3536.74
3911.47	3536.68	3551.43	3568.11
3868.48	3473.78	3420.39	3423.97
3802.40	3488.06	3454.97	3428.24
3407.14	3143.73	3120.24	3126.79
3366.98	3172.93	3104.73	3070.74
3355.25	3225.88	3078.46	3054.10
3344.40	3203.50	3073.71	3050.35
3333.51	3211.81	3058.73	3040.73
3292.39	3223.41	3030.38	3002.27
3286.91	3194.13	3021.18	2993.44
3269.23	3031.36	2922.98	2901.97
3255.35	3141.34	2990.60	2966.30
3201.60	3029.28	2965.05	2916.87

3200.79	2990.60	2911.54	2888.88
1949.17	1786.90	1780.52	1778.43
1913.98	1752.20	1740.75	1739.02
1815.06	1672.38	1653.64	1652.20
1775.68	1617.84	1600.36	1598.79
1763.28	1615.18	1584.45	1579.66
1742.40	1597.43	1579.93	1577.92
1689.66	1543.30	1515.99	1511.86
1646.34	1515.74	1497.43	1495.97
1608.32	1466.28	1450.61	1449.18
1589.48	1474.18	1480.03	1478.71
1586.52	1456.38	1450.10	1448.73
1570.89	1458.02	1474.07	1472.94
1566.41	1448.28	1428.59	1425.50
1551.45	1429.18	1421.08	1419.24
1509.97	1382.72	1374.65	1372.15
1502.43	1372.30	1352.00	1349.26
1482.19	1373.61	1358.74	1357.51
1441.72	1336.63	1320.53	1318.60
1414.20	1388.11	1375.56	1373.79
1408.17	1296.71	1282.84	1281.31
1383.98	1363.24	1349.74	1347.26
1363.06	1338.22	1332.17	1330.27
1354.99	1230.26	1225.08	1223.07
1334.76	1226.99	1214.09	1212.63
1280.16	1179.05	1165.86	1163.72
1258.83	1190.23	1182.94	1180.32
1229.76	1142.71	1134.39	1132.81
1222.58	1156.83	1150.79	1148.80
1206.16	1123.98	1121.73	1117.30
1177.14	1104.79	1095.67	1093.65
1161.89	1076.41	1071.22	1069.85
1150.40	1048.96	1052.78	1050.26
1125.10	1050.54	1036.44	1034.31
1114.37	1019.01	1022.35	1020.68
1105.75	979.64	972.80	968.62
1103.94	1029.32	1027.02	1025.00
1081.88	993.38	1011.28	1008.27
1068.30	933.04	923.20	918.02
1038.27	957.91	952.97	951.31
959.02	869.07	862.28	856.46
948.72	881.13	874.85	874.12
938.98	795.12	785.42	780.41
874.32	814.38	819.13	816.76
856.62	839.21	839.02	838.35
837.36	822.16	831.92	830.27
837.08	842.03	842.86	834.05
820.35	803.90	802.90	802.20
809.31	793.37	795.95	794.72
710.31	696.74	704.78	703.39
702.39	694.60	718.15	713.23
687.64	628.20	637.53	636.43
677.80	609.83	620.30	619.60
635.04	580.27	588.43	588.09
630.67	548.29	550.20	549.83
603.14	662.08	667.99	642.72
582.92	539.15	554.66	552.57
535.90	497.22	522.30	521.05
521.12	687.52	678.20	653.72
502.16	459.78	470.24	469.43

479.00	420.86	424.53	423.41
444.97	439.13	451.03	444.56
388.28	541.99	549.23	534.80
373.99	399.93	425.97	412.74
349.30	384.83	390.35	376.18
335.82	342.20	340.13	334.14
313.47	382.64	388.34	373.11
276.44	266.32	289.43	286.19
251.06	232.33	247.75	247.03
235.51	233.43	248.33	244.54
163.15	162.96	184.48	183.33
157.76	143.52	160.32	159.86
103.75	121.55	154.75	149.23
78.68	91.76	102.39	99.97
69.37	85.54	141.42	141.28
62.09	66.05	83.59	82.22
41.56	55.58	69.31	69.70
25,17	25,17	25.17	25.17
20.59	19.07	6.36	2.26

RESULTS OF VIBRATIONAL SCF CALCULATION: (FREQUENCIES IN CM-1) for AVPO (using HF/MP2 potential with cc-pVDZ basis)

HARMONIC	DIAGONAL	VSCF	PT2-VSCF
3865.84	3471.22	3423.25	3422.50
3841.81	3451.85	3406.30	3411.46
3369.50	3183.88	3111.07	3063.64
3358.79	3226.21	3095.30	3071.16
3350.27	3210.64	3073.91	3047.91
3339.78	3199.41	3072.00	3057.68
3337.17	3199.35	3065.14	3041.17
3331.90	3196.97	3062.34	3039.73
3318.43	3157.53	3022.82	3000.77
3317.13	3230.71	3013.23	2990.34
3277.75	3202.99	3018.51	2997.62
3268.32	3176.20	3008.19	2974.07
3267.62	3200.37	2966.83	2941.13
3262.20	3029.88	2933.26	2921.84
3259.06	3184.02	2975.38	2942.06
3255.69	3151.16	3031.39	2997.36
3249.38	3155.53	3016.26	2988.13
3244.58	3015.37	2937.85	2918.87
3225.60	3060.32	2982.59	2942.11
3223.88	3035.56	2972.75	2927.04
3193.96	3019.15	2957.18	2905.20
3186.00	3027.37	2945.25	2888.69
3178.71	3055.77	2950.48	2924.08
3171.50	2986.07	2900.26	2884.33
1998.19	1800.40	1790.17	1789.47
1949.79	1765.65	1754.63	1752.92
1912.57	1745.67	1731.28	1729.62
1803.93	1648.22	1628.54	1626.23
1775.30	1627.68	1605.30	1603.60
1710.25	1555.66	1528.97	1526.16
1680.52	1527.10	1499.72	1496.38
1650.12	1515.41	1497.30	1496.21
1609.86	1495.81	1491.07	1490.47

1604.94	1491.71	1480.69	1479.07
1601.33	1486.58	1481.01	1480.53
1598.72	1567.22	1559.54	1558.51
1597.74	1475.11	1464.68	1463.72
1593.74	1480.00	1474.59	1474.30
1592.35	1561.67	1549.89	1548.32
1589.88	1477.74	1472.53	1471.27
1583.06	1474.21	1484.48	1482.75
1581.00	1466.53	1466.42	1466.20
1565.81	1454.18	1464.02	1461.97
1539.94	1410.78	1404.95	1403.50
1529.84	1399.85	1391.55	1390.31
1523.81	1395.83	1387.84	1386.24
1513.97	1384.62	1364.53	1362.89
1499.97	1363.17	1345.56	1343.75
1489.76	1367.08	1353.24	1351.83
1478.84	1350.30	1446.23	1447.03
1461.68	1335.70	1324.26	1323.20
1457.23	1332.17	1318.93	1317.93
1424.46	1305.47	1290.70	1289.20
1418.67	1263.36	1245.56	1243.33
1382.86	1271.39	1258.43	1256.10
1371.52	1346.16	1335.52	1333.84
1359.63	1334.61	1325.91	1324.63
1335.90	1312.07	1301.38	1299.46
1316.18	1293.25	1287.69	1285.74
1312.69	1287.03	1280.02	1278.84
1307.18	1282.49	1386.86	1387.77
1301.63	1276.54	1272.94	1272.08
1282.90	1193.34	1184.75	1182.95
1278.84	1254.08	1248.12	1247.12
1273.20	1186.69	1177.03	1172.76
1237.63	1151.32	1142.73	1141.58
1219.01	1133.44	1126.18	1125.33
1204.01	1184.48	1176.89	1175.17
1173.17	1097.50	1090.36	1088.44
1168.51	1078.80	1083.86	1082.56
1148.04	1046.75	1050.44	1047.49
1131.39	1048.92	1155.37	1155.83
1122.79	1042.96	1035.97	1034.39
1108.93	1096.97	1096.96	1092.80
1107.87	1033.45	1028.11	1026.44
1091.39	1083.21	1083.91	1078.90
1083.41	1001.67	993.54	992.22
1079.71	1011.77	1027.69	1024.39
1072.24	992.87	987.02	985.37
1048.16	1027.70	1027.52	1026.17
1040.06	1020.82	1029.78	1028.73
1036.97	1021.79	1027.04	1024.67
1024.14	921.22	926.94	924.49
1006.36	944.06	953.65	952.48
994.32	928.67	945.43	942.82
962.18	888.41	889.90	888.28
946.40	878.12	876.93	871.19
915.49	858.75	857.28	856.38
901.95	828.57	830.16	829.05
855.58	798.02	799.31	798.61
830.42	772.54	774.61	773.81
823.53	746.71	754.05	751.45
774.98	764.78	773.68	770.89

767.50	708.64	715.08	714.09
697.19	643.88	651.24	650.09
692.74	680.25	689.43	686.83
676.66	630.37	654.20	651.49
676.54	617.60	615.34	615.16
660.15	594.97	603.08	602.56
633.19	593.34	620.78	616.39
596.44	721.15	721.65	691.43
562.90	513.95	534.90	531.84
531.60	494.71	499.85	499.06
518.59	666.36	663.92	648.08
490.59	465.10	579.97	575.84
459.84	414.97	431.49	430.71
454.55	412.31	418.26	417.35
432.57	400.90	426.29	423.92
408.21	403.41	414.42	409.55
387.54	361.91	375.88	375.47
376.20	351.68	367.35	366.42
333.83	311.71	327.38	327.14
307.00	273.08	280.89	280.70
286.30	274.90	292.07	291.60
277.17	285.19	314.47	308.02
260.68	304.09	315.53	304.26
236.03	234.30	269.54	268.12
234.63	325.72	328.53	315.87
202.99	205.09	221.69	219.62
181.79	181.42	203.38	202.22
167.88	236.82	242.43	239.19
164.86	199.81	228.86	224.55
143.15	183.74	193.04	189.63
121.00	114.37	137.37	136.29
90.79	114.38	135.02	133.46
81.34	90.06	112.79	112.12
67.35	90.52	97.58	96.57
65.67	82.95	95.64	95.22
63.24	94.75	107.71	107.61
55.89	86.56	302.47	301.74
53.01	73.96	175.40	172.81
43.30	66.43	75.24	73.71
27.34	40.18	47.18	47.78
19.74	26.95	37.47	38.35
14.26	19.72	22.07	22.08

Optimized coordinates of NATA-C5 at MP2/cc-pVDZ

N	7.0	2.0944038867	-2.2504652013	3.6105076247
C	6.0	2.5134311507	-0.9949902008	4.0078138436
C	6.0	2.0360174903	-0.0622560009	3.0338134415
C	6.0	1.3119281064	-0.8136073440	2.0369663171
C	6.0	1.3714860608	-2.1472324565	2.4364928397
C	6.0	3.2626637376	-0.5901811374	5.1307670890
C	6.0	3.5217433408	0.7776977592	5.2666142721
C	6.0	3.0461903739	1.7195208342	4.3138004294
C	6.0	2.3046005695	1.3206984297	3.1983299148
C	6.0	0.6386478012	-0.2297576254	0.8308445564
C	6.0	1.6354392429	0.3977652576	-0.1832312793
N	7.0	0.9597086888	1.2913972485	-1.0957683970
C	6.0	0.6626571412	2.5699481661	-0.7172241618
C	6.0	0.1204022423	3.4579901837	-1.8238837066
C	6.0	2.3290793858	-0.6725286288	-1.0313581696
N	7.0	3.2142719278	-1.4515881362	-0.3422787065
O	8.0	2.1112455517	-0.7909685992	-2.2365661194
O	8.0	0.8300247200	2.9729186581	0.4367523206
H	1.0	3.6241740276	-1.3121519004	5.8714620343
H	1.0	4.0996040023	1.1294567036	6.1278901866
H	1.0	3.2639322299	2.7823849392	4.4627882324
H	1.0	1.9268968298	2.0494084834	2.4711815300
H	1.0	0.9379273609	-3.0319882731	1.9670700155
H	1.0	2.2543457047	-3.1104316642	4.1222314634
H	1.0	0.0197144806	-0.9834998930	0.3111213179
H	1.0	-0.0278504484	0.5894140767	1.1501689537
H	1.0	2.3936741168	0.9620249599	0.3897830120
H	1.0	3.5470694585	-2.2837976817	-0.8203839033
H	1.0	0.9633288124	1.0019385763	-2.0721225681
H	1.0	-0.6473120613	4.1215883133	-1.4005794503
H	1.0	0.9382139972	4.0895721193	-2.2087687038
H	1.0	-0.3051946965	2.8801580557	-2.6586574637
H	1.0	3.1471947674	-1.4789350217	0.6717302348

Optimized coordinates at NATA-C7 at MP2/cc-pVDZ

C	6.0	-1.6885016730	-0.1662461258	0.4609377502
C	6.0	-2.6010527744	-0.7247055354	-0.4940284842
C	6.0	-3.7470009596	-0.0333646634	-0.9358179566
C	6.0	-3.9736677867	1.2420543542	-0.4084643953
C	6.0	-3.0836946295	1.8172942615	0.5389971943
C	6.0	-1.9491131210	1.1295297741	0.9793591140
C	6.0	-0.6416568579	-1.1359599058	0.6737590785
C	6.0	-0.9439079889	-2.2190092989	-0.1464439450
H	1.0	-4.4352637821	-0.4745554070	-1.6653929516
H	1.0	-4.8539044115	1.8075654765	-0.7316968082
H	1.0	-3.2965848756	2.8169915122	0.9326552850
H	1.0	-1.2719849161	1.5831016033	1.7124035894
H	1.0	-0.3815698230	-3.1399986223	-0.2940188042
H	1.0	-2.5467402312	-2.6043350727	-1.4943360653
N	7.0	-2.1169047822	-1.9691779402	-0.8317262352
C	6.0	0.5571351559	-0.9754539734	1.5680953347
H	1.0	0.2946971996	-0.3246634768	2.4200422691
H	1.0	0.8709993948	-1.9509053155	1.9695872350
C	6.0	1.7572096040	-0.3569382019	0.8340693712
H	1.0	2.5233332394	-0.0274957648	1.5614251119
C	6.0	2.4420452905	-1.3957861926	-0.0827155390
O	8.0	2.0932019083	-2.5747991883	-0.1284973386
N	7.0	3.4681532158	-0.8736689554	-0.8096333363
H	1.0	4.0401465020	-1.5227721395	-1.3389088018
H	1.0	3.8176103677	0.0569449859	-0.5793205163
N	7.0	1.3261359967	0.8376415562	0.1184489740
H	1.0	0.3702030348	0.8461169522	-0.2308054973
C	6.0	2.1582170683	1.8768640631	-0.1664433133
O	8.0	3.3654036124	1.8605421601	0.1081103017
C	6.0	1.4998127266	3.0569643152	-0.8574086864
H	1.0	1.8563239346	3.9816339499	-0.3795056842
H	1.0	1.8244858046	3.0795240282	-1.9106366217
H	1.0	0.4003355567	3.0184047872	-0.8167276283

Optimized coordinates of AVPO at MP2/cc-pVDZ

C	6.0	1.4074560215	-1.4677471893	-1.0084177288
C	6.0	1.7870512199	-0.1464511168	-1.7415692846
H	1.0	2.7480019524	-0.3079507824	-2.2575071858
H	1.0	1.0110256366	0.0406448853	-2.4996821193
C	6.0	1.8675181474	1.0002496084	-0.7634099487
C	6.0	0.7145211076	1.7549065239	-0.4568146268
C	6.0	3.0606663688	1.2777904011	-0.0639073379
H	1.0	-0.2114459794	1.5662445718	-1.0123847031
C	6.0	0.7392498044	2.7443716120	0.5407069217
C	6.0	3.0982207770	2.2798788625	0.9205550135
H	1.0	3.9684040632	0.7096489877	-0.3021944429
H	1.0	-0.1797866216	3.2882854476	0.7821689330
C	6.0	1.9351342889	3.0064098922	1.2321532290
H	1.0	4.0340514514	2.4890777422	1.4500806324
H	1.0	1.9616625425	3.7771032389	2.0097475628
H	1.0	1.2508232041	-2.2564667038	-1.7647276923
C	6.0	2.5347867536	-1.8927239910	-0.0793335846
O	8.0	2.4555207604	-1.9382883767	1.1341797154
O	8.0	3.6491864644	-2.1804702387	-0.7823178647
C	6.0	4.7738124498	-2.5469173077	0.0407805751
H	1.0	5.5970527848	-2.7390513763	-0.6581444897
H	1.0	5.0293255199	-1.7271515702	0.7292950079
H	1.0	4.5444928802	-3.4481361941	0.6288489100
N	7.0	0.2251403268	-1.3225835466	-0.1805073196
H	1.0	0.4175536817	-1.1368850781	0.8026706886
C	6.0	-0.9548015256	-0.8902976534	-0.7061020556
O	8.0	-1.1966176196	-0.8893018826	-1.9175658496
C	6.0	-1.9765948333	-0.4158299649	0.3296044475
H	1.0	-1.4663162686	0.2068644867	1.0857103464
C	6.0	-2.6615997519	-1.6027031602	1.0444282258
H	1.0	-1.8527160994	-2.1947089189	1.5163762880
C	6.0	-3.5963380718	-1.0822051119	2.1397887075
H	1.0	-4.0439546511	-1.9208980939	2.6995416342
H	1.0	-3.0606743692	-0.4304918744	2.8497613209
H	1.0	-4.4131824304	-0.4918590224	1.6912966539
C	6.0	-3.4109374617	-2.4969151754	0.0520668954
H	1.0	-4.2114402233	-1.9219131595	-0.4451974125
H	1.0	-2.7436344433	-2.8993577908	-0.7282555311
H	1.0	-3.8809452449	-3.3464238951	0.5757826475
N	7.0	-2.9257364615	0.4467885665	-0.3525518460
H	1.0	-3.0259277869	0.2370027521	-1.3459775954
C	6.0	-3.0557590669	1.7664543292	0.0305638529
O	8.0	-2.6250843641	2.1990138170	1.0985623921
C	6.0	-3.7827647263	2.6387896065	-0.9786568762
H	1.0	-3.0435111906	3.0864161938	-1.6647560674
H	1.0	-4.5104317121	2.0650022122	-1.5731731081
H	1.0	-4.2926623040	3.4529244374	-0.4450889308