

Supplementary Information (SI)

**Deconvolution of Fast Exchange Equilibrium States in NMR Spectroscopy
Using Virtual Reference Standards and Probability Theory**

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1. General Method

Nuclear magnetic resonance (NMR) spectra were recorded on a Bruker-Biospin AVIII 600 MHz spectrometer, nonspinning, using a 1.7 mm CP TCI Z gradient probe. Data were processed by TopSpin. ^1H and ^{13}C chemical shifts are reported in ppm relative to the signals corresponding to the residual non-deuterated solvents (*d*6-DMSO for ^1H NMR: $\delta = 2.50$ ppm; for ^{13}C NMR: $\delta = 39.5$ ppm). ^{15}N chemical shifts were determined based on ^1H - ^{15}N HMBC spectra and reported in ppm relative to an external pyridine reference. Experimental parameters were as follow: for the ^1H spectrum, acquisition time (AQ) = 1.32 s, relaxation delay (RD) = 2.0 s, 90° pulse = 10s, spectral width (SW) = 12376 Hz; for the ^{13}C spectrum, AQ = 0.904 s, RD = 0.5 s, 90° pulse width = 12 us, SW = 36231 Hz; the mixing time for the NOESY spectrum was 0.5 s.

2. Method Screening

Molecular structures were constructed in Maestro. For each molecule, a conformer search was conducted in Maestro with RMSD of 0.5 Å. All conformers within an upper energy limit of 5 kcal/mol were considered stable and used in the next step. Subsequently, each conformer was subjected into geometry optimization step using various Gaussian methods. A total of 45 combinations of functionals (B3LYP, ω B97X, and ω B97XD), basis sets (cc-pVDZ, *aug*-cc-pVDZ, 6-31+G(d,p), 6-311+G(d,p), and 6-311++G(d,p)), and solvation models (PCM, CPCM, and SMD) were tested for each conformer. After obtaining the optimized conformer structure, NMR calculation was further performed on the structure with the same method used for geometry optimization, affording isotropic shielding constants for each ^{13}C , ^1H , and ^{15}N nuclei. Each Gaussian input file including conformer structure and calculation method was generated and submitted automatically with an in-house developed automation Python script. For each molecule, the isotropic shielding constants were extracted from each conformer and weight-average was calculated with a Boltzmann distribution dependent on their energies. The geometry optimization and isotropic shielding constant calculation were performed using the same level of theory for each conformer unless otherwise stated.

The isotropic shielding constants of all molecules were included together in a linear scaling analysis for each calculation method, plotting against the experimental chemical shift values. R^2 and mean-absolute-error (MAE) of the linear scaling was extracted to evaluate the performance of each calculation method.

The method screening procedure was demonstrated in a flowchart (**Figure S1**). Compounds used in method screening were summarized in **Figure S2** and linear scaling results of all calculation methods were summarized in **Table S1~S3**.

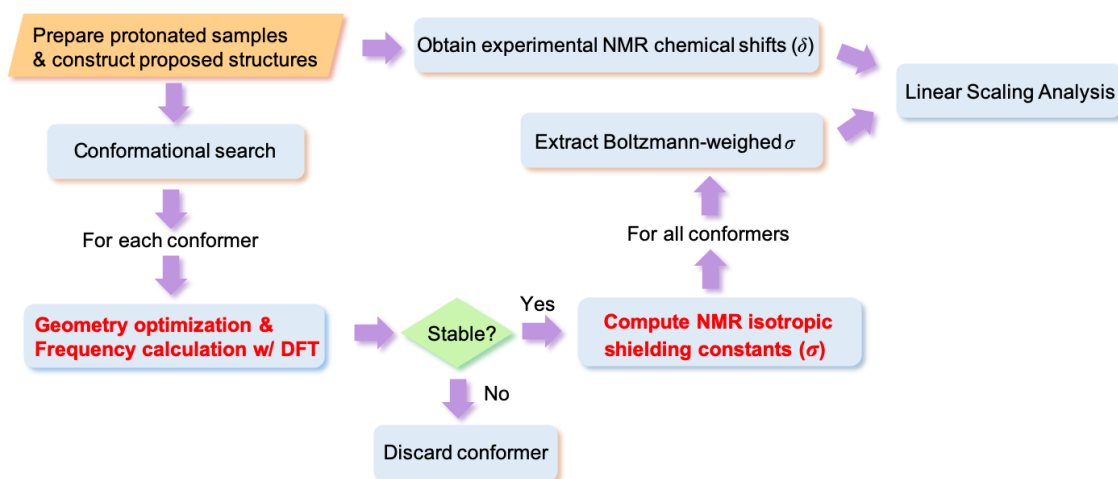


Figure S1. Flowchart diagram of each calculation method for ^1H , ^{13}C , and ^{15}N chemical shifts

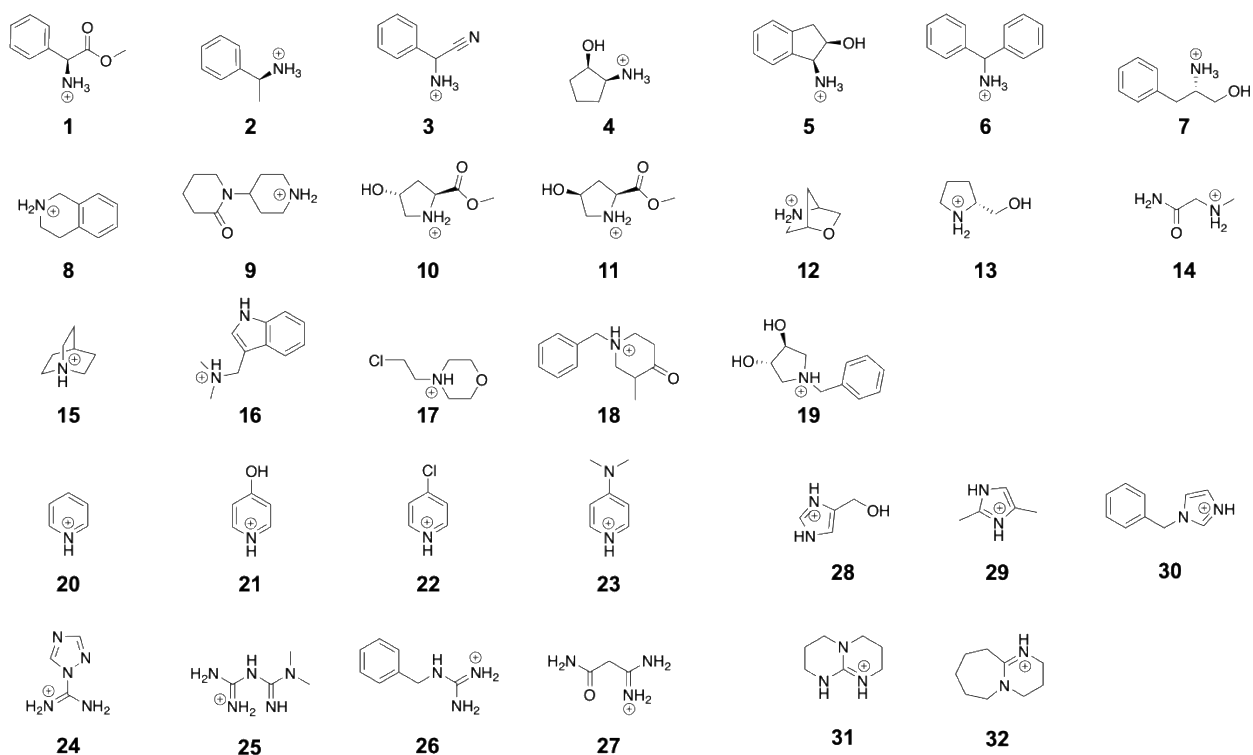


Figure S2. Model molecules used for method screening

Table S1. Linear Scaling Summary of ^{13}C chemical shifts

¹³ C			Slope	Intercept	R ²	MAE (ppm)		Slope	Intercept	R ²	MAE (ppm)		Slope	Intercept	R ²	MAE (ppm)		
B3LYP	6-31+G(d,p)	CPCM	-0.9308	185.53	0.9965	2.15	6-31+G(d,p)	CPCM	-0.9733	196.24	0.9985	1.43	6-31+G(d,p)	CPCM	-0.9610	193.31	0.9982	1.52
		PCM	-0.9300	185.47	0.9965	2.11		PCM	-0.9721	196.14	0.9985	1.43		PCM	-0.9605	193.28	0.9982	1.54
		SMD	-0.9371	185.84	0.9972	1.96		SMD	-0.9798	196.56	0.9991	1.09		SMD	-0.9670	193.57	0.9988	1.25
	6-311+G(d,p)	CPCM	-1.0116	178.00	0.9974	1.81	6-311+G(d,p)	CPCM	-1.0398	189.62	0.9985	1.39	6-311+G(d,p)	CPCM	-1.0294	186.08	0.9984	1.48
		PCM	-1.0115	177.98	0.9974	1.81		PCM	-1.0403	189.69	0.9986	1.38		PCM	-1.0279	185.95	0.9984	1.47
		SMD	-1.0179	178.34	0.9983	1.47		SMD	-1.0471	189.98	0.9993	0.94		SMD	-1.0367	186.53	0.9991	1.02
	6-311++G(d,p)	CPCM	-1.0118	177.98	0.9974	1.81	6-311++G(d,p)	CPCM	-1.0399	189.58	0.9985	1.40	6-311++G(d,p)	CPCM	-1.0288	186.00	0.9985	1.44
		PCM	-1.0099	177.81	0.9974	1.82		PCM	-1.0403	189.67	0.9985	1.41		PCM	-1.0285	185.98	0.9985	1.43
		SMD	-1.0190	178.42	0.9981	1.53		SMD	-1.0471	189.95	0.9993	0.96		SMD	-1.0369	186.48	0.9991	1.04
	cc-pVDZ	CPCM	-0.9521	186.38	0.9969	2.02	cc-pVDZ	CPCM	-0.9951	197.26	0.9981	1.59	cc-pVDZ	CPCM	-0.9821	193.97	0.9980	1.63
		PCM	-0.9521	186.39	0.9969	2.01		PCM	-0.9952	197.27	0.9980	1.63		PCM	-0.9819	193.93	0.9979	1.67
		SMD	-0.9568	186.66	0.9978	1.61		SMD	-0.9995	197.47	0.9990	1.11		SMD	-0.9868	194.22	0.9989	1.16
	aug-cc-PVDZ	CPCM	-0.9797	186.52	0.9931	2.75	aug-cc-PVDZ	CPCM	-1.0141	196.65	0.9954	2.14	aug-cc-PVDZ	CPCM	-1.0022	193.64	0.9948	2.29
		PCM	-0.9795	186.50	0.9931	2.72		PCM	-1.0138	196.62	0.9953	2.16		PCM	-1.0019	193.58	0.9949	2.28
		SMD	-0.9867	186.86	0.9937	2.66		SMD	-1.0210	197.01	0.9962	1.95		SMD	-1.0093	193.98	0.9958	2.07

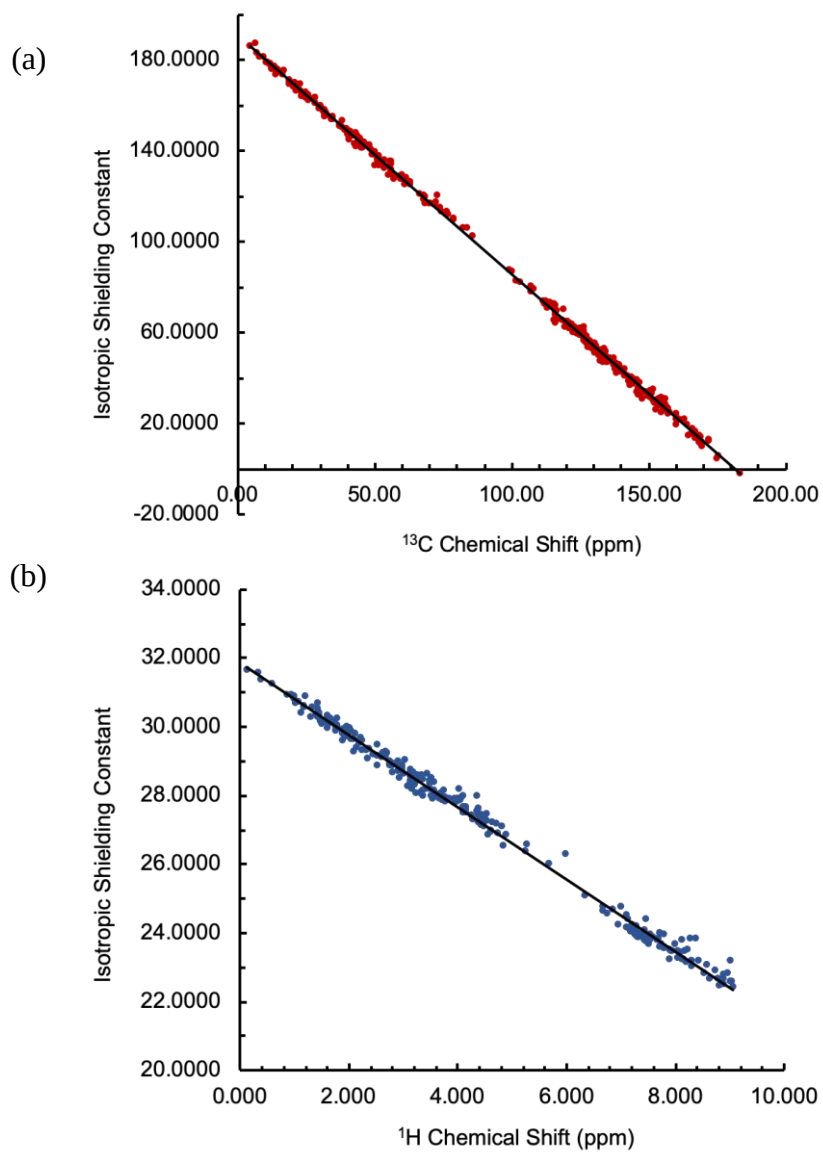
Table S2. Linear Scaling Summary of ^1H chemical shifts

¹ H			Slope	Intercept	R ²	MAE (ppm)			Slope	Intercept	R ²	MAE (ppm)			Slope	Intercept	R ²	MAE (ppm)		
B3LYP	6-31+G(d,p)	CPCM	-0.9778	31.32	0.9837	0.220	ω B97X	6-31+G(d,p)	CPCM	-1.0238	31.54	0.9849	0.229	ω B97XD	6-31+G(d,p)	CPCM	-1.0208	31.55	0.9861	0.221
		PCM	-0.9783	31.32	0.9858	0.216			PCM	-1.0225	31.54	0.9845	0.228			PCM	-1.0196	31.55	0.9858	0.220
		SMD	-1.0050	31.38	0.9900	0.190			SMD	-1.0474	31.58	0.9891	0.198			SMD	-1.0462	31.59	0.9895	0.192
	6-311+G(d,p)	CPCM	-0.9792	31.62	0.9835	0.221		6-311+G(d,p)	CPCM	-1.0181	31.79	0.9849	0.224		6-311+G(d,p)	CPCM	-1.0127	31.78	0.9861	0.218
		PCM	-0.9784	31.62	0.9842	0.221			PCM	-1.0136	31.77	0.9846	0.227			PCM	-1.0127	31.78	0.9867	0.216
		SMD	-1.0057	31.67	0.9897	0.191			SMD	-1.0413	31.81	0.9893	0.194			SMD	-1.0363	31.82	0.9899	0.186
	6-311++G(d,p)	CPCM	-0.9794	31.62	0.9855	0.218		6-311++G(d,p)	CPCM	-1.0160	31.77	0.9847	0.225		6-311++G(d,p)	CPCM	-1.0095	31.77	0.9857	0.220
		PCM	-0.9790	31.62	0.9832	0.222			PCM	-1.0064	31.72	0.9851	0.225			PCM	-1.0098	31.77	0.9866	0.218
		SMD	-1.0048	31.66	0.9897	0.190			SMD	-1.0383	31.80	0.9890	0.196			SMD	-1.0343	31.81	0.9895	0.190
	cc-pVDZ	CPCM	-0.9484	31.11	0.9856	0.214		cc-pVDZ	CPCM	-0.9966	31.38	0.9839	0.231		cc-pVDZ	CPCM	-0.9920	31.38	0.9858	0.221
		PCM	-0.9484	31.11	0.9857	0.214			PCM	-0.9941	31.37	0.9809	0.236			PCM	-0.9896	31.37	0.9840	0.227
		SMD	-0.9698	31.15	0.9901	0.183			SMD	-1.0185	31.42	0.9888	0.200			SMD	-1.0131	31.42	0.9895	0.192
	aug-cc-PVDZ	CPCM	-0.9558	31.15	0.9731	0.280		aug-cc-PVDZ	CPCM	-0.9746	31.29	0.9779	0.249		aug-cc-PVDZ	CPCM	-0.9676	31.29	0.9786	0.245
		PCM	-0.9554	31.15	0.9729	0.278			PCM	-0.9723	31.29	0.9762	0.255			PCM	-0.9668	31.29	0.9783	0.245
		SMD	-0.9775	31.19	0.9772	0.256			SMD	-1.0008	31.34	0.9819	0.223			SMD	-0.9932	31.33	0.9826	0.219

Table S3. Linear Scaling Summary of ¹⁵N chemical shifts

¹⁵ N			Slope	Intercept	R ²	MAE (ppm)			Slope	Intercept	R ²	MAE (ppm)			Slope	Intercept	R ²	MAE (ppm)		
B3LYP	6-31+G(d,p)	CPCM	-0.9271	248.66	0.9827	8.0	ω B97X	6-31+G(d,p)	CPCM	-0.9311	261.03	0.9896	6.0	ω B97XD	6-31+G(d,p)	CPCM	-0.9426	258.60	0.9886	6.3
		PCM	-0.9302	249.12	0.9822	8.2			PCM	-0.9338	261.50	0.9896	6.0			PCM	-0.9428	258.56	0.9886	6.3
		SMD	-0.9206	248.88	0.9841	7.6			SMD	-0.9245	261.28	0.9918	5.4			SMD	-0.9364	258.83	0.9908	5.8
	6-311+G(d,p)	CPCM	-0.9991	237.17	0.9842	7.6		6-311+G(d,p)	CPCM	-0.9908	250.35	0.9898	5.9		6-311+G(d,p)	CPCM	-1.0041	247.10	0.9892	6.1
		PCM	-1.0000	237.21	0.9839	7.7			PCM	-0.9929	250.67	0.9897	5.9			PCM	-1.0059	247.45	0.9890	6.2
		SMD	-0.9908	237.04	0.9866	7.2			SMD	-0.9827	249.98	0.9934	4.9			SMD	-0.9965	247.20	0.9919	5.4
	6-311++G(d,p)	CPCM	-0.9986	237.07	0.9838	7.7		6-311++G(d,p)	CPCM	-0.9920	250.48	0.9897	5.9		6-311++G(d,p)	CPCM	-1.0059	247.42	0.9889	6.2
		PCM	-1.0018	237.51	0.9836	7.9			PCM	-0.9962	251.32	0.9904	5.7			PCM	-1.0066	247.62	0.9889	6.2
		SMD	-0.9907	237.10	0.9861	7.3			SMD	-0.9831	250.07	0.9933	5.0			SMD	-0.9972	247.37	0.9919	5.4
	cc-pVDZ	CPCM	-0.9502	246.75	0.9813	8.1		cc-pVDZ	CPCM	-0.9522	259.38	0.9883	6.2		cc-pVDZ	CPCM	-0.9619	256.64	0.9876	6.4
		PCM	-0.9503	246.74	0.9812	8.2			PCM	-0.9530	259.39	0.9881	6.3			PCM	-0.9629	256.68	0.9873	6.5
		SMD	-0.9435	247.00	0.9842	7.6			SMD	-0.9439	259.33	0.9915	5.4			SMD	-0.9538	256.55	0.9908	5.7
	aug-cc-PVDZ	CPCM	-0.9416	245.00	0.9804	8.6		aug-cc-PVDZ	CPCM	-0.9369	256.53	0.9876	6.7		aug-cc-PVDZ	CPCM	-0.9498	254.35	0.9872	6.8
		PCM	-0.9416	244.85	0.9801	8.8			PCM	-0.9370	256.44	0.9875	6.7			PCM	-0.9490	254.14	0.9867	6.9
		SMD	-0.9312	244.31	0.9833	8.1			SMD	-0.9290	256.33	0.9908	5.8			SMD	-0.9396	253.83	0.9901	6.0

3. Linear Scaling and Statistical Analysis



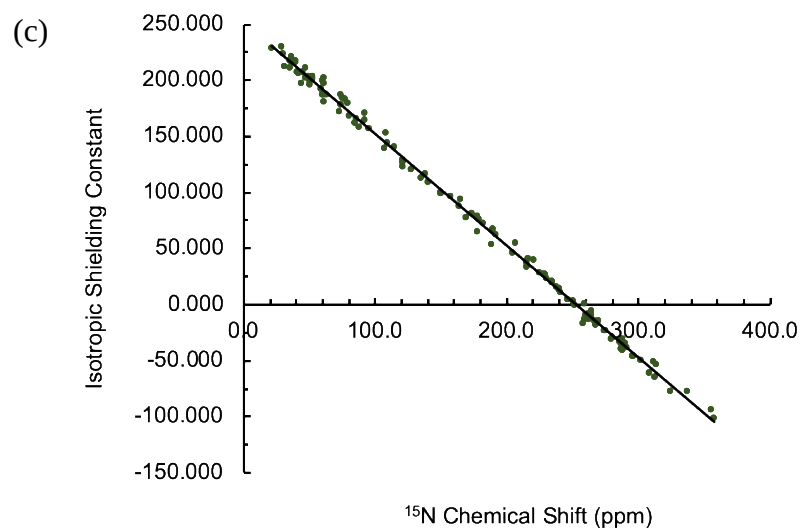
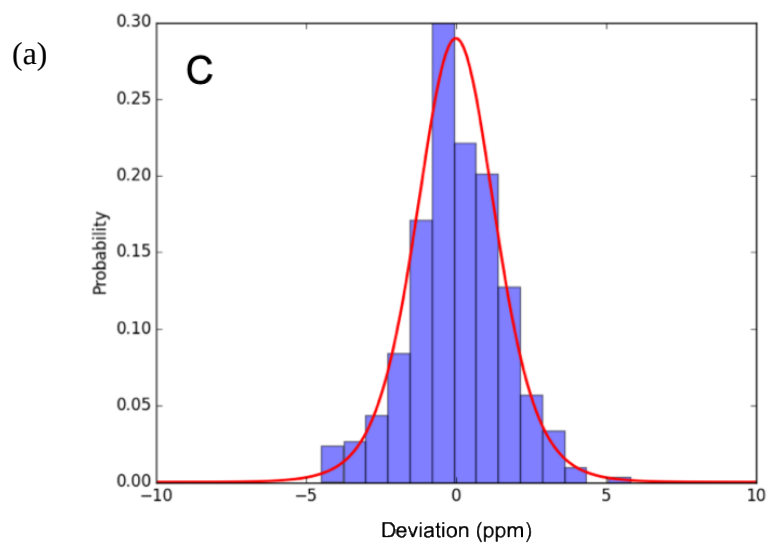


Figure S3. Linear scaling plot of (a) ^{13}C , (b) ^1H , and (c) ^{15}N chemical shifts prediction with $\omega\text{B97X/6-311+G(d,p)/SMD}$.



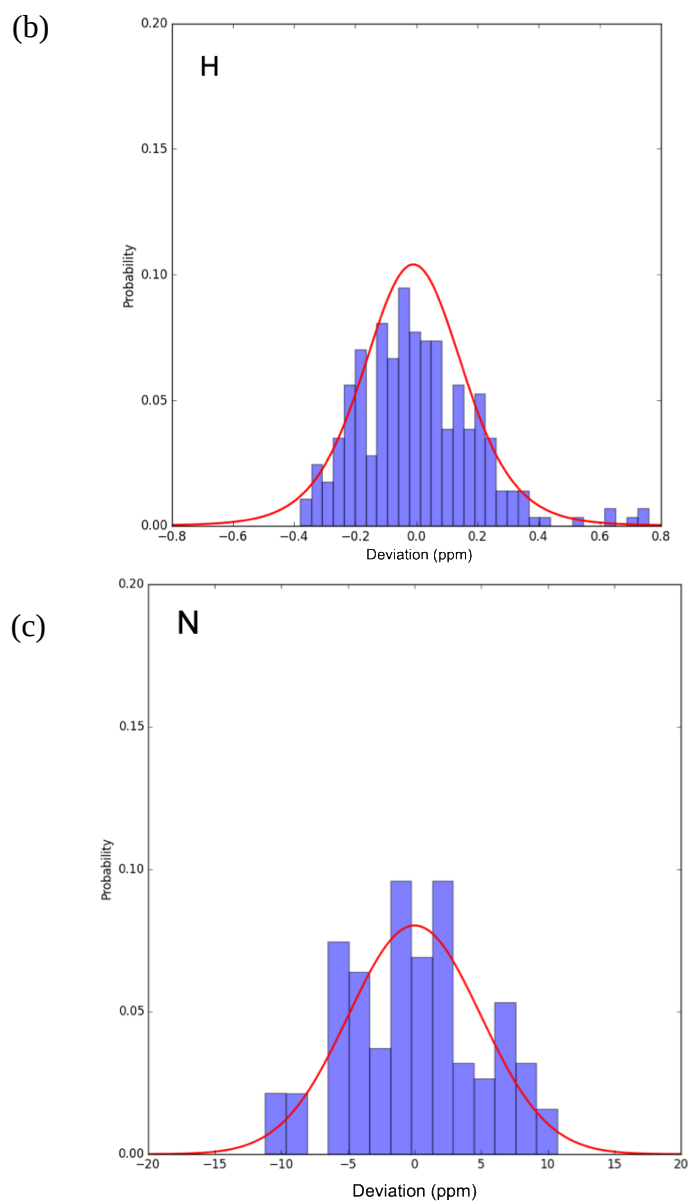


Figure S4. Distribution of calculation errors of (a) ^{13}C , (b) ^1H , and (c) ^{15}N chemical shifts with $\omega\text{B97X/6-311+G(d,p)/SMD}$.

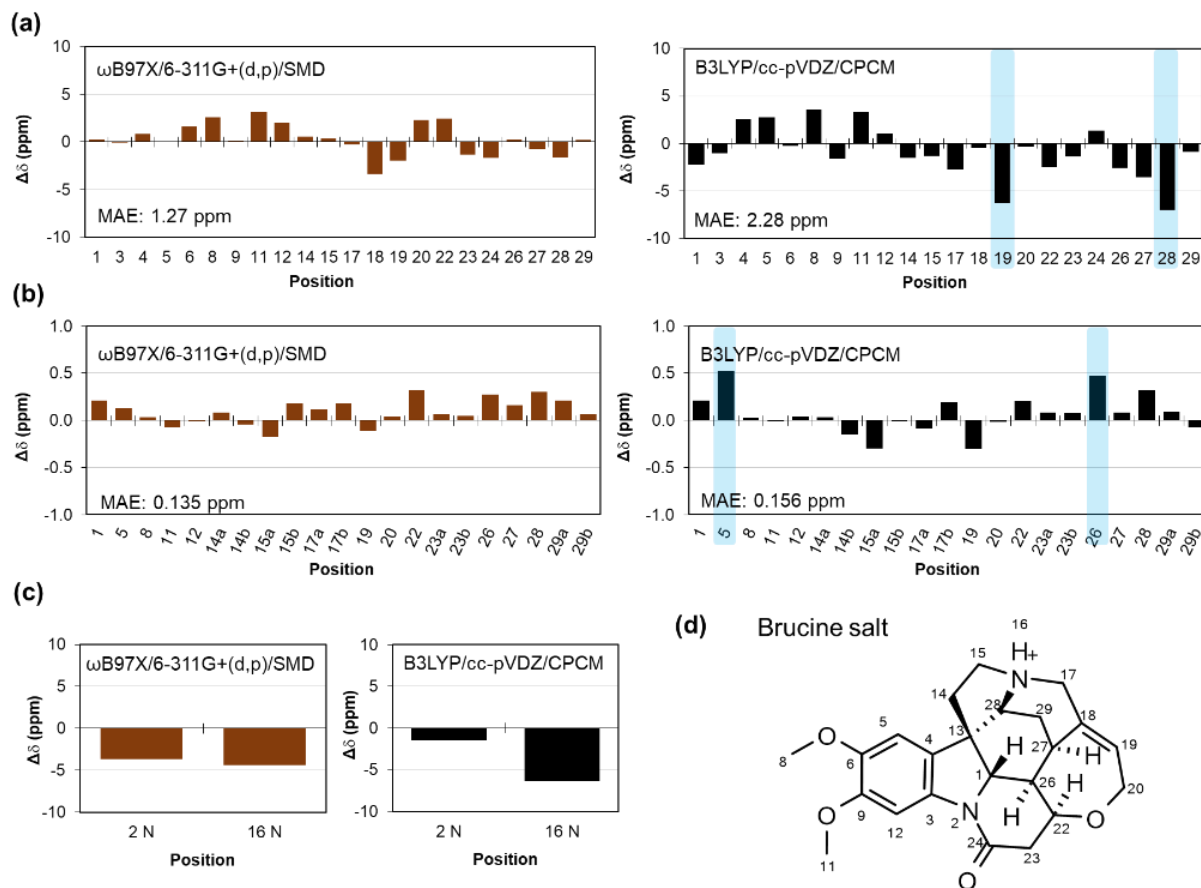


Figure S5. Plots of the differences between the calculated and experimental (a) ^{13}C , (b) ^1H and (c) ^{15}N chemical shifts of protonated Brucine calculated with ω B97X/6-311G+(d,p)/SMD and B3LYP/cc-pVDZ/CPCM.

4. Protonation Ratio Prediction

For model compounds **1** ~ **6**, experimental chemical shifts were collected in their neutral form in DMSO-d₆ and fully protonated form in DMSO-d₆ with excess amount of TFA-d. Chemical shifts were calculated based on their neutral and fully-protonated structures.

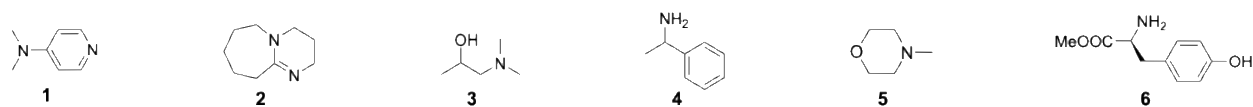


Figure S6. Structure of six model compounds

For each compound, 101 partial salt models were created by calculating the weight-average of experimental data sets, with protonation ratio of 0, 1%, 2%, 3%, ..., 100%. Determination of protonation ratio of each partial salt model was performed according to the procedure showed in **Figure 1**. Results obtained with MAE and DFEQNMR methods were summarized in **Figure 2, Table S4, Figure S7**.

Table S4. Correctness and error analysis of protonation ratio prediction using MAE method

Compound	Correctness percentage (%)			Mean absolute error of 101 cases (%)		
	MAE- ¹³ C	MAE- ¹ H	MAE- ¹⁵ N	MAE- ¹³ C	MAE- ¹ H	MAE- ¹⁵ N
1	100	27.7	100	6	13.6	5.9
2	54.4	9.9	83.1	9.2	37.6	6.8
3	9.9	76.2	22.8	47.3	7.9	14.6
4	88.1	21.8	26.7	4.6	20.1	21.9
5	9.9	9.9	9.9	41.2	16.7	37.2
6	100	68.3	9.9	0.8	8	37.3
Average	60.4	35.6	42.1	18.2	17.3	20.6

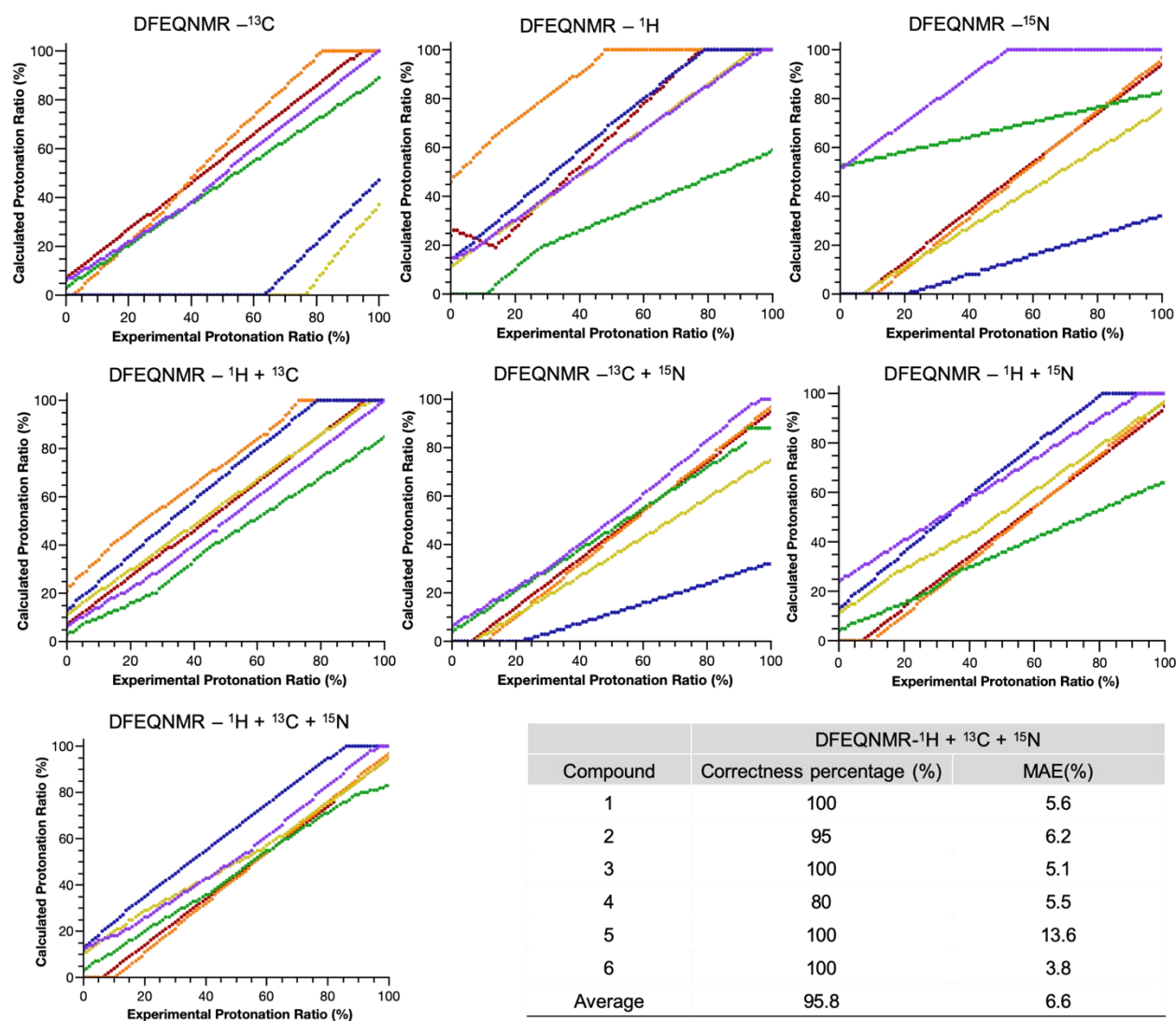
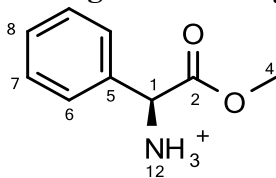
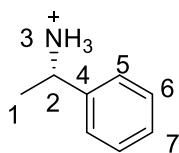


Figure S7. Calculated protonation ratio of 6 model compounds using DFEQNMR method versus experimental protonation ratio from 0% to 100%. Correctness percentages and mean absolute error when using 1H+13C+15N combination were list in the table. (Compound 1: red; 2: orange; 3: yellow; 4: green; 5: blue; 6: purple)

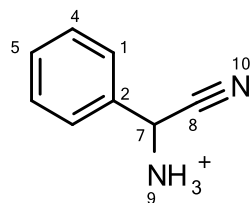
5. Calculated and Experimental Chemical Shifts for Compounds Used in Linear Regression Analysis



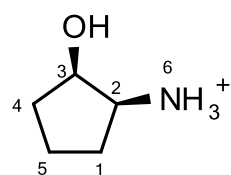
Atom Number	Exptl. Chemical Shifts (ppm)	Isotropic shielding constants	Linearly Scaled Chemical Shifts (ppm)	Delta (ppm)
1 C	55.26	129.2918	58.44	-3.18
2 C	168.80	13.9676	168.03	0.76
4 C	53.10	135.0512	52.97	0.13
5 C	132.56	52.1582	131.74	0.82
6 C	128.23	54.3720	129.64	-1.41
7 C	128.95	54.6040	129.42	-0.47
8 C	129.47	52.7773	131.15	-1.68
1 H	5.251	26.5979	5.011	0.241
4 H	3.707	27.8555	3.816	-0.109
6 H	7.520	23.8533	7.618	-0.099
7 H	7.454	23.8021	7.667	-0.213
8 H	7.445	23.7448	7.722	-0.277
12 N	45.4	207.702	45.0	0.4



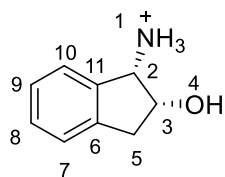
Atom Number	Exptl. Chemical Shifts (ppm)	Isotropic shielding constants	Linearly Scaled Chemical Shifts (ppm)	Delta (ppm)
1 C	20.63	169.7602	19.98	0.65
2 C	49.93	133.8297	54.13	-4.20
4 C	139.22	45.6093	137.97	1.26
5 C	126.72	56.6575	127.47	-0.74
6 C	128.75	55.0197	129.02	-0.27
7 C	128.47	54.4173	129.59	-1.13
1 H	1.498	30.0912	1.691	-0.193
2 H	4.406	27.2433	4.397	0.008
5 H	7.481	23.7945	7.674	-0.193
6 H	7.398	23.8724	7.600	-0.202
7 H	7.427	23.7977	7.671	-0.245
3 N	47.6	202.602	50.1	-2.6



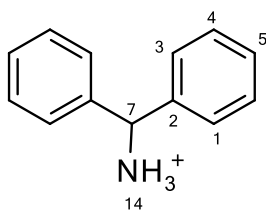
Atom Number	Exptl. Chemical Shifts (ppm)	Isotropic shielding constants	Linearly Scaled Chemical Shifts (ppm)	Delta (ppm)
1 C	128.41	54.1145	129.88	-1.47
2 C	130.50	55.3899	128.67	1.83
4 C	129.14	54.4950	129.52	-0.38
5 C	130.22	51.4008	132.46	-2.25
7 C	43.14	141.8390	46.52	-3.38
8 C	116.30	65.2176	119.33	-3.03
1 H	7.706	23.6114	7.848	-0.143
4 H	7.513	23.7637	7.704	-0.190
5 H	7.509	23.6769	7.786	-0.277
7 H	5.972	26.3120	5.282	0.689
9 N	49.3	204.248	48.5	0.9
10 N	259.2	-12.236	265.5	-6.4



Atom Number	Exptl. Chemical Shifts (ppm)	Isotropic shielding constants	Linearly Scaled Chemical Shifts (ppm)	Delta (ppm)
1 C	27.18	163.0255	26.38	0.79
2 C	53.54	133.1367	54.79	-1.24
3 C	70.02	116.6784	70.43	-0.41
4 C	32.16	156.7885	32.31	-0.15
5 C	20.01	169.5080	20.22	-0.22
1 H	1.618	30.0735	1.708	-0.090
1 H'	1.871	29.5995	2.158	-0.287
2 H	3.230	28.0731	3.609	-0.378
3 H	4.087	27.5060	4.148	-0.061
4 H	1.767	30.0228	1.756	0.011
4 H'	1.624	30.0764	1.705	-0.081
5 H	1.465	30.1528	1.633	-0.168
5 H'	1.742	29.8741	1.897	-0.155
6 N	39.9	217.915	34.8	5.2



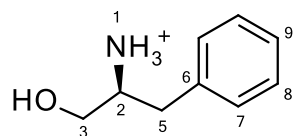
Atom Number	Exptl. Chemical Shifts (ppm)	Isotropic shielding constants	Linearly Scaled Chemical Shifts (ppm)	Delta (ppm)
2 C	56.45	129.6581	58.09	-1.64
3 C	70.21	117.0705	70.06	0.15
5 C	39.21	148.8317	39.87	-0.66
6 C	141.46	41.4173	141.95	-0.49
7 C	125.22	58.7970	125.43	-0.21
8 C	129.08	54.4021	129.61	-0.53
9 C	126.75	57.5767	126.59	0.16
10 C	125.22	60.9130	123.42	1.80
11 C	137.34	48.6822	135.04	2.29
2 H	4.539	26.8639	4.758	-0.219
3 H	4.603	26.9293	4.696	-0.093
5 H	3.121	28.5664	3.140	-0.019
5 H'	2.935	28.7851	2.932	0.003
7 H	7.277	23.9197	7.555	-0.278
8 H	7.320	23.8921	7.582	-0.261
9 H	7.310	23.9801	7.498	-0.188
10 H	7.491	23.8517	7.620	-0.129
1 N	36.4	221.341	31.3	5.1



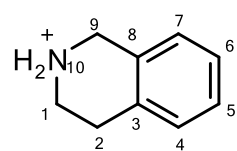
Atom Number	Exptl. Chemical Shifts (ppm)	Isotropic shielding constants	Linearly Scaled Chemical Shifts (ppm)	Delta (ppm)
1 C	127.23	56.8158	127.32	-0.09
2 C	138.13	46.3743	137.24	0.89
4 C	128.84	54.8567	129.18	-0.34
5 C	128.39	54.6738	129.35	-0.96
7 C	56.89	127.8453	59.82	-2.92
1 H	7.491	23.7023	7.762	-0.271
4 H	7.430	23.8611	7.611	-0.181

5 H	7.361	23.9055	7.569	-0.208
7 H	5.668	26.0341	5.546	0.121

*¹⁵N could not be obtained in experiment.

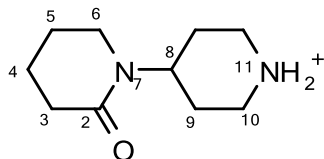


Atom Number	Exptl. Chemical Shifts (ppm)	Isotropic shielding constants	Linearly Scaled Chemical Shifts (ppm)	Delta (ppm)
2 C	53.59	132.1507	55.72	-2.13
3 C	59.58	127.4603	60.18	-0.60
5 C	34.86	154.0507	34.91	-0.05
6 C	136.55	46.8660	136.77	-0.22
7 C	129.25	54.5333	129.48	-0.24
8 C	128.59	55.2827	128.77	-0.18
9 C	126.80	57.1629	126.99	-0.18
2 H	3.325	28.1133	3.571	-0.245
3 H	3.361	27.9847	3.693	-0.332
3 H'	3.500	27.9721	3.705	-0.205
5 H	2.886	28.7215	2.993	-0.107
5 H'	2.809	28.9185	2.806	0.004
7 H	7.258	23.9608	7.516	-0.258
8 H	7.329	23.9179	7.557	-0.228
9 H	7.256	24.0192	7.461	-0.205
1 N	39.8	216.065	36.6	3.2

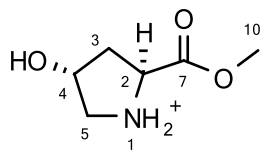


Atom Number	Exptl. Chemical Shifts (ppm)	Isotropic shielding constants	Linearly Scaled Chemical Shifts (ppm)	Delta (ppm)
1 C	40.67	145.1157	43.40	-2.73
2 C	24.62	163.7551	25.69	-1.07
3 C	131.89	51.4308	132.43	-0.54
4 C	128.81	55.6720	128.40	0.41
5 C	127.51	56.4309	127.68	-0.17
6 C	126.59	57.8937	126.29	0.30
7 C	126.77	57.7050	126.47	0.30
8 C	128.90	55.5715	128.50	0.40
9 C	43.75	142.5582	45.83	-2.09

1 H	3.391	28.1956	3.492	-0.101
2 H	2.998	28.6443	3.066	-0.068
4 H	7.213	24.0451	7.436	-0.223
5 H	7.263	24.0463	7.435	-0.172
6 H	7.251	24.0887	7.395	-0.144
7 H	7.203	24.1354	7.350	-0.147
9 H	4.280	27.3051	4.339	-0.059
10 N	35.2	211.433	41.3	-6.1

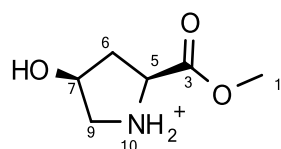


Atom Number	Exptl. Chemical Shifts (ppm)	Isotropic shielding constants	Linearly Scaled Chemical Shifts (ppm)	Delta (ppm)
2 C	168.28	13.6070	168.38	-0.09
3 C	32.15	156.3653	32.71	-0.56
4 C	20.25	168.3983	21.28	-1.03
5 C	22.75	166.1975	23.37	-0.62
6 C	41.67	146.7035	41.90	-0.22
8 C	47.75	141.9233	46.44	1.31
9 C	24.68	163.5845	25.85	-1.17
10 C	42.70	143.3134	45.12	-2.42
3 H	2.230	29.6193	2.140	0.090
4 H	1.651	30.2305	1.559	0.092
5 H	1.702	30.1831	1.604	0.098
6 H	3.126	28.7652	2.951	0.175
8 H	4.510	27.2562	4.385	0.125
9 H	1.597	30.1183	--	--
10 H	2.020	29.8838	1.888	0.132
12 H	2.930	28.5315	--	--
13 H	3.270	28.4594	3.242	0.028
7 N	127.7	121.465	131.5	-3.8
11 N	40.9	208.359	44.3	-3.5

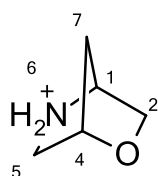


Atom Number	Exptl. Chemical Shifts (ppm)	Isotropic shielding constants	Linearly Scaled Chemical Shifts (ppm)	Delta (ppm)

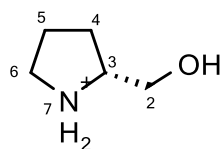
2 C	57.39	129.0335	58.69	-1.30
3 C	36.94	150.6929	38.10	-1.17
4 C	68.37	116.9154	70.20	-1.83
5 C	53.02	134.5139	53.48	-0.46
7 C	169.02	12.3423	169.58	-0.56
10 C	52.97	134.8633	53.15	-0.18
2 H	4.459	27.0957	4.537	-0.079
3 H	2.087	29.2757	2.466	-0.379
3 H'	2.193	29.6765	2.085	0.108
4 H	4.411	27.1570	4.479	-0.069
5 H	3.360	28.1597	3.527	-0.166
5 H'	3.068	28.2757	3.416	-0.349
10 H	3.751	27.8465	3.824	-0.073
1 N	52.9	202.448	50.3	2.6



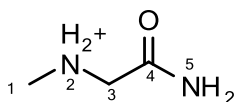
Atom Number	Exptl. Chemical Shifts (ppm)	Isotropic shielding constants	Linearly Scaled Chemical Shifts (ppm)	Delta (ppm)
1 C	53.01	134.8989	53.11	-0.10
3 C	169.63	11.9405	169.96	-0.33
5 C	57.41	129.0335	58.69	-1.28
6 C	37.01	151.4672	37.37	-0.36
7 C	68.11	118.4359	68.76	-0.64
9 C	52.98	134.9618	53.05	-0.07
1 H	3.747	27.8351	3.835	-0.088
5 H	4.485	27.3223	4.322	0.163
6 H	2.310	29.3109	2.433	-0.122
6 H'	2.137	29.4018	2.346	-0.209
7 H	4.366	27.2420	4.399	-0.032
9 H	3.205	28.2996	3.394	-0.188
9 H'	3.151	28.2000	3.488	-0.338
10 N	52.6	203.508	49.2	3.4



Atom Number	Exptl. Chemical Shifts (ppm)	Isotropic shielding constants	Linearly Scaled Chemical Shifts (ppm)	Delta (ppm)
1 C	56.98	129.1000	58.62	-1.64
2 C	68.50	119.8178	67.44	1.05
4 C	73.86	115.0469	71.98	1.88
5 C	51.68	133.7004	54.25	-2.57
7 C	34.84	155.3527	33.68	1.17
1 H	4.355	27.5346	4.120	0.235
2 H	3.651	27.9162	3.758	-0.107
2 H'	3.975	27.8890	3.784	0.191
4 H	4.617	27.2391	4.401	0.216
5 H	3.110	28.3917	3.306	-0.196
7 H	1.871	29.8532	1.917	-0.047
7 H'	1.923	29.7233	2.041	-0.118
6 N	51.0	200.780	51.9	-1.0



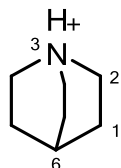
Atom Number	Exptl. Chemical Shifts (ppm)	Isotropic shielding constants	Linearly Scaled Chemical Shifts (ppm)	Delta (ppm)
2 C	60.17	128.5468	59.15	1.02
3 C	60.82	127.2430	60.39	0.43
4 C	25.83	163.3397	26.09	-0.26
5 C	23.33	164.2750	25.20	-1.87
6 C	44.92	141.3861	46.95	-2.03
2 H	3.562	27.9380	3.737	-0.176
3 H	3.535	27.9107	3.763	-0.229
4 H	1.603	29.9678	1.808	-0.205
4 H'	1.951	29.7116	2.052	-0.101
5 H	1.878	29.7840	1.983	-0.105
6 H	3.137	28.3810	3.316	-0.179
7 N	52.9	201.191	51.5	1.3



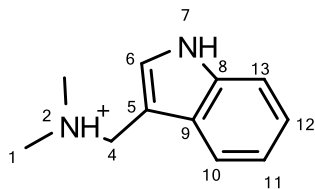
Atom Number	Exptl. Chemical Shifts (ppm)	Isotropic shielding constants	Linearly Scaled Chemical Shifts (ppm)	Delta (ppm)
1 C	32.60	155.4789	33.56	-0.95

3 C	48.86	138.6219	49.58	-0.72
4 C	166.90	16.8112	165.33	1.57
1 H	2.518	28.8792	2.843	-0.324
3 H	3.626	28.0441	3.636	-0.010
5 N	108.3	154.283	98.6	9.7

*Resonance of 2 N was not obtained in experiments.

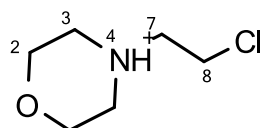


Atom Number	Exptl. Chemical Shifts (ppm)	Isotropic shielding constants	Linearly Scaled Chemical Shifts (ppm)	Delta (ppm)
1 C	22.80	166.3436	23.23	-0.43
2 C	45.73	141.4641	46.87	-1.15
6 C	18.91	169.2382	20.48	-1.57
1 H	1.780	29.9825	1.795	-0.015
2 H	3.214	28.5522	3.154	0.060
6 H	2.012	29.9755	1.801	0.211
3 N	30.8	212.953	39.7	-8.9



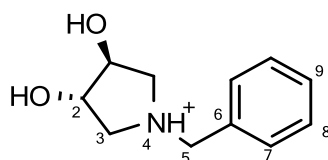
Atom Number	Exptl. Chemical Shifts (ppm)	Isotropic shielding constants	Linearly Scaled Chemical Shifts (ppm)	Delta (ppm)
1 C	41.18	147.5483	41.09	0.08
4 C	51.19	136.2709	51.81	-0.62
5 C	103.01	82.1128	103.28	-0.26
6 C	128.69	54.0986	129.90	-1.21
8 C	136.04	48.8806	134.86	1.18
9 C	127.24	58.1431	126.05	1.19
10 C	118.50	65.7945	118.78	-0.29
11 C	119.60	65.0152	119.52	0.08
12 C	121.75	62.1236	122.27	-0.52
13 C	111.93	72.6225	112.29	-0.36
1 H	2.743	28.9242	2.800	-0.058
3 H	2.743	28.8900	2.833	-0.090
4 H	4.443	27.4059	4.243	0.200

6 H	7.575	23.8814	7.592	-0.017
10 H	7.769	23.5582	7.899	-0.130
11 H	7.103	24.1438	7.342	-0.240
12 H	7.163	24.0567	7.425	-0.262
13 H	7.453	23.8253	7.645	-0.192
2 N	44.4	197.650	55.1	-10.6
7 N	138.2	117.396	135.6	2.7



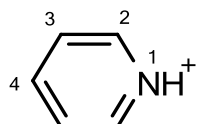
Atom Number	Exptl. Chemical Shifts (ppm)	Isotropic shielding constants	Linearly Scaled Chemical Shifts (ppm)	Delta (ppm)
2 C	62.97	125.3102	62.23	0.74
3 C	51.09	136.6661	51.43	-0.35
7 C	56.09	131.0717	56.75	-0.66
8 C*	36.82	147.9766	40.69	-3.87
2 H	3.828	27.9228	3.752	0.076
3 H	3.938	27.8954	3.778	0.160
5 H	3.431	28.6341	3.076	0.355
6 H	3.127	28.6552	3.056	0.071
7 H	3.493	28.4964	3.207	0.286
8 H	4.063	27.9437	3.732	0.331
4 N	50.6	196.620	56.1	-5.6

*8 C was excluded from linear scaling analysis due to the systematic errors caused by adjacent chlorine substitution.

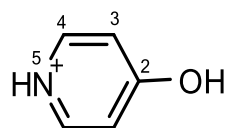


Atom Number	Exptl. Chemical Shifts (ppm)	Isotropic shielding constants	Linearly Scaled Chemical Shifts (ppm)	Delta (ppm)
2 C	74.28	113.1225	73.81	0.48
5 C	59.72	129.2478	58.48	1.24
6 C	131.12	51.8098	132.07	-0.95
7 C	130.62	53.2564	130.70	-0.08
8 C	128.83	54.9383	129.10	-0.27
9 C	129.41	54.0410	129.95	-0.55
2 H	4.117	27.6358	4.024	0.093
3 H	3.353	28.4750	3.227	0.126

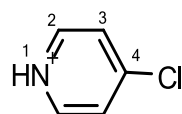
5 H	4.369	27.4167	4.233	0.136
7 H	7.536	23.7786	7.690	-0.154
8 H	7.451	23.8249	7.645	-0.195
9 H	7.448	23.8277	7.643	-0.195
12 H	3.290	28.0839	3.599	-0.308
13 H	4.141	27.5026	4.151	-0.009
4 N	61.2	181.652	71.1	-9.9



Atom Number	Exptl. Chemical Shifts (ppm)	Isotropic shielding constants	Linearly Scaled Chemical Shifts (ppm)	Delta (ppm)
2 C	142.15	41.2520	142.11	0.05
3 C	127.22	58.4008	125.81	1.41
4 C	146.36	32.4861	150.44	-4.08
2 H	8.950	22.8345	8.587	0.363
3 H	8.095	23.4353	8.016	0.079
4 H	8.626	22.6591	8.753	-0.127
1 N	206.2	55.204	197.9	8.3



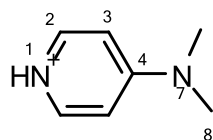
Atom Number	Exptl. Chemical Shifts (ppm)	Isotropic shielding constants	Linearly Scaled Chemical Shifts (ppm)	Delta (ppm)
2 C	171.75	12.3143	169.61	2.14
3 C	113.91	73.1356	111.81	2.10
4 C	142.80	38.9316	144.31	-1.51
3 H	7.271	24.2074	7.282	-0.011
4 H	8.573	23.0924	8.342	0.231
5 N	181.6	73.432	179.6	1.9



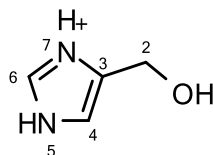
Atom Number	Exptl. Chemical Shifts (ppm)	Isotropic shielding constants	Linearly Scaled Chemical Shifts (ppm)	Delta (ppm)

2 C	144.39	40.0764	143.22	1.17
3 C	127.25	57.7635	126.41	0.83
4 C*	151.28	22.3983	160.02	-8.74
2 H	8.902	22.9406	8.485	0.418
3 H	8.146	23.4496	8.001	0.145
1 N*	218.2	58.301	194.8	23.4

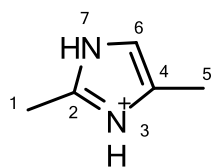
*4 C, and 1 N was excluded from the linear scaling analysis due to the systematic errors caused by chlorine substitution.



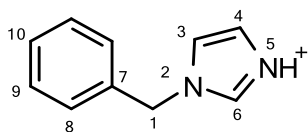
Atom Number	Exptl. Chemical Shifts (ppm)	Isotropic shielding constants	Linearly Scaled Chemical Shifts (ppm)	Delta (ppm)
2 C	139.02	43.8907	139.60	-0.58
3 C	106.95	80.6595	104.66	2.29
4 C	157.01	24.6203	157.91	-0.90
8 C	39.58	149.6288	39.12	0.47
2 H	8.226	23.5040	7.950	0.276
3 H	6.979	24.7610	6.756	0.223
8 H	3.177	28.5832	3.124	0.053
1 N	164.7	94.167	158.8	5.9
7 N	88.0	158.441	94.4	-6.4



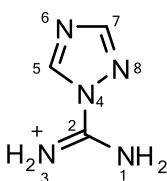
Atom Number	Exptl. Chemical Shifts (ppm)	Isotropic shielding constants	Linearly Scaled Chemical Shifts (ppm)	Delta (ppm)
2 C	53.18	134.2025	53.78	-0.59
3 C	133.85	52.7611	131.17	2.68
4 C	115.88	67.8729	116.81	-0.92
6 C	133.95	48.1079	135.59	-1.64
7 N	177.9	78.778	174.3	3.6



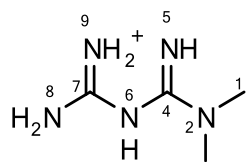
Atom Number	Exptl. Chemical Shifts (ppm)	Isotropic shielding constants	Linearly Scaled Chemical Shifts (ppm)	Delta (ppm)
1 C	10.97	179.1929	11.02	-0.05
2 C	143.16	36.5661	146.56	-3.40
4 C	128.09	53.3414	130.62	-2.53
5 C	9.43	181.1505	9.16	0.27
6 C	114.97	72.0582	112.83	2.14
3 N	178.5	77.296	175.8	2.8
7 N	173.3	82.213	170.8	2.5



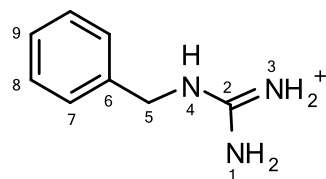
Atom Number	Exptl. Chemical Shifts (ppm)	Isotropic shielding constants	Linearly Scaled Chemical Shifts (ppm)	Delta (ppm)
1 C	51.64	135.6950	52.36	-0.72
3 C	122.06	63.3045	121.15	0.91
4 C	120.28	64.4486	120.06	0.22
6 C	135.43	48.3439	135.37	0.06
7 C	135.13	48.0807	135.62	-0.49
8 C	128.18	54.2750	129.73	-1.55
9 C	128.98	55.2754	128.78	0.20
10 C	128.65	55.0744	128.97	-0.32



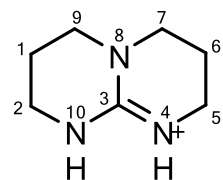
Atom Number	Exptl. Chemical Shifts (ppm)	Isotropic shielding constants	Linearly Scaled Chemical Shifts (ppm)	Delta (ppm)
5 C	146.24	37.9635	145.23	1.01
7 C	153.89	29.7408	153.04	0.85
4 N	215.5	37.413	215.8	-0.3
6 N	261.9	-12.212	265.5	-3.6
8 N	287.5	-30.358	283.7	3.8



Atom Number	Exptl. Chemical Shifts (ppm)	Isotropic shielding constants	Linearly Scaled Chemical Shifts (ppm)	Delta (ppm)
1 C	38.41	153.1640	35.76	2.65
4 C	155.90	30.9847	151.86	4.04
1 H	3.010	29.0227	2.706	0.303

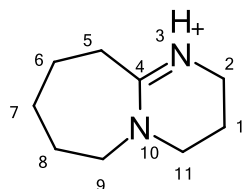


Atom Number	Exptl. Chemical Shifts (ppm)	Isotropic shielding constants	Linearly Scaled Chemical Shifts (ppm)	Delta (ppm)
5 C	43.92	144.7777	43.73	0.20
6 C	137.25	45.6186	137.96	-0.71
7 C	127.19	56.3020	127.80	-0.61
8 C	128.55	55.4485	128.61	-0.07
9 C	127.46	56.4690	127.65	-0.18
5 H	4.385	27.4484	4.202	0.183
7 H	7.310	23.8680	7.605	-0.295
8 H	7.377	23.9016	7.573	-0.196
9 H	7.316	23.9738	7.504	-0.188
4 N	85.5	166.164	86.6	-1.1

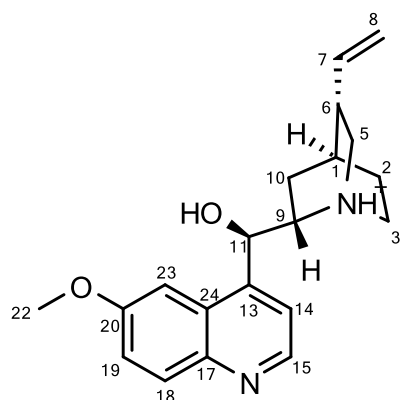


Atom Number	Exptl. Chemical Shifts (ppm)	Isotropic shielding constants	Linearly Scaled Chemical Shifts (ppm)	Delta (ppm)
1 C	20.39	168.9943	20.71	-0.32
2 C	37.64	151.1433	37.68	-0.04
3 C	150.63	34.2408	148.77	1.86
7 C	46.25	143.4826	44.96	1.30
1 H	1.866	29.9183	1.856	0.011

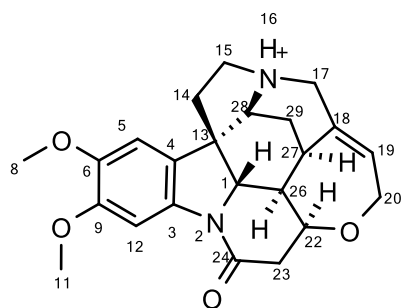
2 H	3.168	28.5676	3.139	0.029
7 H	3.255	28.6073	3.101	0.154
4 N	73.6	179.005	73.8	-0.2
8 N	80.3	168.182	84.6	-4.3



Atom Number	Exptl. Chemical Shifts (ppm)	Isotropic shielding constants	Linearly Scaled Chemical Shifts (ppm)	Delta (ppm)
1 C	18.82	170.0443	19.71	-0.90
2 C	37.45	150.7253	38.07	-0.62
4 C	165.33	15.3392	166.73	-1.40
5 C	31.54	155.0792	33.94	-2.40
6 C	23.29	165.8142	23.73	-0.44
7 C	28.21	160.8471	28.45	-0.25
8 C	25.89	162.9936	26.41	-0.53
9 C	53.35	135.9786	52.09	1.27
11 C	47.85	141.2913	47.04	0.82
1 H	1.914	29.9174	1.856	0.058
2 H	3.248	28.5291	3.175	0.073
5 H	2.658	29.2971	2.446	0.212
6 H	1.623	30.2170	1.572	0.051
7 H	1.670	30.1762	1.610	0.059
8 H	1.610	30.2630	1.528	0.082
9 H	3.550	28.3937	3.304	0.246
11 H	3.477	28.4309	3.269	0.208
3 N	114.7	140.780	112.1	2.6
10 N	121.2	123.046	129.9	-8.7



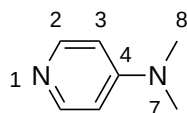
Atom Number	Exptl. Chemical Shifts (ppm)	Isotropic shielding constants	Linearly Scaled Chemical Shifts (ppm)	Delta (ppm)
4 N	42.1	207.087	45.6	-3.5



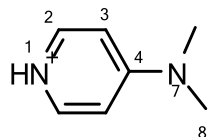
Atom Number	Exptl. Chemical Shifts (ppm)	Isotropic shielding constants	Linearly Scaled Chemical Shifts (ppm)	Delta (ppm)
1 C	58.83	129.0747	58.55	0.29
3 C	135.54	48.1384	135.55	-0.01
4 C	120.34	64.9969	119.51	0.83
5 C	107.00	78.2405	106.91	0.09
6 C	145.93	38.9426	144.30	1.63
8 C	56.04	134.4307	53.45	2.59
9 C	149.37	33.7780	149.21	0.16
11 C	55.69	135.3862	52.54	3.15
12 C	100.33	87.2871	98.30	2.03
14 C	39.68	149.4899	39.12	0.56
15 C	50.55	137.8185	50.23	0.32
17 C	51.45	136.2000	51.77	-0.31
18 C	132.96	47.3296	136.32	-3.36
19 C	134.69	46.9538	136.67	-1.99
20 C	63.14	126.6717	60.83	2.31
22 C	76.12	113.2011	73.65	2.47
23 C	40.81	146.2972	42.16	-1.35
24 C	168.46	11.7487	170.17	-1.71
26 C	46.26	142.3065	45.96	0.30
27 C	29.64	158.6049	30.45	-0.81
28 C	60.88	124.9525	62.47	-1.58
29 C	24.29	165.2961	24.08	0.21
27 H	3.314	28.5752	3.155	0.159
26 H	1.423	30.7017	1.149	0.274
1 H	4.035	27.8689	3.821	0.213
22 H	4.361	27.6364	4.041	0.320

5 H	7.094	24.5358	6.965	0.129
8 H	3.764	27.9666	3.729	0.035
11 H	3.736	27.8852	3.806	-0.070
12 H	7.645	23.8046	7.655	-0.010
14 H	2.099	29.7822	2.017	0.082
14 H'	1.967	29.7895	2.010	-0.043
15 H	3.125	28.4182	3.303	-0.178
15 H'	3.736	28.1515	3.555	0.181
17 H	4.130	27.6689	4.010	0.120
17 H'	3.520	28.3808	3.338	0.182
19 H	6.327	25.0892	6.443	-0.116
20 H	4.144	27.5722	4.101	0.042
23 H	2.612	29.2222	2.545	0.067
23 H'	2.924	28.8719	2.875	0.049
28 H	4.514	27.4538	4.213	0.301
29 H	2.511	29.4773	2.304	0.207
29 H'	1.588	30.3063	1.522	0.066
2 N	149.4	99.075	153.1	-3.7
16 N	59.9	187.638	64.3	-4.4

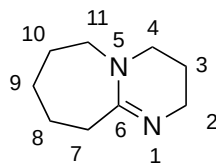
6. Calculated and Experimental Chemical Shifts for Compounds Used in Protonation Ratio Determination



Atom Number	Exptl. Chemical Shifts (ppm)	Isotropic shielding constants	Linearly Scaled Chemical Shifts (ppm)
2 C	149.3238	32.89846315	150.0638
3 C	106.6467	81.73707263	103.5373
4 C	153.8747	29.11850528	153.6647563
8 C	38.5265	151.3431758	37.22683
2 H	8.1035	23.28308631	8.137188
3 H	6.5782	25.00861369	6.510161
8 H	2.9423	28.75261212	2.957001
1 N	276.64	94.167	61.65294065
7 N		158.441	269.8956756



Atom Number	Exptl. Chemical Shifts (ppm)	Isotropic shielding constants	Linearly Scaled Chemical Shifts (ppm)
2 C	139.02	43.8907	139.60
3 C	106.95	80.6595	104.66
4 C	157.01	24.6203	157.91
8 C	39.58	149.6288	39.12
2 H	8.226	23.5040	7.950
3 H	6.979	24.7610	6.756
8 H	3.177	28.5832	3.124
1 N	164.7	94.167	158.8
7 N	88.0	158.441	94.4

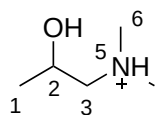


Atom Number	Exptl. Chemical Shifts (ppm)	Isotropic shielding constants	Linearly Scaled Chemical Shifts (ppm)
2 C	43.48	145.2009	43.32334
3 C	22.34	167.6091	22.02883
4 C	47.49	142.5267	45.86463
6 C	159.5	20.2939	162.0223
7 C	36.33	151.0191	37.79426
8 C	25.78	163.6581	25.78345
9 C	29.09	160.328	28.94806
10 C	28.11	160.9866	28.32213
11 C	51.78	138.4437	49.74467
2 H	3.0686	28.67248	3.03926
3 H	1.647	30.23393	1.564558
4 H	3.133	28.74206	3.013992
7 H	2.245	29.62772	2.132202
8 H	1.521	30.32785	1.466113
9 H	1.567	30.28847	1.503998
10 H	1.492	30.33855	1.408826
11 H	3.141	28.53767	2.990864
1 N	207.6	55.42672	197.6968

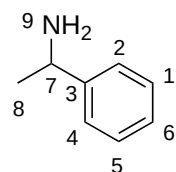
5 N	89.5	154.589	98.25608

Atom Number	Exptl. Chemical Shifts (ppm)	Isotropic shielding constants	Linearly Scaled Chemical Shifts (ppm)
2 C	37.45	150.7253	38.07
3 C	18.82	170.0443	19.71
4 C	47.85	141.2913	47.04
6 C	165.33	15.3392	166.73
7 C	31.54	155.0792	33.94
8 C	23.29	165.8142	23.73
9 C	28.21	160.8471	28.45
10 C	25.89	162.9936	26.41
11 C	53.35	135.9786	52.09
2 H	3.248	28.5291	3.175
3 H	1.914	29.9174	1.856
4 H	3.477	28.4309	3.269
7 H	2.658	29.2971	2.446
8 H	1.623	30.2170	1.572
9 H	1.670	30.1762	1.610
10 H	1.610	30.2630	1.528
11 H	3.550	28.3937	3.304
1 N	114.7	140.780	112.1
5 N	121.2	123.046	129.9

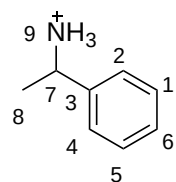
Atom Number	Exptl. Chemical Shifts (ppm)	Isotropic shielding constants	Linearly Scaled Chemical Shifts (ppm)
1 C	21.655	171.1203	18.69213
2 C	63.627	127.378	60.26037
3 C	67.308	124.0662	63.40756
6 C	45.79	146.983	41.62979
1 H	1.0162	30.43864	1.026592
2 H	3.6765	28.08258	3.599795
3 Ha	2.0565	29.81647	1.952236
3 Hb	2.1506	29.75734	2.008421
6 H	2.1377	29.29954	2.158864
5 N	20.71	230.8692	21.76172



Atom Number	Exptl. Chemical Shifts (ppm)	Isotropic shielding constants	Linearly Scaled Chemical Shifts (ppm)
1 C	21.042	170.0709	19.6893
2 C	60.76	127.0361	60.58532
3 C	62.62	126.7712	60.83699
6 C	41.38	149.4109	39.32255
7 C	44.13	145.0637	43.45368
1 H	1.0954	30.37732	1.196651
2 H	4.007	27.56684	4.089854
3 Ha	2.94	28.82947	2.890088
3 Hb	3.05	28.83861	2.881407
6 H	2.7779	29.25669	2.812867
5 N	37.26	210.4	42.28841

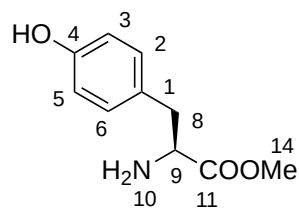


Atom Number	Exptl. Chemical Shifts (ppm)	Isotropic shielding constants	Linearly Scaled Chemical Shifts (ppm)
1 C	127.97	56.06593	128.2791
2 C	125.72	57.30182	125.9634
3 C	148.7	33.80547	149.1823
6 C	126.1	58.00811	126.1825
7 C	50.6	136.869	51.24106
8 C	26.2	163.0169	26.3928
1 H	7.2873	24.01571	7.426679
2 H	7.3633	24.04823	7.640855
6 H	7.1808	24.09462	7.389188
7 H	3.98	27.63514	4.024956
8 H	1.245	30.53151	1.223443
9 N	43.22	216.9991	35.7

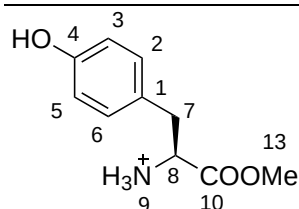


Atom Number	Exptl. Chemical Shifts (ppm)	Isotropic shielding constants	Linearly Scaled Chemical Shifts (ppm)

1 C	128.75	55.0197	129.02
2 C	126.72	56.6575	127.47
3 C	139.22	45.6093	137.97
6 C	128.47	54.4173	129.59
7 C	49.93	133.8297	54.13
8 C	20.63	169.7602	19.98
1 H	7.427	23.7977	7.671
2 H	7.481	23.7945	7.674
6 H	7.398	23.8724	7.600
7 H	4.406	27.2433	4.397
8 H	1.498	30.0912	1.691
9 N	47.6	202.602	50.1

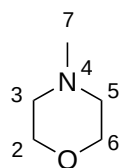


Atom Number	Exptl. Chemical Shifts (ppm)	Isotropic shielding constants	Linearly Scaled Chemical Shifts (ppm)
1 C	127.79	54.25184	127.79
2 C	130.13	52.89915	131.2228
3 C	115.07	71.89744	112.9429
4 C	155.96	28.63165	154.099
8 C	40.05	148.971	39.74057
9 C	55.94	131.8143	56.04459
11 C	175.46	5.6622	175.9268
14 C	51.30	137.9176	50.24463
2 H	6.94	24.24135	7.252085
3 H	6.65	24.62191	6.87284
8 Ha	2.659	29.11903	2.614951
8 Hb	2.738	28.99212	2.735536
9 H	3.48	28.42349	3.275859
14 H	3.56	28.14444	3.520615
10 N	28.7	231.099	21.53132

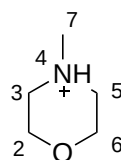


Atom Number	Exptl. Chemical Shifts (ppm)	Isotropic shielding constants	Linearly Scaled Chemical Shifts (ppm)

1 C	124.4	59.63743	124.4
2 C	130.36	51.53148	132.0158
3 C	115.48	70.99565	113.7906
4 C	156.76	27.29168	155.3723
7 C	35.07	153.6223	35.32042
8 C	53.55	131.5387	56.30645
10 C	169.43	13.7286	168.2613
13 C	52.51	135.5732	52.47245
2 H	6.999	24.12151	7.336131
3 H	6.738	24.52751	6.95083
7 Ha	2.999	28.73188	2.982816
7 Hb	3.098	28.5612	3.144999
8 H	4.104	27.60492	4.053673
13 H	3.635	27.90377	3.786969
9 N	41.7	217.2253	35.44399



Atom Number	Exptl. Chemical Shifts (ppm)	Isotropic shielding constants	Linearly Scaled Chemical Shifts (ppm)
2 C	66	123.0695	64.35524
3 C	55	135.3081	52.72369
7 C	46	145.7994	42.75454
2 Ha	3.549	28.32054	3.4794
2 Hb	3.549	28.09805	3.4794
3 Ha	2.269	29.33581	2.141227
3 Hb	2.269	29.89929	2.141227
7 H	2.148	29.72288	2.135871
4 N	36.1	215.3871	37.28726



Atom Number	Exptl. Chemical Shifts (ppm)	Isotropic shielding constants	Linearly Scaled Chemical Shifts (ppm)
2 C	63.4	125.202	62.32808
3 C	52.4	135.1054	52.91485
7 C	42.4	146.3548	42.22672
2 Ha	3.629	28.09471	3.58829
2 Hb	3.963	27.82369	3.845837

3 Ha	3.37	28.59822	3.10978
3 Hb	3.063	28.82186	2.897345
7 H	2.814	28.97027	2.790087
4 N	41.91	201.0497	51.66498

7. Gaussian Output: Coordinates, Energies and Shielding Constants

Dimethylaminopyridine_neutral

Dimethylaminopyridine_protonated

1-(dimethylamino)propan-2-ol_neutral

1-(dimethylamino)propan-2-ol_protonated

1,2,3,4-tetrahydroisoquinoline_neutral

1,2,3,4-tetrahydroisoquinoline_protonated

1-benzylguanidine_neutral

1-benzylguanidine_protonated

Methyl L-tyrosinate_neutral

Methyl L-tyrosinate_protonated

2-(pyrrolidin-1-yl)ethan-1-ol_neutral

2-(pyrrolidin-1-yl)ethan-1-ol_protonated

2,3,4,6,7,8,9,10-octahydropyrimido[1,2-a]azepine_neutral

2,3,4,6,7,8,9,10-octahydropyrimido[1,2-a]azepine_protonated

4-amino-butan-1-ol_neutral

4-amino-butan-1-ol_protonated

Cyclohexanamine_neutral

Cyclohexanamine_protonated

1-phenylethan-1-amine_neutral

1-phenylethan-1-amine_protonated

4-methylmorpholine_neutral

4-methylmorpholine_protonated

Piperidine_neutral

Piperidine_protonated

Quinuclidine_neutral

Quinuclidine_protonated

Brucine_neutral

Brucine_protonated

Dimethylaminopyridine_neutral

Conformer 1

C	0.065056728010	-0.008430379785	0.012554329566
C	-0.729594201745	-0.577475270543	-1.009194434336
C	-2.105042051587	-0.573906141642	-0.880713096858
N	-2.777005846625	-0.063116041109	0.159054816419
C	-2.021823099268	0.475094071022	1.125278455379
C	-0.641607181762	0.531642072011	1.111736125503
N	1.419152276137	0.017711741882	-0.057291250801
C	2.100539387705	-0.551155867945	-1.207053593355
C	2.192834644459	0.613326042206	1.018120895830
H	-0.285342506063	-1.017494860107	-1.893015887175
H	-2.708602260530	-1.014083969011	-1.672154845425
H	-2.557280262263	0.893333795089	1.975444725000
H	-0.126073597456	0.990050814507	1.946124389496
H	3.175185126790	-0.432977270786	-1.075546006773
H	1.884970100173	-1.620459575498	-1.314344350391
H	1.812403862325	-0.046107217725	-2.136175283135
H	1.947911216200	1.673402884362	1.150785218695
H	2.022060043992	0.097898159274	1.970263206350
H	3.251957621509	0.537347013798	0.776026586011

SCF Done: E(RwB97X) = -382.263379204

Zero-point correction=	0.163515
Thermal correction to Energy=	0.171136
Thermal correction to Enthalpy=	0.172080
Thermal correction to Gibbs Free Energy=	0.131327
Sum of electronic and zero-point Energies=	-382.099864
Sum of electronic and thermal Energies=	-382.092243
Sum of electronic and thermal Enthalpies=	-382.091299
Sum of electronic and thermal Free Energies=	-382.132052

1	C	Isotropic =	29.1198	Anisotropy =	189.8498
2	C	Isotropic =	81.7369	Anisotropy =	142.9432

3	C	Isotropic =	32.8976	Anisotropy =	174.7200
4	N	Isotropic =	-16.7758	Anisotropy =	469.6526
5	C	Isotropic =	32.8976	Anisotropy =	174.7201
6	C	Isotropic =	81.7369	Anisotropy =	142.9432
7	N	Isotropic =	190.8200	Anisotropy =	89.5635
8	C	Isotropic =	151.3405	Anisotropy =	57.1497
9	C	Isotropic =	151.3405	Anisotropy =	57.1497
10	H	Isotropic =	25.0087	Anisotropy =	8.6128
11	H	Isotropic =	23.2830	Anisotropy =	6.5270
12	H	Isotropic =	23.2830	Anisotropy =	6.5270
13	H	Isotropic =	25.0087	Anisotropy =	8.6128
14	H	Isotropic =	28.8700	Anisotropy =	8.0149
15	H	Isotropic =	28.7314	Anisotropy =	9.4061
16	H	Isotropic =	28.7289	Anisotropy =	9.4066
17	H	Isotropic =	28.7295	Anisotropy =	9.4039
18	H	Isotropic =	28.7308	Anisotropy =	9.4088
19	H	Isotropic =	28.8700	Anisotropy =	8.0149

Conformer 2

SCF Done: E(RwB97X) = -382.263379216

Zero-point correction=	0.163590
Thermal correction to Energy=	0.172084
Thermal correction to Enthalpy=	0.173028
Thermal correction to Gibbs Free Energy=	0.129578
Sum of electronic and zero-point Energies=	-382.099790
Sum of electronic and thermal Energies=	-382.091296
Sum of electronic and thermal Enthalpies=	-382.090351
Sum of electronic and thermal Free Energies=	-382.133802

1	C	Isotropic =	29.1183	Anisotropy =	189.8507
2	C	Isotropic =	81.7371	Anisotropy =	142.9430
3	C	Isotropic =	32.8986	Anisotropy =	174.7204
4	N	Isotropic =	-16.7745	Anisotropy =	469.6486
5	C	Isotropic =	32.8986	Anisotropy =	174.7205
6	C	Isotropic =	81.7377	Anisotropy =	142.9427
7	N	Isotropic =	190.8205	Anisotropy =	89.5696
8	C	Isotropic =	151.3436	Anisotropy =	57.1444
9	C	Isotropic =	151.3441	Anisotropy =	57.1444
10	H	Isotropic =	25.0086	Anisotropy =	8.6130
11	H	Isotropic =	23.2831	Anisotropy =	6.5270
12	H	Isotropic =	23.2831	Anisotropy =	6.5270
13	H	Isotropic =	25.0086	Anisotropy =	8.6128

14	H	Isotropic =	28.7340	Anisotropy =	9.3912
15	H	Isotropic =	28.8700	Anisotropy =	8.0154
16	H	Isotropic =	28.7267	Anisotropy =	9.4214
17	H	Isotropic =	28.7265	Anisotropy =	9.4213
18	H	Isotropic =	28.7342	Anisotropy =	9.3914
19	H	Isotropic =	28.8700	Anisotropy =	8.0154

Dimethylaminopyridine_protonated
Conformer 1

```

-----
N   -2.676269320043   -0.342442072615   -0.318345301909
C   -1.993743165124   -1.213421578386    0.454790233001
C   -0.647291526305   -1.100250677825    0.619132651378
C    0.065363130517   -0.049020492285   -0.031483035090
C   -0.702977575646    0.843712757527   -0.837050580510
C   -2.047756547350    0.668852546283   -0.954299814052
N    1.384326270735    0.092131615006    0.106535706442
C    2.088018984987    1.168600474569   -0.583061178566
C    2.141321642440   -0.827954016979    0.949105265125
H   -3.677655408335   -0.449618335590   -0.423127439976
H   -2.576454183505   -1.994337427493    0.926929245919
H   -0.142207163590   -1.821207973566    1.245890927284
H   -0.242692875701    1.668001683491   -1.362789431211
H   -2.671786856023    1.320620586323   -1.552699058092
H    1.731987884422    2.147709573544   -0.248752968943
H    3.150052073144    1.091434168066   -0.360303144234
H    1.955768102836    1.091986599703   -1.666259335120
H    1.777216855099   -0.804192819067    1.980390460135
H    2.074071353893   -1.852409573135    0.570768380345
H    3.186308323551   -0.525495037571    0.946628418074

```

SCF Done: E(RwB97X) = -382.734188284

```

Zero-point correction=          0.177592
Thermal correction to Energy=      0.186137
Thermal correction to Enthalpy=    0.187082
Thermal correction to Gibbs Free Energy= 0.144360
Sum of electronic and zero-point Energies= -382.556596
Sum of electronic and thermal Energies= -382.548051
Sum of electronic and thermal Enthalpies= -382.547107
Sum of electronic and thermal Free Energies= -382.589829

```

1	N	Isotropic =	94.1669	Anisotropy =	201.1307
2	C	Isotropic =	43.8909	Anisotropy =	175.0926

3 C	Isotropic =	80.6593	Anisotropy =	147.4794
4 C	Isotropic =	24.6209	Anisotropy =	193.0503
5 C	Isotropic =	80.6600	Anisotropy =	147.4791
6 C	Isotropic =	43.8904	Anisotropy =	175.0934
7 N	Isotropic =	158.4411	Anisotropy =	65.9250
8 C	Isotropic =	149.6277	Anisotropy =	59.3428
9 C	Isotropic =	149.6265	Anisotropy =	59.3418
10 H	Isotropic =	22.5078	Anisotropy =	7.8925
11 H	Isotropic =	23.5040	Anisotropy =	4.5997
12 H	Isotropic =	24.7611	Anisotropy =	7.9116
13 H	Isotropic =	24.7611	Anisotropy =	7.9111
14 H	Isotropic =	23.5040	Anisotropy =	4.5997
15 H	Isotropic =	28.5122	Anisotropy =	9.0619
16 H	Isotropic =	28.6969	Anisotropy =	7.8461
17 H	Isotropic =	28.5401	Anisotropy =	8.9507
18 H	Isotropic =	28.5403	Anisotropy =	8.9513
19 H	Isotropic =	28.5120	Anisotropy =	9.0612
20 H	Isotropic =	28.6970	Anisotropy =	7.8460

Conformer 2

SCF Done: E(RwB97X) = -382.734188274

Zero-point correction=	0.177593
Thermal correction to Energy=	0.186137
Thermal correction to Enthalpy=	0.187082
Thermal correction to Gibbs Free Energy=	0.144368
Sum of electronic and zero-point Energies=	-382.556595
Sum of electronic and thermal Energies=	-382.548051
Sum of electronic and thermal Enthalpies=	-382.547107
Sum of electronic and thermal Free Energies=	-382.589820

1 N	Isotropic =	94.1707	Anisotropy =	201.1242
2 C	Isotropic =	43.8906	Anisotropy =	175.0927
3 C	Isotropic =	80.6623	Anisotropy =	147.4769
4 C	Isotropic =	24.6221	Anisotropy =	193.0506
5 C	Isotropic =	80.6591	Anisotropy =	147.4749
6 C	Isotropic =	43.8920	Anisotropy =	175.0905
7 N	Isotropic =	158.4393	Anisotropy =	65.9155
8 C	Isotropic =	149.6308	Anisotropy =	59.3456
9 C	Isotropic =	149.6243	Anisotropy =	59.3400
10 H	Isotropic =	22.5080	Anisotropy =	7.8926
11 H	Isotropic =	23.5041	Anisotropy =	4.5996
12 H	Isotropic =	24.7614	Anisotropy =	7.9102

13	H	Isotropic =	24.7610	Anisotropy =	7.9122
14	H	Isotropic =	23.5041	Anisotropy =	4.5996
15	H	Isotropic =	28.5119	Anisotropy =	9.0622
16	H	Isotropic =	28.6967	Anisotropy =	7.8464
17	H	Isotropic =	28.5406	Anisotropy =	8.9509
18	H	Isotropic =	28.5407	Anisotropy =	8.9487
19	H	Isotropic =	28.5118	Anisotropy =	9.0629
20	H	Isotropic =	28.6970	Anisotropy =	7.8460

Conformer 3

SCF Done: E(RwB97X) = -382.734188276

Zero-point correction=	0.177592
Thermal correction to Energy=	0.186137
Thermal correction to Enthalpy=	0.187081
Thermal correction to Gibbs Free Energy=	0.144356
Sum of electronic and zero-point Energies=	-382.556597
Sum of electronic and thermal Energies=	-382.548051
Sum of electronic and thermal Enthalpies=	-382.547107
Sum of electronic and thermal Free Energies=	-382.589832

1	N	Isotropic =	94.1640	Anisotropy =	201.1352
2	C	Isotropic =	43.8908	Anisotropy =	175.0929
3	C	Isotropic =	80.6591	Anisotropy =	147.4834
4	C	Isotropic =	24.6170	Anisotropy =	193.0516
5	C	Isotropic =	80.6576	Anisotropy =	147.4818
6	C	Isotropic =	43.8900	Anisotropy =	175.0939
7	N	Isotropic =	158.4426	Anisotropy =	65.9425
8	C	Isotropic =	149.6289	Anisotropy =	59.3343
9	C	Isotropic =	149.6322	Anisotropy =	59.3384
10	H	Isotropic =	22.5076	Anisotropy =	7.8924
11	H	Isotropic =	23.5039	Anisotropy =	4.5997
12	H	Isotropic =	24.7609	Anisotropy =	7.9111
13	H	Isotropic =	24.7607	Anisotropy =	7.9121
14	H	Isotropic =	23.5039	Anisotropy =	4.5999
15	H	Isotropic =	28.5407	Anisotropy =	8.9509
16	H	Isotropic =	28.6972	Anisotropy =	7.8465
17	H	Isotropic =	28.5120	Anisotropy =	9.0616
18	H	Isotropic =	28.5125	Anisotropy =	9.0615
19	H	Isotropic =	28.5402	Anisotropy =	8.9518
20	H	Isotropic =	28.6968	Anisotropy =	7.8468

Conformer 4

SCF Done: E(RwB97X) = -382.734188274

Zero-point correction= 0.177593
 Thermal correction to Energy= 0.186137
 Thermal correction to Enthalpy= 0.187081
 Thermal correction to Gibbs Free Energy= 0.144372
 Sum of electronic and zero-point Energies= -382.556595
 Sum of electronic and thermal Energies= -382.548051
 Sum of electronic and thermal Enthalpies= -382.547107
 Sum of electronic and thermal Free Energies= -382.589817

1	N	Isotropic =	94.1662	Anisotropy =	201.1315
2	C	Isotropic =	43.8871	Anisotropy =	175.0997
3	C	Isotropic =	80.6589	Anisotropy =	147.4796
4	C	Isotropic =	24.6214	Anisotropy =	193.0496
5	C	Isotropic =	80.6601	Anisotropy =	147.4799
6	C	Isotropic =	43.8937	Anisotropy =	175.0871
7	N	Isotropic =	158.4428	Anisotropy =	65.9268
8	C	Isotropic =	149.6305	Anisotropy =	59.3390
9	C	Isotropic =	149.6292	Anisotropy =	59.3362
10	H	Isotropic =	22.5078	Anisotropy =	7.8924
11	H	Isotropic =	23.5038	Anisotropy =	4.5997
12	H	Isotropic =	24.7610	Anisotropy =	7.9119
13	H	Isotropic =	24.7611	Anisotropy =	7.9111
14	H	Isotropic =	23.5041	Anisotropy =	4.5996
15	H	Isotropic =	28.5408	Anisotropy =	8.9493
16	H	Isotropic =	28.6970	Anisotropy =	7.8467
17	H	Isotropic =	28.5118	Anisotropy =	9.0634
18	H	Isotropic =	28.5119	Anisotropy =	9.0633
19	H	Isotropic =	28.5406	Anisotropy =	8.9490
20	H	Isotropic =	28.6969	Anisotropy =	7.8466

1-(dimethylamino)propan-2-ol_neutral
 Conformer_1

C	-0.223850856838	1.215078147459	0.684969744896
C	0.524486762133	-0.088604722511	0.860477714923
C	1.626231562758	-0.258000968421	-0.181821102866
O	-0.396566188896	-1.170950934076	0.739908891223
N	2.193006412344	-1.602647644735	-0.132097550307
C	2.847811295672	-1.951605372077	-1.383121581144
C	3.110130347172	-1.765958998051	0.986717178607

H	-1.016155680643	1.308085135399	1.432991855134
H	0.455720728008	2.064955699199	0.802603019650
H	-0.678843675820	1.267361643722	-0.309569517510
H	0.968265242038	-0.110541663243	1.866488092969
H	2.399184593191	0.518019060791	-0.044201499706
H	1.179996213979	-0.116405738363	-1.172641778245
H	0.149556099294	-1.928278593694	0.483376353245
H	3.217020865322	-2.979903126614	-1.332972050109
H	2.135652907427	-1.882939483460	-2.209747158811
H	3.704250748888	-1.291493152777	-1.606727252606
H	2.605534846290	-1.562668151975	1.934629877529
H	3.980474888731	-1.090880907969	0.908284310055
H	3.476292888949	-2.795720228605	1.016152453072

SCF Done: E(RwB97X) = -328.343630500

Zero-point correction=	0.183691
Thermal correction to Energy=	0.192464
Thermal correction to Enthalpy=	0.193408
Thermal correction to Gibbs Free Energy=	0.150754
Sum of electronic and zero-point Energies=	-328.159939
Sum of electronic and thermal Energies=	-328.151167
Sum of electronic and thermal Enthalpies=	-328.150223
Sum of electronic and thermal Free Energies=	-328.192876

1 C	Isotropic = 171.1930	Anisotropy = 35.6826
2 C	Isotropic = 127.5723	Anisotropy = 53.6587
3 C	Isotropic = 124.0487	Anisotropy = 53.8802
4 O	Isotropic = 284.6393	Anisotropy = 44.4524
5 N	Isotropic = 230.9512	Anisotropy = 37.0726
6 C	Isotropic = 144.3884	Anisotropy = 71.6406
7 C	Isotropic = 149.7824	Anisotropy = 64.2136
8 H	Isotropic = 30.4260	Anisotropy = 10.0114
9 H	Isotropic = 30.8862	Anisotropy = 9.6369
10 H	Isotropic = 31.0720	Anisotropy = 7.9873
11 H	Isotropic = 28.0859	Anisotropy = 5.6210
12 H	Isotropic = 29.8247	Anisotropy = 4.6861
13 H	Isotropic = 29.7571	Anisotropy = 6.6583
14 H	Isotropic = 29.0162	Anisotropy = 17.2331
15 H	Isotropic = 29.3765	Anisotropy = 10.3379
16 H	Isotropic = 29.4567	Anisotropy = 9.8723
17 H	Isotropic = 29.7344	Anisotropy = 9.1510
18 H	Isotropic = 29.1992	Anisotropy = 8.8583
19 H	Isotropic = 30.2327	Anisotropy = 9.0255
20 H	Isotropic = 29.5817	Anisotropy = 10.3167

Conformer_10

C	-0.394726144360	0.166638470601	-0.273215961359
C	0.647575159749	0.146216038383	0.831726951936
C	2.059513073408	-0.177038714873	0.333659179795
O	0.228887342911	-0.679494525265	1.925771632311
N	2.188947854468	-1.270546267638	-0.623866936706
C	3.538445411295	-1.285619450891	-1.168852263996
C	1.872412924751	-2.569491795741	-0.050350100758
H	-1.352144948761	0.524910185031	0.115129049403
H	-0.081267428564	0.829737830655	-1.085150911385
H	-0.544023875766	-0.832005485121	-0.696761597002
H	0.713687358847	1.145383337487	1.274133723910
H	2.701160784940	-0.348815452336	1.218599620862
H	2.432148654491	0.726336324737	-0.161409886923
H	-0.046681752194	-1.532407601656	1.578091315118
H	4.302707046003	-1.475194902504	-0.393029917486
H	3.624256702146	-2.068118828188	-1.927898851489
H	3.764159130234	-0.324596792859	-1.639260313001
H	2.436823743024	-2.768242624948	0.878221554782
H	2.117412490970	-3.353741343089	-0.771729526028
H	0.803906472406	-2.662708401785	0.163093238017

SCF Done: E(RwB97X) = -328.336358726

Zero-point correction=	0.183814
Thermal correction to Energy=	0.192561
Thermal correction to Enthalpy=	0.193505
Thermal correction to Gibbs Free Energy=	0.151313
Sum of electronic and zero-point Energies=	-328.152545
Sum of electronic and thermal Energies=	-328.143798
Sum of electronic and thermal Enthalpies=	-328.142854
Sum of electronic and thermal Free Energies=	-328.185046

1	C	Isotropic =	171.2138	Anisotropy =	30.6320
2	C	Isotropic =	120.1382	Anisotropy =	49.4224
3	C	Isotropic =	124.1973	Anisotropy =	39.7454
4	O	Isotropic =	262.2105	Anisotropy =	28.9987
5	N	Isotropic =	229.9014	Anisotropy =	35.8371
6	C	Isotropic =	143.4873	Anisotropy =	73.6325
7	C	Isotropic =	146.3438	Anisotropy =	62.8184
8	H	Isotropic =	30.5032	Anisotropy =	9.5072
9	H	Isotropic =	30.6816	Anisotropy =	9.6422
10	H	Isotropic =	30.5412	Anisotropy =	5.2082
11	H	Isotropic =	28.1473	Anisotropy =	6.4349

12	H	Isotropic =	29.6927	Anisotropy =	5.4334
13	H	Isotropic =	29.2714	Anisotropy =	6.2312
14	H	Isotropic =	31.1991	Anisotropy =	12.5361
15	H	Isotropic =	29.9004	Anisotropy =	8.7411
16	H	Isotropic =	29.5042	Anisotropy =	10.1860
17	H	Isotropic =	29.5331	Anisotropy =	10.1414
18	H	Isotropic =	30.0839	Anisotropy =	7.6647
19	H	Isotropic =	29.5088	Anisotropy =	9.7997
20	H	Isotropic =	29.4257	Anisotropy =	7.2931

Conformer_11

C	-0.277413841178	0.949442518390	0.360870193120
C	0.682791140680	-0.173550451430	0.720496271750
C	1.523433400749	-0.580315156781	-0.482594984426
O	-0.045725146242	-1.319970454888	1.180324211489
N	2.765576489133	-1.279249925094	-0.170689619902
C	2.545198040830	-2.628160401347	0.330467533534
C	3.621907176749	-1.324815552033	-1.345694976785
H	-0.926075368287	1.188304747541	1.210171203270
H	0.270771193231	1.857246615774	0.092432104516
H	-0.911280106210	0.661168064142	-0.484546030979
H	1.360461697218	0.164311053304	1.516873416366
H	1.795848039431	0.337851830121	-1.012372832003
H	0.886881777587	-1.174680255756	-1.166456921968
H	-0.598334455867	-1.039968326158	1.916127143031
H	1.941282375115	-2.607200350576	1.237580289313
H	2.025936474119	-3.264172588170	-0.410465453358
H	3.509148306179	-3.092022209334	0.559696092607
H	4.570212196229	-1.808173688261	-1.094286555278
H	3.162370742289	-1.889118677841	-2.177957340337
H	3.835309868247	-0.311826791603	-1.698273743960

SCF Done: E(RwB97X) = -328.337588831

Zero-point correction=	0.183162
Thermal correction to Energy=	0.192157
Thermal correction to Enthalpy=	0.193102
Thermal correction to Gibbs Free Energy=	0.149865
Sum of electronic and zero-point Energies=	-328.154427
Sum of electronic and thermal Energies=	-328.145431
Sum of electronic and thermal Enthalpies=	-328.144487
Sum of electronic and thermal Free Energies=	-328.187724

1	C	Isotropic =	166.6922	Anisotropy =	39.8333

2	C	Isotropic =	118.5901	Anisotropy =	40.9066
3	C	Isotropic =	125.0035	Anisotropy =	54.8983
4	O	Isotropic =	267.2652	Anisotropy =	63.7657
5	N	Isotropic =	220.5875	Anisotropy =	47.0332
6	C	Isotropic =	146.8434	Anisotropy =	61.7450
7	C	Isotropic =	143.6049	Anisotropy =	73.1729
8	H	Isotropic =	30.8271	Anisotropy =	9.3516
9	H	Isotropic =	30.7393	Anisotropy =	9.5755
10	H	Isotropic =	30.6813	Anisotropy =	6.9543
11	H	Isotropic =	27.8682	Anisotropy =	4.2266
12	H	Isotropic =	29.4317	Anisotropy =	6.4132
13	H	Isotropic =	29.9926	Anisotropy =	4.3965
14	H	Isotropic =	31.2602	Anisotropy =	18.2281
15	H	Isotropic =	28.5592	Anisotropy =	7.1178
16	H	Isotropic =	30.2504	Anisotropy =	7.7544
17	H	Isotropic =	29.6105	Anisotropy =	9.9015
18	H	Isotropic =	29.5066	Anisotropy =	10.2115
19	H	Isotropic =	29.9589	Anisotropy =	8.4176
20	H	Isotropic =	29.4579	Anisotropy =	9.7592

Conformer_12

C	-0.343856726780	0.973428144902	0.339574521573
C	0.720186478502	-0.016342015804	0.790070187024
C	1.422738355062	-0.643063304371	-0.413724616045
O	0.147005276828	-0.993806387826	1.666366932912
N	2.729384743602	-1.229854931018	-0.141376426122
C	2.651631177743	-2.440542958214	0.663018022207
C	3.421541760674	-1.510791911199	-1.389659245792
H	0.102753895358	1.802199013972	-0.217254900137
H	-1.079157907976	0.484008586027	-0.310697994633
H	-0.870645257701	1.383784863311	1.205076806961
H	1.469019696762	0.498538471852	1.400299079913
H	1.573382525126	0.149460934367	-1.153884923383
H	0.738222095259	-1.384768191492	-0.874758891820
H	-0.548754853501	-1.449102062293	1.180269413547
H	2.196236114326	-2.231854369700	1.631008992009
H	2.053731445132	-3.227910012061	0.166704066886
H	3.659857647125	-2.832124764004	0.826719285200
H	4.420270790820	-1.903483443271	-1.178940804925
H	2.886295847142	-2.254782763582	-2.007899073425
H	3.529156896496	-0.594692899594	-1.977110431948

SCF Done: E(RwB97X) = -328.337446073

Zero-point correction=	0.183060
Thermal correction to Energy=	0.192089
Thermal correction to Enthalpy=	0.193033
Thermal correction to Gibbs Free Energy=	0.149802
Sum of electronic and zero-point Energies=	-328.154386
Sum of electronic and thermal Energies=	-328.145357
Sum of electronic and thermal Enthalpies=	-328.144413
Sum of electronic and thermal Free Energies=	-328.187644

1 C	Isotropic =	167.4598	Anisotropy =	39.8982
2 C	Isotropic =	117.6723	Anisotropy =	42.3978
3 C	Isotropic =	122.6240	Anisotropy =	51.8571
4 O	Isotropic =	262.8401	Anisotropy =	55.1618
5 N	Isotropic =	220.8073	Anisotropy =	46.6966
6 C	Isotropic =	146.8806	Anisotropy =	60.8502
7 C	Isotropic =	143.5670	Anisotropy =	73.3012
8 H	Isotropic =	30.7105	Anisotropy =	9.6097
9 H	Isotropic =	30.8025	Anisotropy =	6.7601
10 H	Isotropic =	30.6439	Anisotropy =	9.4395
11 H	Isotropic =	28.1249	Anisotropy =	3.7864
12 H	Isotropic =	29.3086	Anisotropy =	6.1352
13 H	Isotropic =	30.1805	Anisotropy =	4.3815
14 H	Isotropic =	31.8885	Anisotropy =	14.1570
15 H	Isotropic =	28.5082	Anisotropy =	7.2678
16 H	Isotropic =	30.2826	Anisotropy =	7.7020
17 H	Isotropic =	29.5932	Anisotropy =	9.8188
18 H	Isotropic =	29.5093	Anisotropy =	10.1894
19 H	Isotropic =	29.9898	Anisotropy =	8.4080
20 H	Isotropic =	29.4707	Anisotropy =	9.7661

Conformer_13

C	0.545631700955	0.680516912468	1.269061888746
C	0.560910949498	-0.761324957165	0.786623165460
C	1.445169177405	-0.998079963361	-0.442388716980
O	-0.763579201876	-1.166970206289	0.413120695396
N	2.720990868943	-1.639406085608	-0.140626436554
C	3.394483118537	-2.006992603497	-1.375805880051
C	3.586504332500	-0.792865104900	0.665406701433
H	0.162007221129	1.338494981135	0.482411219925
H	-0.092015860401	0.787491897066	2.153326109615
H	1.549679037205	1.019365678028	1.538714909423
H	0.916253560770	-1.418018434159	1.592731750153
H	1.604887730642	-0.043888458808	-0.980777814883
H	0.895964975058	-1.661841969806	-1.115816736786

H	-1.354966556289	-0.942824980541	1.138128700443
H	3.630515618959	-1.128432138572	-2.003644424493
H	2.762815948832	-2.682328945365	-1.959788490125
H	4.331850307909	-2.522331454003	-1.148218076469
H	4.538535375910	-1.303070190349	0.836341919051
H	3.798235393014	0.175372427741	0.175229507122
H	3.137026301299	-0.592666404014	1.641170009573

SCF Done: E(RwB97X) = -328.335480709

Zero-point correction=	0.183358
Thermal correction to Energy=	0.192248
Thermal correction to Enthalpy=	0.193192
Thermal correction to Gibbs Free Energy=	0.150220
Sum of electronic and zero-point Energies=	-328.152122
Sum of electronic and thermal Energies=	-328.143233
Sum of electronic and thermal Enthalpies=	-328.142289
Sum of electronic and thermal Free Energies=	-328.185261

1 C	Isotropic = 165.4179	Anisotropy = 38.2958
2 C	Isotropic = 119.2909	Anisotropy = 49.0548
3 C	Isotropic = 123.2675	Anisotropy = 50.5778
4 O	Isotropic = 266.7953	Anisotropy = 88.7420
5 N	Isotropic = 222.9016	Anisotropy = 44.7884
6 C	Isotropic = 144.1699	Anisotropy = 73.1110
7 C	Isotropic = 147.2703	Anisotropy = 59.3304
8 H	Isotropic = 30.7324	Anisotropy = 7.1067
9 H	Isotropic = 30.6265	Anisotropy = 9.5954
10 H	Isotropic = 30.3649	Anisotropy = 6.7123
11 H	Isotropic = 28.0292	Anisotropy = 3.9474
12 H	Isotropic = 30.0331	Anisotropy = 3.6356
13 H	Isotropic = 29.2160	Anisotropy = 5.5470
14 H	Isotropic = 31.4818	Anisotropy = 18.1769
15 H	Isotropic = 30.0263	Anisotropy = 8.4730
16 H	Isotropic = 29.4244	Anisotropy = 9.8900
17 H	Isotropic = 29.4816	Anisotropy = 10.3063
18 H	Isotropic = 29.5612	Anisotropy = 9.8506
19 H	Isotropic = 30.3903	Anisotropy = 7.6689
20 H	Isotropic = 29.4302	Anisotropy = 7.6571

Conformer_14

C	0.507705239158	0.806744450437	1.081225687980
C	0.584495151157	-0.709111834502	0.986993638361
C	1.347856978184	-1.215059704669	-0.248899708708

O	-0.737404283843	-1.260818606564	1.022825203613
N	2.720352422693	-1.631640936755	0.025267525773
C	3.288830089023	-2.266116891210	-1.153303214074
C	3.563623996033	-0.525813463907	0.450869861440
H	-0.050641337567	1.210053792329	0.227508870122
H	-0.001019085908	1.109542011066	2.000571604142
H	1.501017623886	1.262484443317	1.069433078424
H	1.074951184900	-1.117626383884	1.876453222765
H	1.324283898354	-0.447363100573	-1.047832252503
H	0.814477885189	-2.092258292758	-0.626058937608
H	-1.256762606216	-0.826215136332	0.338355471188
H	2.680531038626	-3.126948229048	-1.444898123298
H	3.345188522702	-1.577058873953	-2.015762948332
H	4.300860882218	-2.617819903371	-0.933993767554
H	3.591320182318	0.290560578537	-0.294276672725
H	3.216154060050	-0.113135250004	1.401098436597
H	4.585578159043	-0.885298668156	0.599723024397

SCF Done: E(RwB97X) = -328.334827866

Zero-point correction=	0.183155
Thermal correction to Energy=	0.192172
Thermal correction to Enthalpy=	0.193116
Thermal correction to Gibbs Free Energy=	0.149957
Sum of electronic and zero-point Energies=	-328.151672
Sum of electronic and thermal Energies=	-328.142656
Sum of electronic and thermal Enthalpies=	-328.141712
Sum of electronic and thermal Free Energies=	-328.184871

1 C	Isotropic =	165.6472	Anisotropy =	37.6260
2 C	Isotropic =	119.0791	Anisotropy =	50.6774
3 C	Isotropic =	120.4312	Anisotropy =	52.1597
4 O	Isotropic =	256.4200	Anisotropy =	49.3653
5 N	Isotropic =	223.0876	Anisotropy =	45.2518
6 C	Isotropic =	144.0531	Anisotropy =	73.3528
7 C	Isotropic =	147.3780	Anisotropy =	58.1456
8 H	Isotropic =	30.8981	Anisotropy =	7.0024
9 H	Isotropic =	30.4617	Anisotropy =	9.7106
10 H	Isotropic =	30.3752	Anisotropy =	6.6679
11 H	Isotropic =	28.2920	Anisotropy =	3.2266
12 H	Isotropic =	30.0113	Anisotropy =	3.3793
13 H	Isotropic =	29.1506	Anisotropy =	5.7355
14 H	Isotropic =	31.3158	Anisotropy =	14.4437
15 H	Isotropic =	29.4496	Anisotropy =	9.8621
16 H	Isotropic =	30.0559	Anisotropy =	8.4247
17 H	Isotropic =	29.4848	Anisotropy =	10.2859

18 H	Isotropic =	30.4035	Anisotropy =	7.6440
19 H	Isotropic =	29.4097	Anisotropy =	7.6440
20 H	Isotropic =	29.5623	Anisotropy =	9.7752

Conformer_15

C	-0.169812599440	1.147724078101	0.920887892557
C	0.522471695471	-0.194858458523	0.795133025040
C	1.728394220391	-0.090518509029	-0.145409735603
O	-0.462970723017	-1.119297320851	0.315863119763
N	2.640182466950	-1.224084580773	-0.244993988220
C	2.137768271477	-2.388067098605	-0.950683157861
C	3.269088260492	-1.586641006436	1.010827739594
H	0.505658512562	1.893443119808	1.348985086385
H	-0.498126452281	1.502568728329	-0.062222552699
H	-1.047084219077	1.066643104891	1.567923380592
H	0.860731783359	-0.517024265789	1.789717629273
H	2.320660288410	0.770888698598	0.187797369491
H	1.356282209656	0.139007225697	-1.151442672963
H	-0.082399188526	-2.001364051547	0.317559847547
H	1.468988596427	-3.028505566443	-0.346099968647
H	1.601584838006	-2.080216661833	-1.852063521186
H	2.977936257796	-3.022192996416	-1.254378068707
H	2.581237546013	-2.084752039125	1.716483300791
H	3.671459429762	-0.694075022565	1.499516248055
H	4.099348805571	-2.274377377487	0.819799026801

SCF Done: E(RwB97X) = -328.336322688

Zero-point correction=	0.183099
Thermal correction to Energy=	0.192088
Thermal correction to Enthalpy=	0.193032
Thermal correction to Gibbs Free Energy=	0.150095
Sum of electronic and zero-point Energies=	-328.153223
Sum of electronic and thermal Energies=	-328.144235
Sum of electronic and thermal Enthalpies=	-328.143291
Sum of electronic and thermal Free Energies=	-328.186228

1 C	Isotropic =	170.6701	Anisotropy =	36.1507
2 C	Isotropic =	125.2766	Anisotropy =	68.2886
3 C	Isotropic =	124.5962	Anisotropy =	42.8153
4 O	Isotropic =	267.9215	Anisotropy =	59.1521
5 N	Isotropic =	235.5163	Anisotropy =	37.9870
6 C	Isotropic =	146.4848	Anisotropy =	61.9546
7 C	Isotropic =	150.2623	Anisotropy =	60.3041

8 H	Isotropic =	31.0475	Anisotropy =	9.7531
9 H	Isotropic =	30.9290	Anisotropy =	7.3966
10 H	Isotropic =	30.7207	Anisotropy =	9.7188
11 H	Isotropic =	27.4347	Anisotropy =	3.6237
12 H	Isotropic =	29.1829	Anisotropy =	5.7926
13 H	Isotropic =	29.2859	Anisotropy =	6.0096
14 H	Isotropic =	31.0570	Anisotropy =	16.4118
15 H	Isotropic =	29.4745	Anisotropy =	7.6629
16 H	Isotropic =	29.0591	Anisotropy =	8.2554
17 H	Isotropic =	29.2037	Anisotropy =	10.3564
18 H	Isotropic =	29.4326	Anisotropy =	7.5965
19 H	Isotropic =	29.4928	Anisotropy =	9.4216
20 H	Isotropic =	29.3712	Anisotropy =	9.9221

Conformer_16

C	-0.097555104398	0.616757722584	-0.350574563107
C	0.552331151785	-0.036945924660	0.851086787243
C	1.998251871512	-0.474291114459	0.604655936599
O	-0.300221805033	-1.115410069545	1.257811034643
N	2.265592637062	-1.167135049213	-0.648436861248
C	3.700141912968	-1.262623374352	-0.867142171546
C	1.664529839354	-2.491357060378	-0.696157404730
H	0.510953009910	1.455178173104	-0.701889030373
H	-0.206455640503	-0.095949309163	-1.172527198555
H	-1.087692954675	0.997319376264	-0.085160463051
H	0.596961291493	0.693562080879	1.671325167686
H	2.331261845959	-1.081925816033	1.470789736055
H	2.607371698839	0.436239389606	0.611295486598
H	0.089523084644	-1.524251870044	2.036528503463
H	4.207082010984	-1.845128652727	-0.075690057463
H	3.897424195524	-1.751610480263	-1.825390253673
H	4.145690838854	-0.264130900199	-0.893663268597
H	1.908137171415	-2.968246372769	-1.650130843120
H	2.035394519473	-3.143076160943	0.117522860174
H	0.579778424834	-2.425574587690	-0.606253396997

SCF Done: E(RwB97X) = -328.337345799

Zero-point correction=	0.183227
Thermal correction to Energy=	0.192101
Thermal correction to Enthalpy=	0.193045
Thermal correction to Gibbs Free Energy=	0.150501
Sum of electronic and zero-point Energies=	-328.154119
Sum of electronic and thermal Energies=	-328.145245

Sum of electronic and thermal Enthalpies= -328.144300
Sum of electronic and thermal Free Energies= -328.186845

1 C	Isotropic =	173.3154	Anisotropy =	26.3507
2 C	Isotropic =	120.6029	Anisotropy =	47.1467
3 C	Isotropic =	124.2946	Anisotropy =	40.5703
4 O	Isotropic =	269.7230	Anisotropy =	90.9912
5 N	Isotropic =	229.7119	Anisotropy =	33.1331
6 C	Isotropic =	143.7081	Anisotropy =	73.5224
7 C	Isotropic =	146.3563	Anisotropy =	62.2233
8 H	Isotropic =	30.8597	Anisotropy =	9.5182
9 H	Isotropic =	30.4491	Anisotropy =	5.4791
10 H	Isotropic =	30.5732	Anisotropy =	9.8587
11 H	Isotropic =	27.8588	Anisotropy =	6.8993
12 H	Isotropic =	29.8557	Anisotropy =	5.4116
13 H	Isotropic =	29.2951	Anisotropy =	6.2318
14 H	Isotropic =	31.3259	Anisotropy =	16.8190
15 H	Isotropic =	29.9808	Anisotropy =	8.6991
16 H	Isotropic =	29.5060	Anisotropy =	10.1831
17 H	Isotropic =	29.5167	Anisotropy =	10.1748
18 H	Isotropic =	29.6061	Anisotropy =	9.9530
19 H	Isotropic =	30.3061	Anisotropy =	7.8950
20 H	Isotropic =	28.7496	Anisotropy =	6.5942

Conformer_17

C	0.726334741857	0.537172458970	1.444173095147
C	0.463062617431	-0.890180362034	0.999301243136
C	1.291701084944	-1.329536658790	-0.209945944160
O	-0.925661149534	-1.085432845661	0.714497652442
N	2.733816077606	-1.295248281314	0.032934675851
C	3.375946157297	-0.147202806233	-0.588147122209
C	3.391106037086	-2.527259841571	-0.374527560954
H	0.098735673540	0.785902032462	2.304736677449
H	0.501024360758	1.244350553165	0.636219172296
H	1.771965667875	0.670509440219	1.735080936292
H	0.680300566180	-1.574774873662	1.825975626643
H	1.022500692031	-0.702726790655	-1.077071908350
H	0.987166087205	-2.351938811752	-0.454898030188
H	-1.182930708180	-0.436717808873	0.050766440961
H	3.323413256140	-0.187710980034	-1.691138098606
H	4.430408053245	-0.109265471681	-0.298905565563
H	2.904012887066	0.782361459345	-0.261787580882
H	2.951598362626	-3.379936676590	0.149550834708
H	3.313571727428	-2.710909188466	-1.461320698614

H 4.453227807398 -2.481254546845 -0.115993845398

SCF Done: E(RwB97X) = -328.336230198

Zero-point correction= 0.183221
Thermal correction to Energy= 0.192213
Thermal correction to Enthalpy= 0.193157
Thermal correction to Gibbs Free Energy= 0.150010
Sum of electronic and zero-point Energies= -328.153009
Sum of electronic and thermal Energies= -328.144017
Sum of electronic and thermal Enthalpies= -328.143073
Sum of electronic and thermal Free Energies= -328.186220

1 C	Isotropic =	168.4480	Anisotropy =	29.8613
2 C	Isotropic =	119.7627	Anisotropy =	63.9625
3 C	Isotropic =	124.2096	Anisotropy =	64.1061
4 O	Isotropic =	270.0310	Anisotropy =	41.9136
5 N	Isotropic =	234.4365	Anisotropy =	54.7010
6 C	Isotropic =	144.9768	Anisotropy =	66.6826
7 C	Isotropic =	143.7635	Anisotropy =	69.8391
8 H	Isotropic =	30.4984	Anisotropy =	9.5948
9 H	Isotropic =	31.1370	Anisotropy =	6.8742
10 H	Isotropic =	30.3041	Anisotropy =	7.0282
11 H	Isotropic =	28.3410	Anisotropy =	4.1694
12 H	Isotropic =	30.1555	Anisotropy =	4.6243
13 H	Isotropic =	29.3216	Anisotropy =	4.8340
14 H	Isotropic =	31.7597	Anisotropy =	14.9000
15 H	Isotropic =	29.9039	Anisotropy =	8.3769
16 H	Isotropic =	29.6254	Anisotropy =	10.2647
17 H	Isotropic =	29.3515	Anisotropy =	7.1889
18 H	Isotropic =	29.3592	Anisotropy =	9.7276
19 H	Isotropic =	29.6535	Anisotropy =	8.8038
20 H	Isotropic =	29.5980	Anisotropy =	10.3418

Conformer_18

C	0.353994478813	0.827081199196	0.122871660083
C	0.467587010939	-0.431740687448	0.965243696135
C	1.894363612861	-0.956963339846	1.092693373947
O	-0.372190869383	-1.475457725623	0.452103053290
N	2.676448914200	-1.017659406207	-0.136300351626
C	4.082431142588	-1.214536114361	0.178266427063
C	2.218680437353	-2.063275467458	-1.039192771749
H	1.002424136028	1.614079671561	0.520801881254
H	0.642209617718	0.632688711199	-0.913599611181

H	-0.674816435090	1.202601695215	0.134235951205
H	0.141398982393	-0.203406534409	1.989642142662
H	1.854699666470	-1.945411240939	1.588298959384
H	2.416310025989	-0.278380963544	1.775299265195
H	-1.272131305136	-1.137637258771	0.422065473678
H	4.264960168334	-2.166673988959	0.710139872528
H	4.670739129485	-1.225565359400	-0.743773688363
H	4.447288679807	-0.398023819174	0.807921905998
H	1.178955345085	-1.897965204782	-1.322835890717
H	2.835312917860	-2.061200518535	-1.942967747763
H	2.289034343687	-3.066153647715	-0.577613601021

SCF Done: E(RwB97X) = -328.337072387

Zero-point correction=	0.183016
Thermal correction to Energy=	0.192020
Thermal correction to Enthalpy=	0.192964
Thermal correction to Gibbs Free Energy=	0.149800
Sum of electronic and zero-point Energies=	-328.154056
Sum of electronic and thermal Energies=	-328.145053
Sum of electronic and thermal Enthalpies=	-328.144109
Sum of electronic and thermal Free Energies=	-328.187272

1 C	Isotropic = 170.3107	Anisotropy = 31.1338
2 C	Isotropic = 120.5642	Anisotropy = 47.5544
3 C	Isotropic = 127.4734	Anisotropy = 42.7185
4 O	Isotropic = 268.6633	Anisotropy = 66.1456
5 N	Isotropic = 230.2104	Anisotropy = 32.3782
6 C	Isotropic = 143.6188	Anisotropy = 73.5280
7 C	Isotropic = 146.1678	Anisotropy = 63.2746
8 H	Isotropic = 30.7544	Anisotropy = 9.7295
9 H	Isotropic = 30.3600	Anisotropy = 5.1527
10 H	Isotropic = 30.6884	Anisotropy = 9.2747
11 H	Isotropic = 27.8709	Anisotropy = 6.7770
12 H	Isotropic = 29.6444	Anisotropy = 5.6194
13 H	Isotropic = 29.3912	Anisotropy = 6.6162
14 H	Isotropic = 31.2781	Anisotropy = 18.1795
15 H	Isotropic = 29.9289	Anisotropy = 8.7294
16 H	Isotropic = 29.4927	Anisotropy = 10.1957
17 H	Isotropic = 29.5097	Anisotropy = 10.1522
18 H	Isotropic = 28.7567	Anisotropy = 6.5576
19 H	Isotropic = 29.6199	Anisotropy = 10.0291
20 H	Isotropic = 30.2629	Anisotropy = 7.9532

Conformer_19

C	-0.137977297592	0.985984734383	1.013025122480
C	0.711761073481	-0.275032745089	0.975639478898
C	1.687325546893	-0.231093359900	-0.206345736965
O	-0.115399587751	-1.442847057842	0.949236740602
N	2.718586591093	-1.255621067844	-0.301093884578
C	2.246817833538	-2.581097432578	-0.665847478178
C	3.602128249094	-1.299293896148	0.848946498388
H	-0.852251467934	0.939280120260	1.839357621076
H	0.484603899145	1.875765504609	1.146508478530
H	-0.700544078865	1.101868303752	0.078447217369
H	1.273203091591	-0.357450724500	1.911659578882
H	2.192849474309	0.742134273643	-0.170556971009
H	1.102428131841	-0.250757635832	-1.136302092368
H	-0.615378785613	-1.429825573040	0.126067805373
H	1.704712983034	-3.090784549627	0.144890924283
H	1.579675520536	-2.512116658281	-1.530469542385
H	3.103258927905	-3.203036079243	-0.948882192613
H	4.474243268236	-1.919563060924	0.617744256361
H	3.126181207100	-1.719257261410	1.751906223950
H	3.955875419958	-0.291355834387	1.087467951903

SCF Done: E(RwB97X) = -328.336308839

Zero-point correction=	0.183094
Thermal correction to Energy=	0.192127
Thermal correction to Enthalpy=	0.193071
Thermal correction to Gibbs Free Energy=	0.150008
Sum of electronic and zero-point Energies=	-328.153215
Sum of electronic and thermal Energies=	-328.144182
Sum of electronic and thermal Enthalpies=	-328.143238
Sum of electronic and thermal Free Energies=	-328.186301

1 C	Isotropic =	168.2208	Anisotropy =	39.9878
2 C	Isotropic =	124.8040	Anisotropy =	68.6425
3 C	Isotropic =	124.9070	Anisotropy =	44.3144
4 O	Isotropic =	262.9487	Anisotropy =	50.8640
5 N	Isotropic =	234.6800	Anisotropy =	37.5103
6 C	Isotropic =	146.7442	Anisotropy =	61.8839
7 C	Isotropic =	150.2886	Anisotropy =	60.3038
8 H	Isotropic =	30.6477	Anisotropy =	9.2916
9 H	Isotropic =	30.9076	Anisotropy =	9.9600
10 H	Isotropic =	31.0081	Anisotropy =	6.9570
11 H	Isotropic =	27.6835	Anisotropy =	3.5707
12 H	Isotropic =	29.0731	Anisotropy =	5.8217
13 H	Isotropic =	29.4019	Anisotropy =	5.9003

14	H	Isotropic =	32.0208	Anisotropy =	13.9238
15	H	Isotropic =	29.0190	Anisotropy =	6.8394
16	H	Isotropic =	29.3075	Anisotropy =	8.5454
17	H	Isotropic =	29.4358	Anisotropy =	10.1892
18	H	Isotropic =	29.3850	Anisotropy =	9.9313
19	H	Isotropic =	29.4083	Anisotropy =	7.5721
20	H	Isotropic =	29.4963	Anisotropy =	9.4969

Conformer_2

C	-0.270951574311	0.572713475294	-0.176577081348
C	0.496476541109	0.079000611965	1.041018501937
C	1.982558445263	-0.189501054171	0.788877705993
O	-0.100825545985	-1.110976142041	1.556375034390
N	2.177659795739	-1.363110993491	-0.066540784664
C	2.473894106390	-1.004547054270	-1.446982892595
C	3.201865522450	-2.261848593791	0.446688530169
H	-0.294562205241	-0.189602894427	-0.961797305277
H	-1.304015793522	0.800648930119	0.101447003257
H	0.181856657956	1.482082988559	-0.585395433299
H	0.420033408041	0.827424359180	1.836847443048
H	2.449545791514	-0.380879107092	1.759893030696
H	2.464952927812	0.704222511865	0.366370462865
H	0.241122455419	-1.815787298309	0.988678812140
H	1.716633484871	-0.326255899866	-1.844185937497
H	3.456553471262	-0.509111741681	-1.539740961666
H	2.485205956121	-1.903690904498	-2.070026581668
H	3.263673108375	-3.149366294084	-0.189926260381
H	4.199837090195	-1.790275840566	0.472584218712
H	2.948686356541	-2.586139058696	1.459292495188

SCF Done: E(RwB97X) = -328.339224751

Zero-point correction=	0.183984
Thermal correction to Energy=	0.192655
Thermal correction to Enthalpy=	0.193600
Thermal correction to Gibbs Free Energy=	0.151348
Sum of electronic and zero-point Energies=	-328.155241
Sum of electronic and thermal Energies=	-328.146569
Sum of electronic and thermal Enthalpies=	-328.145625
Sum of electronic and thermal Free Energies=	-328.187877

1	C	Isotropic =	168.2520	Anisotropy =	31.8852
2	C	Isotropic =	123.4029	Anisotropy =	46.2145
3	C	Isotropic =	127.5585	Anisotropy =	43.0709

4 O	Isotropic =	284.2692	Anisotropy =	48.5042
5 N	Isotropic =	241.0924	Anisotropy =	37.6837
6 C	Isotropic =	143.8957	Anisotropy =	68.3950
7 C	Isotropic =	142.9356	Anisotropy =	71.0733
8 H	Isotropic =	30.6200	Anisotropy =	4.8324
9 H	Isotropic =	30.6112	Anisotropy =	9.4639
10 H	Isotropic =	30.9216	Anisotropy =	9.5873
11 H	Isotropic =	28.3038	Anisotropy =	6.5957
12 H	Isotropic =	29.3681	Anisotropy =	6.9771
13 H	Isotropic =	29.6039	Anisotropy =	5.2824
14 H	Isotropic =	29.5085	Anisotropy =	14.5032
15 H	Isotropic =	29.2861	Anisotropy =	7.5223
16 H	Isotropic =	29.8143	Anisotropy =	8.6398
17 H	Isotropic =	29.4786	Anisotropy =	10.2529
18 H	Isotropic =	29.4725	Anisotropy =	10.2702
19 H	Isotropic =	29.6240	Anisotropy =	9.1349
20 H	Isotropic =	29.4773	Anisotropy =	9.7376

Conformer_21

C	0.834642953765	0.046536410878	1.738096932603
C	0.437600041590	-1.008049921578	0.719785064510
C	1.279299307195	-1.013788728069	-0.568469021654
O	-0.938266519307	-0.860006019514	0.349180978358
N	2.706019408687	-1.289726029084	-0.482356056386
C	3.031233443484	-2.509354322516	0.231174665815
C	3.560439005248	-0.180704226952	-0.098340658451
H	1.815794678703	-0.168208488110	2.169394718344
H	0.871352476230	1.043130016887	1.281703217000
H	0.106610867199	0.066893936873	2.554503151531
H	0.487581847009	-1.996434778240	1.187634853064
H	1.153186780119	-0.043259117805	-1.066223438273
H	0.829239004358	-1.770975832127	-1.222884745671
H	-1.046547926486	0.019397649914	-0.028703353903
H	4.079023619420	-2.771811482593	0.052130043933
H	2.890553497305	-2.429185483879	1.323150168797
H	2.408780460494	-3.332842675784	-0.132836411025
H	4.594664033541	-0.409138014326	-0.379127503763
H	3.556578774505	0.040389398090	0.981191774444
H	3.258414246942	0.724237707936	-0.633004379273

SCF Done: E(RwB97X) = -328.334705747

Zero-point correction=	0.183137
Thermal correction to Energy=	0.192184

Thermal correction to Enthalpy=	0.193128
Thermal correction to Gibbs Free Energy=	0.149928
Sum of electronic and zero-point Energies=	-328.151569
Sum of electronic and thermal Energies=	-328.142522
Sum of electronic and thermal Enthalpies=	-328.141578
Sum of electronic and thermal Free Energies=	-328.184778

1 C	Isotropic =	166.1224	Anisotropy =	33.0375
2 C	Isotropic =	123.7092	Anisotropy =	57.6115
3 C	Isotropic =	125.1704	Anisotropy =	51.3561
4 O	Isotropic =	267.1411	Anisotropy =	42.4076
5 N	Isotropic =	238.5725	Anisotropy =	41.9262
6 C	Isotropic =	151.5171	Anisotropy =	58.2634
7 C	Isotropic =	147.2958	Anisotropy =	63.9797
8 H	Isotropic =	30.4447	Anisotropy =	6.8165
9 H	Isotropic =	30.9520	Anisotropy =	6.3868
10 H	Isotropic =	30.4587	Anisotropy =	9.3584
11 H	Isotropic =	28.0116	Anisotropy =	4.2513
12 H	Isotropic =	29.6029	Anisotropy =	5.1201
13 H	Isotropic =	28.7236	Anisotropy =	5.7650
14 H	Isotropic =	31.6648	Anisotropy =	14.7242
15 H	Isotropic =	29.4706	Anisotropy =	10.1300
16 H	Isotropic =	29.6034	Anisotropy =	7.5337
17 H	Isotropic =	29.3557	Anisotropy =	9.3429
18 H	Isotropic =	29.4009	Anisotropy =	10.2686
19 H	Isotropic =	29.2711	Anisotropy =	6.7496
20 H	Isotropic =	29.3764	Anisotropy =	8.6180

Conformer_22

C	-0.306373725706	0.089325828089	-0.217507912321
C	0.637183439551	0.191039560735	0.970501124345
C	2.128420730959	-0.001259570366	0.645657369548
O	0.201129742064	-0.662555414326	2.036457322999
N	2.589975401519	-1.170055951166	-0.090139752514
C	2.401130535605	-1.151239328600	-1.528750927208
C	2.265734773658	-2.455363369891	0.493129618236
H	-1.314757156780	0.393626491455	0.077520253138
H	0.022157255836	0.737155626588	-1.035855313683
H	-0.360047818796	-0.936843826180	-0.595241520231
H	0.561595589648	1.199868212561	1.392318787512
H	2.655196648010	0.017148188777	1.608411403955
H	2.456896627487	0.882706233570	0.086932786577
H	0.112837174960	-1.555320657103	1.689873909783
H	2.659755936378	-0.164898551165	-1.924564400880

H	3.073084425795	-1.884452900369	-1.989360803053
H	1.377122627369	-1.395542416936	-1.852840191421
H	2.467973458255	-2.443800785282	1.568091676839
H	2.892721326543	-3.231273489825	0.040222354655
H	1.215263007644	-2.763363880567	0.336544213725

SCF Done: E(RwB97X) = -328.333250288

Zero-point correction=	0.183403
Thermal correction to Energy=	0.192280
Thermal correction to Enthalpy=	0.193224
Thermal correction to Gibbs Free Energy=	0.150592
Sum of electronic and zero-point Energies=	-328.149847
Sum of electronic and thermal Energies=	-328.140971
Sum of electronic and thermal Enthalpies=	-328.140027
Sum of electronic and thermal Free Energies=	-328.182658

1 C	Isotropic = 167.5392	Anisotropy = 26.6475
2 C	Isotropic = 114.7558	Anisotropy = 43.1398
3 C	Isotropic = 127.7002	Anisotropy = 29.4695
4 O	Isotropic = 255.9375	Anisotropy = 25.5101
5 N	Isotropic = 233.8760	Anisotropy = 46.6186
6 C	Isotropic = 146.1141	Anisotropy = 64.0342
7 C	Isotropic = 149.3084	Anisotropy = 56.1455
8 H	Isotropic = 30.3798	Anisotropy = 9.4383
9 H	Isotropic = 30.4827	Anisotropy = 7.9806
10 H	Isotropic = 30.5855	Anisotropy = 4.5301
11 H	Isotropic = 28.2535	Anisotropy = 5.9965
12 H	Isotropic = 28.7770	Anisotropy = 7.4482
13 H	Isotropic = 29.1792	Anisotropy = 6.3419
14 H	Isotropic = 31.2604	Anisotropy = 12.2046
15 H	Isotropic = 29.2202	Anisotropy = 8.4935
16 H	Isotropic = 29.3216	Anisotropy = 10.1743
17 H	Isotropic = 29.0257	Anisotropy = 6.5540
18 H	Isotropic = 29.0049	Anisotropy = 7.8647
19 H	Isotropic = 29.2920	Anisotropy = 10.1325
20 H	Isotropic = 29.2651	Anisotropy = 6.9758

Conformer_23

C	0.717416545823	-0.054854815663	1.786631488027
C	0.482284588972	-0.879048885662	0.532112332823
C	1.476744371447	-0.619920362075	-0.608428606443
O	-0.796519633475	-0.564015216965	-0.035959905123
N	2.832324958023	-1.135009843850	-0.491968783647

C	3.709123015674	-0.435446345854	0.429069152814
C	2.911093978814	-2.574298091896	-0.330668251247
H	-0.114949231045	-0.185571413939	2.487678086896
H	0.797950500363	1.009962809555	1.542707343776
H	1.628237128668	-0.364304461452	2.304576035949
H	0.499494631731	-1.946741075410	0.791096848214
H	1.533361254417	0.462241300564	-0.777497192396
H	1.032966602161	-1.064431115994	-1.507081458173
H	-1.454836666012	-0.630783096743	0.661812259480
H	3.585078646243	0.645038775748	0.313670385831
H	4.750849938995	-0.683852456761	0.197569660676
H	3.539797166062	-0.691949427216	1.487422055228
H	2.618825830790	-2.919853636902	0.675967744430
H	2.264407498130	-3.068684587206	-1.062151789403
H	3.939448874218	-2.906878052279	-0.507057407711

SCF Done: E(RwB97X) = -328.334577161

Zero-point correction=	0.183323
Thermal correction to Energy=	0.192296
Thermal correction to Enthalpy=	0.193240
Thermal correction to Gibbs Free Energy=	0.149928
Sum of electronic and zero-point Energies=	-328.151254
Sum of electronic and thermal Energies=	-328.142281
Sum of electronic and thermal Enthalpies=	-328.141337
Sum of electronic and thermal Free Energies=	-328.184649

1 C	Isotropic =	164.8668	Anisotropy =	36.9654
2 C	Isotropic =	127.2687	Anisotropy =	60.0936
3 C	Isotropic =	126.4363	Anisotropy =	46.2868
4 O	Isotropic =	270.4011	Anisotropy =	73.8794
5 N	Isotropic =	238.7917	Anisotropy =	35.9684
6 C	Isotropic =	147.4484	Anisotropy =	61.1946
7 C	Isotropic =	149.9659	Anisotropy =	61.1330
8 H	Isotropic =	30.6303	Anisotropy =	9.2349
9 H	Isotropic =	30.7727	Anisotropy =	6.7002
10 H	Isotropic =	30.3333	Anisotropy =	7.0221
11 H	Isotropic =	27.7181	Anisotropy =	5.5740
12 H	Isotropic =	29.3391	Anisotropy =	5.0339
13 H	Isotropic =	28.8580	Anisotropy =	5.3670
14 H	Isotropic =	31.6115	Anisotropy =	17.7314
15 H	Isotropic =	29.3475	Anisotropy =	8.3335
16 H	Isotropic =	29.3586	Anisotropy =	10.1940
17 H	Isotropic =	29.3633	Anisotropy =	7.0171
18 H	Isotropic =	29.5642	Anisotropy =	7.6934
19 H	Isotropic =	29.3661	Anisotropy =	9.2965

20 H Isotropic = 29.4042 Anisotropy = 10.0637

Conformer_25

```
-----  
C      0.689669282619    1.017936686431    0.516717256575  
C      0.403648581558   -0.389051115336    1.001997446986  
C      1.637592917455   -1.278695218358    1.226112699636  
O     -0.520006295803   -0.963865642909    0.069630613861  
N      2.635831736178   -1.461517575053    0.184823361806  
C      3.571836934553   -0.371644641957   -0.018493824053  
C      2.154738060459   -2.018417809592   -1.064057604746  
H     -0.227779778947    1.613401754139    0.532474780540  
H      1.426485299978    1.508001536462    1.159440875979  
H      1.069754463913    1.009297058529   -0.507949701976  
H     -0.087940513421   -0.324712682880    1.985350998482  
H      1.259884482925   -2.275125864986    1.498947529974  
H      2.154731581179   -0.893346308480    2.112925968429  
H     -0.722464983050   -1.857420713484    0.362707221087  
H      3.902167934567    0.021466373671    0.947535520481  
H      4.454754223175   -0.749832400987   -0.546601316477  
H      3.169098779849    0.464726740504   -0.611172046471  
H      1.583116042169   -1.302525204333   -1.676081000847  
H      3.008795720533   -2.364201760943   -1.657447180980  
H      1.509585530113   -2.879673210438   -0.865561598287
```

SCF Done: E(RwB97X) = -328.333023809

```
Zero-point correction=          0.183460  
Thermal correction to Energy=      0.192332  
Thermal correction to Enthalpy=     0.193276  
Thermal correction to Gibbs Free Energy= 0.150845  
Sum of electronic and zero-point Energies= -328.149564  
Sum of electronic and thermal Energies= -328.140692  
Sum of electronic and thermal Enthalpies= -328.139748  
Sum of electronic and thermal Free Energies= -328.182178
```

```
1 C Isotropic = 170.2604 Anisotropy = 22.7713  
2 C Isotropic = 115.8029 Anisotropy = 40.6193  
3 C Isotropic = 127.0162 Anisotropy = 31.2318  
4 O Isotropic = 267.5151 Anisotropy = 88.3330  
5 N Isotropic = 233.9833 Anisotropy = 46.1718  
6 C Isotropic = 146.2927 Anisotropy = 63.3408  
7 C Isotropic = 148.3690 Anisotropy = 55.0623  
8 H Isotropic = 30.4739 Anisotropy = 9.8465  
9 H Isotropic = 30.6360 Anisotropy = 7.8147
```

10	H	Isotropic =	30.4964	Anisotropy =	5.0629
11	H	Isotropic =	27.9734	Anisotropy =	6.4477
12	H	Isotropic =	28.9344	Anisotropy =	7.3298
13	H	Isotropic =	29.1105	Anisotropy =	6.3567
14	H	Isotropic =	31.2175	Anisotropy =	16.4744
15	H	Isotropic =	29.2011	Anisotropy =	8.3711
16	H	Isotropic =	29.3229	Anisotropy =	10.1854
17	H	Isotropic =	29.0283	Anisotropy =	6.6133
18	H	Isotropic =	29.0348	Anisotropy =	6.7384
19	H	Isotropic =	29.4085	Anisotropy =	10.0086
20	H	Isotropic =	29.1838	Anisotropy =	8.0377

Conformer_26

C	-0.195328218539	0.138685825466	-0.340445001292
C	0.567272085309	-0.069438481447	0.956192800576
C	2.069129837649	-0.274710776771	0.787557286399
O	0.059848182818	-1.203194101657	1.669097776173
N	2.451221930940	-1.310187681986	-0.171929873488
C	2.842048763097	-0.748756530899	-1.455663338911
C	3.506097114073	-2.169197889952	0.340706643031
H	-1.259521384915	0.296849588823	-0.133641443895
H	0.172589632673	1.022362925013	-0.871096521773
H	-0.096348472552	-0.733508090590	-0.992893529990
H	0.444776740364	0.824487507672	1.585654672466
H	2.464029795388	-0.536501822103	1.774570881209
H	2.520883931585	0.692822998509	0.516355844384
H	-0.899077114605	-1.135464651162	1.688002023389
H	2.046682459019	-0.120051689689	-1.861416241780
H	3.756696206518	-0.132464803640	-1.377222935694
H	3.035282019012	-1.553457517216	-2.171510591777
H	3.730314247183	-2.953072353983	-0.389131966184
H	4.442581863395	-1.618089491983	0.544499155284
H	3.184220381591	-2.650712962404	1.267814361873

SCF Done: E(RwB97X) = -328.334877936

Zero-point correction=	0.183036
Thermal correction to Energy=	0.192102
Thermal correction to Enthalpy=	0.193046
Thermal correction to Gibbs Free Energy=	0.149340
Sum of electronic and zero-point Energies=	-328.151842
Sum of electronic and thermal Energies=	-328.142776
Sum of electronic and thermal Enthalpies=	-328.141832
Sum of electronic and thermal Free Energies=	-328.185538

1	C	Isotropic =	169.8301	Anisotropy =	28.1425
2	C	Isotropic =	120.8989	Anisotropy =	46.5609
3	C	Isotropic =	128.0217	Anisotropy =	48.0763
4	O	Isotropic =	271.5427	Anisotropy =	68.1540
5	N	Isotropic =	239.5584	Anisotropy =	42.3654
6	C	Isotropic =	144.0001	Anisotropy =	68.2067
7	C	Isotropic =	142.9076	Anisotropy =	71.0594
8	H	Isotropic =	30.7830	Anisotropy =	9.3927
9	H	Isotropic =	30.7074	Anisotropy =	9.1880
10	H	Isotropic =	30.4121	Anisotropy =	4.7298
11	H	Isotropic =	28.0776	Anisotropy =	6.5874
12	H	Isotropic =	29.2553	Anisotropy =	6.2210
13	H	Isotropic =	29.7424	Anisotropy =	5.4925
14	H	Isotropic =	31.4967	Anisotropy =	17.8534
15	H	Isotropic =	29.3419	Anisotropy =	7.4737
16	H	Isotropic =	29.9949	Anisotropy =	8.4813
17	H	Isotropic =	29.5358	Anisotropy =	10.2307
18	H	Isotropic =	29.5143	Anisotropy =	10.2781
19	H	Isotropic =	29.6692	Anisotropy =	8.9662
20	H	Isotropic =	29.4124	Anisotropy =	9.6100

Conformer_27

C	0.447412102504	0.771079892225	0.687117258798
C	0.529647504935	-0.664670682348	1.174959490320
C	1.898957462811	-1.316479076594	1.012810533546
O	-0.418952889916	-1.490444463812	0.489845074987
N	2.475983293620	-1.225462318173	-0.327927854049
C	3.470361467001	-0.168209859334	-0.424655278078
C	3.045097038811	-2.489454920825	-0.765977727919
H	-0.558320838543	1.171888002602	0.854878996449
H	1.151535885229	1.408218023612	1.231271982308
H	0.668819285665	0.830603004638	-0.382297496197
H	0.300979633141	-0.686026066169	2.250869978344
H	1.779581763982	-2.371116013969	1.281454863395
H	2.579813469929	-0.878394489168	1.759985585144
H	-1.265661281412	-1.034884408698	0.495281756751
H	3.046341719429	0.790973518868	-0.120214720590
H	4.351544695851	-0.368568120661	0.212465988723
H	3.814044416653	-0.072797350060	-1.459110749316
H	3.425811851558	-2.388080494421	-1.786848490482
H	3.880618254643	-2.825235642564	-0.124559425345
H	2.278985164108	-3.269238535151	-0.765349766788

SCF Done: E(RwB97X) = -328.334877932

Zero-point correction=	0.183035
Thermal correction to Energy=	0.192102
Thermal correction to Enthalpy=	0.193046
Thermal correction to Gibbs Free Energy=	0.149339
Sum of electronic and zero-point Energies=	-328.151842
Sum of electronic and thermal Energies=	-328.142776
Sum of electronic and thermal Enthalpies=	-328.141832
Sum of electronic and thermal Free Energies=	-328.185539

1 C	Isotropic =	169.8297	Anisotropy =	28.1411
2 C	Isotropic =	120.8989	Anisotropy =	46.5624
3 C	Isotropic =	128.0218	Anisotropy =	48.0771
4 O	Isotropic =	271.5426	Anisotropy =	68.1547
5 N	Isotropic =	239.5573	Anisotropy =	42.3632
6 C	Isotropic =	143.9995	Anisotropy =	68.2074
7 C	Isotropic =	142.9073	Anisotropy =	71.0599
8 H	Isotropic =	30.7830	Anisotropy =	9.3928
9 H	Isotropic =	30.7073	Anisotropy =	9.1880
10 H	Isotropic =	30.4120	Anisotropy =	4.7295
11 H	Isotropic =	28.0775	Anisotropy =	6.5876
12 H	Isotropic =	29.2552	Anisotropy =	6.2210
13 H	Isotropic =	29.7425	Anisotropy =	5.4925
14 H	Isotropic =	31.4969	Anisotropy =	17.8529
15 H	Isotropic =	29.3419	Anisotropy =	7.4736
16 H	Isotropic =	29.9949	Anisotropy =	8.4812
17 H	Isotropic =	29.5358	Anisotropy =	10.2306
18 H	Isotropic =	29.5143	Anisotropy =	10.2781
19 H	Isotropic =	29.6692	Anisotropy =	8.9661
20 H	Isotropic =	29.4124	Anisotropy =	9.6102

Conformer_28

C	0.580482953908	0.777416066862	0.459681909747
C	0.515804505867	-0.608026434026	1.081662627605
C	1.859830469310	-1.326785779916	1.245644297420
O	-0.355420537997	-1.463095153925	0.329741797331
N	2.787316979851	-1.448852720299	0.131362888082
C	3.580165836633	-0.276030917421	-0.186514225697
C	2.272178397287	-2.106520619198	-1.053211973443
H	1.281545494158	1.417426145500	1.004232348702
H	0.891103402263	0.726059520862	-0.587050446310
H	-0.404853710083	1.255209188883	0.498119668231
H	0.111801282703	-0.512854418685	2.101050315124

H	1.622408641806	-2.339674441787	1.595626677459
H	2.395842112626	-0.828194105553	2.060856355434
H	-1.197790031482	-1.009926712293	0.229732618012
H	4.455757162754	-0.581077049626	-0.771232539311
H	3.044794252870	0.487065732561	-0.773343130256
H	3.940085748288	0.191446806258	0.734746754396
H	3.109272577316	-2.389036204711	-1.701876755390
H	1.584147467848	-1.477699616339	-1.641452293506
H	1.733526994076	-3.015349287149	-0.771876893630

SCF Done: E(RwB97X) = -328.332751704

Zero-point correction=	0.183442
Thermal correction to Energy=	0.192360
Thermal correction to Enthalpy=	0.193304
Thermal correction to Gibbs Free Energy=	0.150517
Sum of electronic and zero-point Energies=	-328.149310
Sum of electronic and thermal Energies=	-328.140392
Sum of electronic and thermal Enthalpies=	-328.139448
Sum of electronic and thermal Free Energies=	-328.182234

1 C	Isotropic =	167.6466	Anisotropy =	26.7225
2 C	Isotropic =	116.3034	Anisotropy =	40.3794
3 C	Isotropic =	130.1183	Anisotropy =	34.4430
4 O	Isotropic =	266.3360	Anisotropy =	67.2587
5 N	Isotropic =	234.3105	Anisotropy =	46.1266
6 C	Isotropic =	146.0870	Anisotropy =	64.1379
7 C	Isotropic =	148.6183	Anisotropy =	54.5934
8 H	Isotropic =	30.5043	Anisotropy =	8.0397
9 H	Isotropic =	30.4164	Anisotropy =	4.8105
10 H	Isotropic =	30.5864	Anisotropy =	9.2851
11 H	Isotropic =	27.9961	Anisotropy =	6.3740
12 H	Isotropic =	28.7414	Anisotropy =	7.5417
13 H	Isotropic =	29.1860	Anisotropy =	6.7961
14 H	Isotropic =	31.3319	Anisotropy =	17.6112
15 H	Isotropic =	29.3251	Anisotropy =	10.2247
16 H	Isotropic =	29.0171	Anisotropy =	6.6386
17 H	Isotropic =	29.2112	Anisotropy =	8.4349
18 H	Isotropic =	29.4447	Anisotropy =	10.0583
19 H	Isotropic =	29.1058	Anisotropy =	6.6581
20 H	Isotropic =	29.1142	Anisotropy =	7.9947

Conformer_3

C	-0.333213976485	1.188896229979	0.331820183461

C	0.799839508224	0.233996639309	0.639620761011
C	1.076011869090	-0.716034991822	-0.522371477320
O	0.458707497718	-0.532697002411	1.792914048628
N	2.019513242508	-1.760210586818	-0.133509744215
C	3.389934160712	-1.270120983467	-0.098625105958
C	1.915780119973	-2.922753117297	-1.001473987798
H	-0.521777033556	1.849738065761	1.182505053401
H	-1.252978875144	0.637226734166	0.111476316401
H	-0.084359504663	1.811516332603	-0.533256419831
H	1.706559581508	0.817292621233	0.856653715655
H	1.432295124597	-0.147301404564	-1.398872341114
H	0.131654051719	-1.199724537208	-0.796396219143
H	0.994160852028	-1.336028765286	1.718649104984
H	3.484976125497	-0.433651629305	0.598352384211
H	3.731824377692	-0.930826956641	-1.092296574137
H	4.057926796118	-2.066414308445	0.240565152461
H	2.597549960422	-3.704733838453	-0.655175361323
H	0.897388836623	-3.319444768651	-0.975123480891
H	2.169907285420	-2.687523732683	-2.049956008483

SCF Done: E(RwB97X) = -328.343630602

Zero-point correction=	0.183690
Thermal correction to Energy=	0.192463
Thermal correction to Enthalpy=	0.193407
Thermal correction to Gibbs Free Energy=	0.150751
Sum of electronic and zero-point Energies=	-328.159941
Sum of electronic and thermal Energies=	-328.151167
Sum of electronic and thermal Enthalpies=	-328.150223
Sum of electronic and thermal Free Energies=	-328.192880

1 C	Isotropic =	171.1932	Anisotropy =	35.6818
2 C	Isotropic =	127.5729	Anisotropy =	53.6580
3 C	Isotropic =	124.0556	Anisotropy =	53.8754
4 O	Isotropic =	284.6607	Anisotropy =	44.4414
5 N	Isotropic =	230.9651	Anisotropy =	37.0834
6 C	Isotropic =	149.7800	Anisotropy =	64.2142
7 C	Isotropic =	144.3934	Anisotropy =	71.6366
8 H	Isotropic =	30.4260	Anisotropy =	10.0115
9 H	Isotropic =	31.0721	Anisotropy =	7.9874
10 H	Isotropic =	30.8863	Anisotropy =	9.6365
11 H	Isotropic =	28.0858	Anisotropy =	5.6216
12 H	Isotropic =	29.8245	Anisotropy =	4.6866
13 H	Isotropic =	29.7577	Anisotropy =	6.6596
14 H	Isotropic =	29.0182	Anisotropy =	17.2327
15 H	Isotropic =	29.1993	Anisotropy =	8.8580

16 H	Isotropic =	30.2323	Anisotropy =	9.0253
17 H	Isotropic =	29.5817	Anisotropy =	10.3170
18 H	Isotropic =	29.3768	Anisotropy =	10.3375
19 H	Isotropic =	29.4567	Anisotropy =	9.8732
20 H	Isotropic =	29.7345	Anisotropy =	9.1516

Conformer_4

C	0.520072287825	0.846386027976	0.561078504129
C	0.600957869597	-0.604090281686	0.999103911265
C	1.336352232307	-1.490886938665	-0.007614332077
O	-0.702329820856	-1.149339244559	1.223826082210
N	2.686923520631	-1.050607506959	-0.328934044879
C	3.214676184397	-1.818652699913	-1.444824256872
C	3.576386436009	-1.153654478552	0.817401012149
H	1.518347321494	1.281944261053	0.467633731048
H	0.023710348912	0.926985249403	-0.413867770495
H	-0.048240627510	1.431977209099	1.289240409607
H	1.089342318572	-0.662836101435	1.976171432755
H	0.753969696193	-1.494814222219	-0.938372658496
H	1.339307355785	-2.526541441071	0.381901032736
H	-1.203814650705	-1.057143271184	0.406570654466
H	4.211732428255	-1.454599362527	-1.708399586591
H	3.294019090037	-2.896642009551	-1.212504093178
H	2.566200640146	-1.705795901317	-2.318218588205
H	4.587272708793	-0.858515569423	0.523234409271
H	3.621013500620	-2.183239813772	1.217676763933
H	3.256801159497	-0.488133904699	1.623397387224

SCF Done: E(RwB97X) = -328.338929783

Zero-point correction=	0.183193
Thermal correction to Energy=	0.192217
Thermal correction to Enthalpy=	0.193161
Thermal correction to Gibbs Free Energy=	0.149805
Sum of electronic and zero-point Energies=	-328.155737
Sum of electronic and thermal Energies=	-328.146713
Sum of electronic and thermal Enthalpies=	-328.145769
Sum of electronic and thermal Free Energies=	-328.189125

1 C	Isotropic =	169.2940	Anisotropy =	34.0773
2 C	Isotropic =	123.0690	Anisotropy =	58.8313
3 C	Isotropic =	122.9993	Anisotropy =	59.1847
4 O	Isotropic =	272.3684	Anisotropy =	42.5813
5 N	Isotropic =	226.6169	Anisotropy =	39.1309

6 C	Isotropic =	144.0986	Anisotropy =	73.1642
7 C	Isotropic =	148.9908	Anisotropy =	63.9189
8 H	Isotropic =	30.3150	Anisotropy =	7.4079
9 H	Isotropic =	31.1381	Anisotropy =	7.5102
10 H	Isotropic =	30.5399	Anisotropy =	9.5617
11 H	Isotropic =	28.1282	Anisotropy =	4.0922
12 H	Isotropic =	29.8062	Anisotropy =	5.2977
13 H	Isotropic =	29.7329	Anisotropy =	3.8378
14 H	Isotropic =	31.7698	Anisotropy =	15.2070
15 H	Isotropic =	29.4662	Anisotropy =	10.2805
16 H	Isotropic =	29.9507	Anisotropy =	8.7743
17 H	Isotropic =	29.4739	Anisotropy =	9.8082
18 H	Isotropic =	29.6173	Anisotropy =	10.1309
19 H	Isotropic =	30.3273	Anisotropy =	8.5827
20 H	Isotropic =	29.4219	Anisotropy =	8.3450

Conformer_5

C	-0.238015510521	1.172569463008	0.424816344276
C	0.547171063266	-0.091794345654	0.713139516657
C	1.405677784700	-0.493567049636	-0.488805486633
O	-0.424869259648	-1.088586803773	1.055464970713
N	2.624607169286	-1.225870255309	-0.158686336476
C	2.364919327856	-2.487768517633	0.514961683256
C	3.408027390283	-1.449404330630	-1.363492689463
H	-0.890004219724	1.416664197850	1.267562353797
H	0.437848081917	2.014559161294	0.254018149071
H	-0.861692290469	1.041689035637	-0.466181454974
H	1.209796352662	0.079341875062	1.573138332741
H	1.713916712018	0.417445269709	-1.011821190122
H	0.767933654186	-1.070505122742	-1.186651122864
H	0.028068885876	-1.908706682468	1.268228066527
H	1.958746166308	-2.321450595299	1.518072279740
H	1.673705423803	-3.137758571033	-0.052629694138
H	3.304918268408	-3.030018602107	0.646181257921
H	4.352083753721	-1.938579567037	-1.108087819949
H	3.635148859074	-0.492901063862	-1.842635727718
H	2.879312387000	-2.084757495377	-2.097091432363

SCF Done: E(RwB97X) = -328.336835853

Zero-point correction=	0.183242
Thermal correction to Energy=	0.192197
Thermal correction to Enthalpy=	0.193141
Thermal correction to Gibbs Free Energy=	0.150127

Sum of electronic and zero-point Energies=	-328.153594
Sum of electronic and thermal Energies=	-328.144639
Sum of electronic and thermal Enthalpies=	-328.143694
Sum of electronic and thermal Free Energies=	-328.186709

1 C	Isotropic =	169.1681	Anisotropy =	35.2174
2 C	Isotropic =	120.0757	Anisotropy =	43.9941
3 C	Isotropic =	121.7079	Anisotropy =	50.0902
4 O	Isotropic =	268.9696	Anisotropy =	45.3497
5 N	Isotropic =	222.7589	Anisotropy =	48.8665
6 C	Isotropic =	148.4156	Anisotropy =	60.8310
7 C	Isotropic =	144.5081	Anisotropy =	72.3339
8 H	Isotropic =	30.6717	Anisotropy =	9.9131
9 H	Isotropic =	30.8149	Anisotropy =	9.3540
10 H	Isotropic =	30.7000	Anisotropy =	7.2127
11 H	Isotropic =	27.9148	Anisotropy =	3.8192
12 H	Isotropic =	29.2008	Anisotropy =	6.1806
13 H	Isotropic =	30.0383	Anisotropy =	3.9773
14 H	Isotropic =	30.4285	Anisotropy =	15.9327
15 H	Isotropic =	29.2778	Anisotropy =	8.0612
16 H	Isotropic =	30.0726	Anisotropy =	7.5891
17 H	Isotropic =	29.4263	Anisotropy =	9.7443
18 H	Isotropic =	29.5019	Anisotropy =	10.2738
19 H	Isotropic =	29.4898	Anisotropy =	9.8335
20 H	Isotropic =	29.9935	Anisotropy =	8.5077

Conformer_6

C	0.592439192399	0.778299305814	0.705817434049
C	0.546083839550	-0.735902882798	0.790493472766
C	1.353332170060	-1.423026664542	-0.305787359801
O	-0.789626731130	-1.223494178814	0.619376958044
N	2.752130531320	-1.023200667311	-0.360940793324
C	3.374352384866	-1.542818148882	-1.567663924460
C	3.491406447053	-1.460799059027	0.812848537998
H	0.263130963407	1.119845543133	-0.281520638813
H	-0.060481642621	1.224715337871	1.463661029942
H	1.607839012760	1.145476816978	0.878436667884
H	0.910329872722	-1.053623815146	1.776367645997
H	0.888428623387	-1.169227116986	-1.265295936031
H	1.259312071079	-2.517510468846	-0.173255071548
H	-1.336887009332	-0.830974675325	1.305638024545
H	3.373200581469	-2.648046333288	-1.598119776747
H	2.843094411775	-1.178153429021	-2.451293727878
H	4.412344783444	-1.203378595611	-1.626742979622

H	3.441149426461	-2.556526167832	0.951352154677
H	3.107538259677	-0.984771012584	1.718621532401
H	4.542782811654	-1.178983787783	0.708506749921

SCF Done: E(RwB97X) = -328.338775867

Zero-point correction=	0.183057
Thermal correction to Energy=	0.192103
Thermal correction to Enthalpy=	0.193047
Thermal correction to Gibbs Free Energy=	0.149739
Sum of electronic and zero-point Energies=	-328.155719
Sum of electronic and thermal Energies=	-328.146673
Sum of electronic and thermal Enthalpies=	-328.145729
Sum of electronic and thermal Free Energies=	-328.189037

1 C	Isotropic = 168.6842	Anisotropy = 34.2319
2 C	Isotropic = 123.8752	Anisotropy = 57.6048
3 C	Isotropic = 125.6194	Anisotropy = 55.7054
4 O	Isotropic = 277.3219	Anisotropy = 62.8062
5 N	Isotropic = 228.1867	Anisotropy = 36.8581
6 C	Isotropic = 143.9199	Anisotropy = 73.3942
7 C	Isotropic = 148.7065	Anisotropy = 64.3830
8 H	Isotropic = 30.9902	Anisotropy = 7.6471
9 H	Isotropic = 30.7155	Anisotropy = 9.3876
10 H	Isotropic = 30.3935	Anisotropy = 7.4144
11 H	Isotropic = 27.8716	Anisotropy = 4.5911
12 H	Isotropic = 29.6903	Anisotropy = 5.3030
13 H	Isotropic = 29.7479	Anisotropy = 4.0443
14 H	Isotropic = 31.1667	Anisotropy = 18.5752
15 H	Isotropic = 29.9263	Anisotropy = 8.8112
16 H	Isotropic = 29.4404	Anisotropy = 9.8672
17 H	Isotropic = 29.4435	Anisotropy = 10.3090
18 H	Isotropic = 30.3322	Anisotropy = 8.6086
19 H	Isotropic = 29.4475	Anisotropy = 8.3601
20 H	Isotropic = 29.6113	Anisotropy = 10.1348

Conformer_7

C	0.615994404559	1.004390737458	0.658918694107
C	0.524346595766	-0.493131218800	0.851983071429
C	1.269959115626	-1.279408297614	-0.227701142658
O	-0.863244751097	-0.843711900318	0.801345292544
N	2.693199666261	-0.986314990325	-0.319482934888
C	3.252376824180	-1.588841972550	-1.518665897093
C	3.421200688583	-1.440011379671	0.855556963221

H	0.241832463159	1.287397753311	-0.331084871836
H	0.023322109079	1.524527931471	1.416606944678
H	1.653076704128	1.338784091000	0.742312567643
H	0.914836309208	-0.755046532777	1.843852146351
H	0.807571939534	-1.035511843211	-1.190826235181
H	1.106178377117	-2.362020170569	-0.050406557220
H	-0.938715935742	-1.788337522342	0.968487704937
H	3.166962900156	-2.690970961203	-1.512553020745
H	2.734823047772	-1.211407658960	-2.404970418529
H	4.311878920483	-1.331480683001	-1.604555822888
H	3.299111373222	-2.525775920875	1.024970093944
H	3.085838625137	-0.914069451119	1.752561409050
H	4.487250622870	-1.233060009905	0.727452013134

SCF Done: E(RwB97X) = -328.338901099

Zero-point correction=	0.183098
Thermal correction to Energy=	0.192102
Thermal correction to Enthalpy=	0.193046
Thermal correction to Gibbs Free Energy=	0.149918
Sum of electronic and zero-point Energies=	-328.155803
Sum of electronic and thermal Energies=	-328.146799
Sum of electronic and thermal Enthalpies=	-328.145855
Sum of electronic and thermal Free Energies=	-328.188983

1 C	Isotropic =	171.7601	Anisotropy =	31.0148
2 C	Isotropic =	123.9466	Anisotropy =	58.2675
3 C	Isotropic =	122.6776	Anisotropy =	58.2723
4 O	Isotropic =	283.1922	Anisotropy =	87.6120
5 N	Isotropic =	226.7565	Anisotropy =	39.0611
6 C	Isotropic =	143.8937	Anisotropy =	73.4002
7 C	Isotropic =	148.7565	Anisotropy =	64.4421
8 H	Isotropic =	31.0356	Anisotropy =	7.9293
9 H	Isotropic =	30.5912	Anisotropy =	9.9683
10 H	Isotropic =	30.4308	Anisotropy =	7.2957
11 H	Isotropic =	27.8885	Anisotropy =	4.6883
12 H	Isotropic =	29.6632	Anisotropy =	4.9823
13 H	Isotropic =	29.9291	Anisotropy =	3.7776
14 H	Isotropic =	31.3067	Anisotropy =	18.3868
15 H	Isotropic =	29.9731	Anisotropy =	8.7360
16 H	Isotropic =	29.4533	Anisotropy =	9.8231
17 H	Isotropic =	29.4721	Anisotropy =	10.2898
18 H	Isotropic =	30.3530	Anisotropy =	8.4979
19 H	Isotropic =	29.4210	Anisotropy =	8.3782
20 H	Isotropic =	29.6165	Anisotropy =	10.1190

Conformer_8

C	-0.133449343871	0.639186766656	-0.473725269151
C	0.506133439876	0.183798160467	0.829656342550
C	1.960761916252	-0.275034123365	0.696636050784
O	-0.254145625741	-0.874255571879	1.413539363652
N	2.058548963603	-1.541730347091	-0.033477264506
C	2.465843593428	-1.356933164651	-1.419798551045
C	2.940651166550	-2.496049129219	0.623229964398
H	-1.145059506554	1.008971281519	-0.282978148225
H	0.444617668443	1.446787130216	-0.934959747092
H	-0.207006157657	-0.189019423225	-1.185712680452
H	0.478277828048	1.010681902880	1.547158352413
H	2.351304914370	-0.421519342912	1.708365040622
H	2.567006069600	0.512173047119	0.224712647897
H	0.030221469611	-1.665666406467	0.935231314174
H	2.401370337210	-2.308374683311	-1.955877375574
H	1.816492306136	-0.638984034785	-1.923970551317
H	3.504169075589	-0.988525762777	-1.496149285326
H	2.598938123858	-2.687971331324	1.643536874126
H	3.985041258089	-2.140754571360	0.668033660123
H	2.928882503160	-3.443280396492	0.076049261950

SCF Done: E(RwB97X) = -328.339224745

Zero-point correction=	0.183983
Thermal correction to Energy=	0.192655
Thermal correction to Enthalpy=	0.193599
Thermal correction to Gibbs Free Energy=	0.151346
Sum of electronic and zero-point Energies=	-328.155242
Sum of electronic and thermal Energies=	-328.146570
Sum of electronic and thermal Enthalpies=	-328.145626
Sum of electronic and thermal Free Energies=	-328.187879

1 C	Isotropic = 168.2500	Anisotropy = 31.8903
2 C	Isotropic = 123.4036	Anisotropy = 46.2151
3 C	Isotropic = 127.5637	Anisotropy = 43.0736
4 O	Isotropic = 284.2738	Anisotropy = 48.5022
5 N	Isotropic = 241.1044	Anisotropy = 37.6839
6 C	Isotropic = 143.8991	Anisotropy = 68.3909
7 C	Isotropic = 142.9402	Anisotropy = 71.0671
8 H	Isotropic = 30.6113	Anisotropy = 9.4638
9 H	Isotropic = 30.9216	Anisotropy = 9.5882
10 H	Isotropic = 30.6197	Anisotropy = 4.8319
11 H	Isotropic = 28.3038	Anisotropy = 6.5959

12	H	Isotropic =	29.3684	Anisotropy =	6.9776
13	H	Isotropic =	29.6039	Anisotropy =	5.2830
14	H	Isotropic =	29.5078	Anisotropy =	14.5039
15	H	Isotropic =	29.4783	Anisotropy =	10.2535
16	H	Isotropic =	29.2864	Anisotropy =	7.5216
17	H	Isotropic =	29.8141	Anisotropy =	8.6412
18	H	Isotropic =	29.4773	Anisotropy =	9.7373
19	H	Isotropic =	29.6241	Anisotropy =	9.1355
20	H	Isotropic =	29.4723	Anisotropy =	10.2707

Conformer_9

C	0.602612457039	0.942898476639	1.206201120441
C	0.525014423458	-0.535639112534	0.878510983418
C	1.348817796033	-0.944507739755	-0.354703031500
O	-0.864899657760	-0.814314847937	0.668912339048
N	2.621146374268	-1.584303138563	-0.034699122828
C	3.229701338137	-2.111187143436	-1.245872348480
C	3.544815129402	-0.681741401290	0.634509450985
H	0.189591780151	1.530155046167	0.379435757846
H	0.029940847955	1.166308933718	2.110460951877
H	1.635884287844	1.260453643008	1.364688234338
H	0.881655604038	-1.126454717080	1.733861090531
H	1.502693112182	-0.066077887465	-1.011332582925
H	0.762187409312	-1.669564218268	-0.928510635006
H	-0.962011844558	-1.760906552285	0.528005635480
H	4.160814615395	-2.628753581510	-0.998595273344
H	2.554170506911	-2.826550095727	-1.723486157343
H	3.463203978409	-1.317435378733	-1.978667276715
H	3.149891049091	-0.366618669957	1.603286380893
H	3.755585875691	0.222211374272	0.033824237890
H	4.491384917002	-1.198972989261	0.814170245391

SCF Done: E(RwB97X) = -328.335424068

Zero-point correction=	0.183414
Thermal correction to Energy=	0.192296
Thermal correction to Enthalpy=	0.193241
Thermal correction to Gibbs Free Energy=	0.150426
Sum of electronic and zero-point Energies=	-328.152010
Sum of electronic and thermal Energies=	-328.143128
Sum of electronic and thermal Enthalpies=	-328.142183
Sum of electronic and thermal Free Energies=	-328.184998

1	C	Isotropic =	168.1055	Anisotropy =	34.6558

2	C	Isotropic =	119.1993	Anisotropy =	49.4654
3	C	Isotropic =	120.1285	Anisotropy =	53.1093
4	O	Isotropic =	266.5458	Anisotropy =	91.7937
5	N	Isotropic =	223.3153	Anisotropy =	43.8804
6	C	Isotropic =	144.1282	Anisotropy =	73.2833
7	C	Isotropic =	147.3145	Anisotropy =	58.6878
8	H	Isotropic =	30.7976	Anisotropy =	7.4023
9	H	Isotropic =	30.5356	Anisotropy =	10.0781
10	H	Isotropic =	30.5252	Anisotropy =	6.4558
11	H	Isotropic =	28.0345	Anisotropy =	3.7083
12	H	Isotropic =	29.9036	Anisotropy =	3.2546
13	H	Isotropic =	29.3777	Anisotropy =	5.6518
14	H	Isotropic =	31.1569	Anisotropy =	17.1329
15	H	Isotropic =	29.4913	Anisotropy =	10.2558
16	H	Isotropic =	29.4666	Anisotropy =	9.8590
17	H	Isotropic =	30.0354	Anisotropy =	8.4678
18	H	Isotropic =	29.4473	Anisotropy =	7.6371
19	H	Isotropic =	30.3997	Anisotropy =	7.6853
20	H	Isotropic =	29.5805	Anisotropy =	9.7899

1-(dimethylamino)propan-2-ol_protonated

Conformer_1

C	-1.362148683454	-1.017187158878	0.420149071935
C	0.092007374433	-1.414883989456	0.585307642256
C	0.999495073254	-0.406105512906	-0.094709437342
O	0.386339141669	-2.665730490893	-0.041771319318
N	2.423054865902	-0.861564016061	-0.104974325528
C	3.034884478194	-0.887004731609	1.249138893494
C	3.238237421492	-0.046505032947	-1.042593402229
H	-2.012549698519	-1.756128754148	0.896514627339
H	-1.626436170186	-0.948007195912	-0.639348547036
H	-1.548318536749	-0.048990373324	0.894228258954
H	0.330925206776	-1.477413428920	1.653572610429
H	0.701935281575	-0.288261759830	-1.138970316126
H	0.964711295272	0.563759282336	0.404448581932
H	-0.091243380397	-3.364190788159	0.416236728385
H	2.412189538304	-1.824672467558	-0.455080397402
H	2.988498605859	0.119353018777	1.665907768698
H	2.492676650844	-1.586771148649	1.882383845548
H	4.070137991400	-1.209860991259	1.149549550079
H	4.253179711397	-0.441757990644	-1.052761318790
H	2.796747901654	-0.109841725509	-2.036281895792
H	3.237375931280	0.985765255550	-0.691246619487

SCF Done: E(RwB97X) = -328.814722958

Zero-point correction=	0.199604
Thermal correction to Energy=	0.208645
Thermal correction to Enthalpy=	0.209589
Thermal correction to Gibbs Free Energy=	0.166485
Sum of electronic and zero-point Energies=	-328.615119
Sum of electronic and thermal Energies=	-328.606078
Sum of electronic and thermal Enthalpies=	-328.605134
Sum of electronic and thermal Free Energies=	-328.648238

1	C	Isotropic =	170.0839	Anisotropy =	37.2268
2	C	Isotropic =	127.0657	Anisotropy =	54.0043
3	C	Isotropic =	126.7520	Anisotropy =	56.9809
4	O	Isotropic =	284.5085	Anisotropy =	51.4537
5	N	Isotropic =	210.3911	Anisotropy =	12.1833
6	C	Isotropic =	149.5148	Anisotropy =	64.7984
7	C	Isotropic =	145.0496	Anisotropy =	72.1690
8	H	Isotropic =	30.3749	Anisotropy =	9.7820
9	H	Isotropic =	30.7748	Anisotropy =	7.8930
10	H	Isotropic =	30.6896	Anisotropy =	10.0715
11	H	Isotropic =	27.5679	Anisotropy =	4.8700
12	H	Isotropic =	28.8325	Anisotropy =	6.5981
13	H	Isotropic =	28.8433	Anisotropy =	5.1409
14	H	Isotropic =	30.5689	Anisotropy =	19.7026
15	H	Isotropic =	26.5005	Anisotropy =	12.6580
16	H	Isotropic =	29.2671	Anisotropy =	8.7664
17	H	Isotropic =	28.5951	Anisotropy =	8.5963
18	H	Isotropic =	28.9361	Anisotropy =	10.1929
19	H	Isotropic =	28.8267	Anisotropy =	10.2675
20	H	Isotropic =	28.9165	Anisotropy =	9.9139
21	H	Isotropic =	28.9330	Anisotropy =	8.6420

Conformer_2

C	-0.747168469778	-1.034188956993	-0.750616269614
C	-0.121020114737	-1.311445483460	0.605285869120
C	1.120000967705	-0.501314592676	0.944387726279
O	0.286695511507	-2.677990604671	0.714687244941
N	2.275109981600	-0.840739034977	0.044879308297
C	3.548035138917	-0.970762856081	0.803804935064
C	2.435626701016	0.124734255883	-1.076389478005
H	-1.674689077410	-1.606664485398	-0.847693987499
H	-0.997313630619	0.025579132209	-0.851370271336

H	-0.087435307646	-1.325843987077	-1.573523408043
H	-0.850424826749	-1.076199550951	1.389892095969
H	1.425329447113	-0.736906702194	1.964019009600
H	0.932281940318	0.570201525530	0.869729268867
H	-0.424683059851	-3.237995742556	0.388287619484
H	2.074392002495	-1.763612969067	-0.354384785373
H	3.752671306713	-0.020081636458	1.296599569207
H	3.437119651093	-1.764705084830	1.540973520430
H	4.345598916709	-1.213861359184	0.102771793336
H	1.488687363909	0.239935578484	-1.599590809008
H	2.748021906634	1.080347421299	-0.654916475671
H	3.197463651061	-0.257684866831	-1.754632476046

SCF Done: E(RwB97X) = -328.810545117

Zero-point correction=	0.199673
Thermal correction to Energy=	0.208563
Thermal correction to Enthalpy=	0.209507
Thermal correction to Gibbs Free Energy=	0.166836
Sum of electronic and zero-point Energies=	-328.610873
Sum of electronic and thermal Energies=	-328.601982
Sum of electronic and thermal Enthalpies=	-328.601038
Sum of electronic and thermal Free Energies=	-328.643709

1 C	Isotropic = 169.8785	Anisotropy = 30.7415
2 C	Isotropic = 124.4983	Anisotropy = 49.3070
3 C	Isotropic = 127.1211	Anisotropy = 51.5301
4 O	Isotropic = 279.3981	Anisotropy = 49.0389
5 N	Isotropic = 215.9224	Anisotropy = 12.2744
6 C	Isotropic = 143.0547	Anisotropy = 71.0465
7 C	Isotropic = 143.4710	Anisotropy = 69.3460
8 H	Isotropic = 30.3860	Anisotropy = 9.7429
9 H	Isotropic = 30.5237	Anisotropy = 9.8013
10 H	Isotropic = 30.4499	Anisotropy = 5.3408
11 H	Isotropic = 27.6366	Anisotropy = 7.3520
12 H	Isotropic = 28.5056	Anisotropy = 6.7831
13 H	Isotropic = 28.6766	Anisotropy = 5.6903
14 H	Isotropic = 30.8034	Anisotropy = 18.4494
15 H	Isotropic = 26.4960	Anisotropy = 12.4017
16 H	Isotropic = 28.8434	Anisotropy = 8.6359
17 H	Isotropic = 28.8975	Anisotropy = 9.6640
18 H	Isotropic = 28.9038	Anisotropy = 10.1976
19 H	Isotropic = 28.6652	Anisotropy = 7.2546
20 H	Isotropic = 28.9660	Anisotropy = 8.3548
21 H	Isotropic = 28.8277	Anisotropy = 10.2024

Conformer_3

C	-1.269555143731	-1.195815613654	0.652906596256
C	0.222718171314	-1.460510902682	0.534817564017
C	0.921564581115	-0.190843499696	0.087207881281
O	0.496397733949	-2.477873744511	-0.428403314423
N	2.423705203385	-0.234800285057	0.072623116082
C	3.005111914797	-1.011005001134	-1.057839042054
C	3.017009230683	-0.644518573094	1.372309561125
H	-1.790512757442	-2.115459738927	0.935052668682
H	-1.471052479215	-0.445449719402	1.422352902377
H	-1.677512548089	-0.843646847133	-0.299627784692
H	0.605494143892	-1.771839022314	1.514669949232
H	0.655208630540	0.618247973916	0.769368776969
H	0.609408954463	0.080259516401	-0.923522362108
H	0.017300233058	-3.270670682364	-0.166896149695
H	2.705412657755	0.736331839274	-0.078176203999
H	2.571590945294	-0.645538927944	-1.987864983491
H	4.082757521746	-0.849276800630	-1.054245803252
H	2.770778072906	-2.063611712563	-0.920461423912
H	4.085372579777	-0.435207683620	1.338346554487
H	2.546324111272	-0.072782552691	2.171561216393
H	2.856378242531	-1.711688022177	1.518120280726

SCF Done: E(RwB97X) = -328.810423669

Zero-point correction=	0.199651
Thermal correction to Energy=	0.208640
Thermal correction to Enthalpy=	0.209584
Thermal correction to Gibbs Free Energy=	0.166611
Sum of electronic and zero-point Energies=	-328.610773
Sum of electronic and thermal Energies=	-328.601783
Sum of electronic and thermal Enthalpies=	-328.600839
Sum of electronic and thermal Free Energies=	-328.643813

1 C	Isotropic =	168.3040	Anisotropy =	39.4954
2 C	Isotropic =	126.8340	Anisotropy =	59.9502
3 C	Isotropic =	127.8520	Anisotropy =	48.1486
4 O	Isotropic =	272.9939	Anisotropy =	57.9880
5 N	Isotropic =	207.6676	Anisotropy =	15.0178
6 C	Isotropic =	145.4368	Anisotropy =	66.1299
7 C	Isotropic =	149.2442	Anisotropy =	61.8277
8 H	Isotropic =	30.5454	Anisotropy =	9.4537
9 H	Isotropic =	30.7418	Anisotropy =	10.2250
10 H	Isotropic =	30.6543	Anisotropy =	7.6284

11	H	Isotropic =	27.3154	Anisotropy =	4.2779
12	H	Isotropic =	28.6742	Anisotropy =	6.7307
13	H	Isotropic =	28.6634	Anisotropy =	6.3785
14	H	Isotropic =	30.8941	Anisotropy =	18.6282
15	H	Isotropic =	26.8102	Anisotropy =	15.4393
16	H	Isotropic =	28.8625	Anisotropy =	9.3161
17	H	Isotropic =	28.9296	Anisotropy =	10.1529
18	H	Isotropic =	28.1859	Anisotropy =	5.1775
19	H	Isotropic =	28.7902	Anisotropy =	10.0103
20	H	Isotropic =	29.0102	Anisotropy =	9.7717
21	H	Isotropic =	28.7954	Anisotropy =	6.8885

Conformer_4

C	-0.397923043611	-1.483428940973	-0.797702518531
C	-0.039769634652	-1.263897880127	0.663627019598
C	1.007834235491	-0.204507276348	0.971565849327
O	0.366955902989	-2.480969761776	1.290380805877
N	2.339697358503	-0.265062643390	0.272430924638
C	2.332003267432	0.250634267677	-1.124560517643
C	3.030511021008	-1.580192669733	0.362685375704
H	-0.640777144628	-0.536159799236	-1.287247833843
H	0.412134059117	-1.973239109386	-1.344371397280
H	-1.280778277437	-2.127067355836	-0.860537585314
H	-0.931947191255	-0.881338151678	1.178053330320
H	1.234654559036	-0.248832180663	2.038438410244
H	0.599805290242	0.781512154218	0.745723161070
H	-0.319498174476	-3.137190555528	1.135019722079
H	2.918902867142	0.391736988150	0.799804932296
H	1.790687146905	1.195672539429	-1.145999062208
H	3.367098992969	0.405329895067	-1.427712294065
H	1.861285959356	-0.476920403595	-1.780784256687
H	4.045265553922	-1.448483410458	-0.012280631369
H	3.046983564060	-1.898240969746	1.403310304501
H	2.494173687884	-2.305954736067	-0.244543738713

SCF Done: E(RwB97X) = -328.805982796

Zero-point correction=	0.200088
Thermal correction to Energy=	0.208899
Thermal correction to Enthalpy=	0.209843
Thermal correction to Gibbs Free Energy=	0.167605
Sum of electronic and zero-point Energies=	-328.605895
Sum of electronic and thermal Energies=	-328.597084
Sum of electronic and thermal Enthalpies=	-328.596140

Sum of electronic and thermal Free Energies= -328.638378

1	C	Isotropic =	169.1016	Anisotropy =	25.7202
2	C	Isotropic =	122.5307	Anisotropy =	48.8513
3	C	Isotropic =	129.0007	Anisotropy =	38.6190
4	O	Isotropic =	270.7295	Anisotropy =	65.6274
5	N	Isotropic =	206.0812	Anisotropy =	17.4964
6	C	Isotropic =	144.6798	Anisotropy =	67.6050
7	C	Isotropic =	146.8887	Anisotropy =	56.5022
8	H	Isotropic =	30.3504	Anisotropy =	8.5750
9	H	Isotropic =	30.2098	Anisotropy =	5.1099
10	H	Isotropic =	30.3212	Anisotropy =	9.5618
11	H	Isotropic =	27.6188	Anisotropy =	7.0141
12	H	Isotropic =	28.2271	Anisotropy =	7.8090
13	H	Isotropic =	28.6260	Anisotropy =	7.1878
14	H	Isotropic =	30.9766	Anisotropy =	18.2025
15	H	Isotropic =	26.7937	Anisotropy =	15.3837
16	H	Isotropic =	28.8647	Anisotropy =	9.1385
17	H	Isotropic =	28.8009	Anisotropy =	10.0775
18	H	Isotropic =	28.4377	Anisotropy =	5.2037
19	H	Isotropic =	28.8939	Anisotropy =	9.9153
20	H	Isotropic =	28.7291	Anisotropy =	8.4272
21	H	Isotropic =	28.5554	Anisotropy =	5.1666

Conformer_5

C	-0.275315709829	-1.245908058301	-1.102273816075
C	-0.005288024175	-1.294086290806	0.393285739113
C	1.059781575926	-0.354396109195	0.938541927661
O	0.312689344704	-2.617932897390	0.824412222732
N	2.431164103670	-0.360811610371	0.317581179476
C	2.534311225764	0.382791558817	-0.968537230527
C	3.064169143253	-1.704269971278	0.221073791240
H	-0.449014960135	-0.218830075569	-1.435282522537
H	0.549287982849	-1.675577690036	-1.677069241084
H	-1.176276485321	-1.825613276830	-1.325564492754
H	-0.913847378823	-0.960736391023	0.913237112361
H	1.214643604184	-0.589381129277	1.993250957177
H	0.705383600617	0.674341914711	0.862143977329
H	-0.386444834314	-3.204249523378	0.518740709978
H	2.999250846403	0.168793716978	0.982265890895
H	2.031513356830	1.342910261057	-0.859260640793
H	3.592118791552	0.536250327286	-1.180054297534
H	2.080456643119	-0.200209085458	-1.765814782984
H	4.105558362502	-1.560663991860	-0.066270719091

H	3.000530298431	-2.193638752228	1.191028086039
H	2.541528512791	-2.290382925848	-0.531533850619

SCF Done: E(RwB97X) = -328.805982648

Zero-point correction=	0.200087
Thermal correction to Energy=	0.208898
Thermal correction to Enthalpy=	0.209842
Thermal correction to Gibbs Free Energy=	0.167602
Sum of electronic and zero-point Energies=	-328.605896
Sum of electronic and thermal Energies=	-328.597085
Sum of electronic and thermal Enthalpies=	-328.596140
Sum of electronic and thermal Free Energies=	-328.638381

1 C	Isotropic = 169.1016	Anisotropy = 25.7190
2 C	Isotropic = 122.5273	Anisotropy = 48.8520
3 C	Isotropic = 128.9970	Anisotropy = 38.6219
4 O	Isotropic = 270.7276	Anisotropy = 65.6294
5 N	Isotropic = 206.0762	Anisotropy = 17.4953
6 C	Isotropic = 144.6770	Anisotropy = 67.6017
7 C	Isotropic = 146.8902	Anisotropy = 56.5143
8 H	Isotropic = 30.3500	Anisotropy = 8.5741
9 H	Isotropic = 30.2099	Anisotropy = 5.1106
10 H	Isotropic = 30.3211	Anisotropy = 9.5619
11 H	Isotropic = 27.6189	Anisotropy = 7.0139
12 H	Isotropic = 28.2275	Anisotropy = 7.8079
13 H	Isotropic = 28.6259	Anisotropy = 7.1885
14 H	Isotropic = 30.9770	Anisotropy = 18.2001
15 H	Isotropic = 26.7935	Anisotropy = 15.3832
16 H	Isotropic = 28.8646	Anisotropy = 9.1363
17 H	Isotropic = 28.8006	Anisotropy = 10.0773
18 H	Isotropic = 28.4380	Anisotropy = 5.2030
19 H	Isotropic = 28.8936	Anisotropy = 9.9158
20 H	Isotropic = 28.7293	Anisotropy = 8.4285
21 H	Isotropic = 28.5559	Anisotropy = 5.1685

Conformer_6

C	-0.658714696246	-0.796576873783	0.655180288387
C	0.418820776023	-1.835232647803	0.398743629601
C	1.555838012203	-1.329094109035	-0.482879049088
O	-0.088668142969	-2.942446793381	-0.343456523027
N	2.259116071044	-0.121637183423	0.044154693855
C	2.869737382375	-0.338086632764	1.383281116184
C	3.278322087936	0.344551096841	-0.934956398696

H	-1.494713966184	-1.251152285798	1.195044477432
H	-0.285737859716	0.024251714052	1.277717509657
H	-1.034065739717	-0.384893771764	-0.287231943444
H	0.820527643877	-2.196377059078	1.352935129744
H	1.157997051977	-1.057909972239	-1.463124519037
H	2.315030706235	-2.104155592414	-0.605322517895
H	-0.795268412419	-3.345052223532	0.170696162483
H	1.573190112011	0.632328105721	0.135430247351
H	3.444642582198	0.549541141271	1.643958792761
H	2.083514145703	-0.496339714581	2.119783962401
H	3.522027480235	-1.209814666620	1.324938776370
H	3.717528478796	1.268393549742	-0.561154423960
H	4.041380971987	-0.428358737983	-1.029352138053
H	2.789995314651	0.517162656571	-1.892987273026

SCF Done: E(RwB97X) = -328.810727346

Zero-point correction=	0.199735
Thermal correction to Energy=	0.208664
Thermal correction to Enthalpy=	0.209609
Thermal correction to Gibbs Free Energy=	0.166850
Sum of electronic and zero-point Energies=	-328.610992
Sum of electronic and thermal Energies=	-328.602063
Sum of electronic and thermal Enthalpies=	-328.601119
Sum of electronic and thermal Free Energies=	-328.643877

1 C	Isotropic = 170.7277	Anisotropy = 33.8852
2 C	Isotropic = 126.6133	Anisotropy = 58.3084
3 C	Isotropic = 127.3806	Anisotropy = 54.2849
4 O	Isotropic = 280.3066	Anisotropy = 62.0982
5 N	Isotropic = 208.7325	Anisotropy = 11.6057
6 C	Isotropic = 148.5121	Anisotropy = 64.4470
7 C	Isotropic = 143.9890	Anisotropy = 74.1509
8 H	Isotropic = 30.4474	Anisotropy = 9.6834
9 H	Isotropic = 30.4868	Anisotropy = 7.7617
10 H	Isotropic = 30.7960	Anisotropy = 7.9596
11 H	Isotropic = 27.6301	Anisotropy = 4.7423
12 H	Isotropic = 28.9458	Anisotropy = 5.3850
13 H	Isotropic = 28.6910	Anisotropy = 4.5159
14 H	Isotropic = 30.9311	Anisotropy = 18.9134
15 H	Isotropic = 27.1597	Anisotropy = 12.8130
16 H	Isotropic = 28.9620	Anisotropy = 10.0299
17 H	Isotropic = 28.8581	Anisotropy = 8.0429
18 H	Isotropic = 29.2078	Anisotropy = 8.4506
19 H	Isotropic = 28.8250	Anisotropy = 10.2556
20 H	Isotropic = 28.9246	Anisotropy = 8.4784

21 H Isotropic = 28.8540 Anisotropy = 9.8171

Conformer_7

```
-----
C      -0.656437417787   -0.737854227044   -0.332775420700
C      0.261063746225   -1.697068689927    0.404345530565
C      1.736228730517   -1.607750009216    0.024848996209
O     -0.066631821881   -3.052960865055    0.113692507595
N      2.367588791199   -0.302450669098    0.413144907287
C      2.408243813407    0.675944620967   -0.709359301211
C      3.732928287590   -0.504381683979    0.972118588639
H     -1.697947419969   -0.959331513552   -0.078544456200
H     -0.534205225115   -0.831647558502   -1.416248712037
H     -0.472926996727    0.300065297071   -0.038451637442
H      0.175898863796   -1.521673365553    1.486750396456
H      1.876427360946   -1.736496009670   -1.050076384027
H      2.273447502045   -2.398342915607    0.548438144914
H     -1.009616663864   -3.170209887157    0.264878279179
H      1.805392861674    0.112525056988    1.161432073622
H      3.075729265471    0.281592241198   -1.475460937305
H      1.407072126990    0.808858775583   -1.113370908692
H      2.786992618869    1.622468153912   -0.325518544619
H      4.142858349823    0.467723719735    1.243067823707
H      3.658317163593   -1.143617408499    1.850508619633
H      4.347976063200   -0.977193062594    0.206280434426
```

SCF Done: E(RwB97X) = -328.807490903

```
Zero-point correction=          0.199641
Thermal correction to Energy=      0.208638
Thermal correction to Enthalpy=     0.209582
Thermal correction to Gibbs Free Energy= 0.166438
Sum of electronic and zero-point Energies= -328.607850
Sum of electronic and thermal Energies= -328.598853
Sum of electronic and thermal Enthalpies= -328.597909
Sum of electronic and thermal Free Energies= -328.641053
```

```
1 C Isotropic = 167.8667 Anisotropy = 30.5954
2 C Isotropic = 124.0844 Anisotropy = 59.7201
3 C Isotropic = 126.1179 Anisotropy = 61.6553
4 O Isotropic = 274.2224 Anisotropy = 67.9715
5 N Isotropic = 210.3098 Anisotropy = 19.8861
6 C Isotropic = 144.3261 Anisotropy = 68.3447
7 C Isotropic = 142.6629 Anisotropy = 71.5089
8 H Isotropic = 30.4514 Anisotropy = 9.4617
```


9 H	Isotropic =	30.6511	Anisotropy =	7.2057
10 H	Isotropic =	30.3319	Anisotropy =	7.4800
11 H	Isotropic =	27.7324	Anisotropy =	4.8704
12 H	Isotropic =	28.9426	Anisotropy =	4.2697
13 H	Isotropic =	28.5743	Anisotropy =	4.8575
14 H	Isotropic =	31.0752	Anisotropy =	18.4607
15 H	Isotropic =	27.3914	Anisotropy =	12.0218
16 H	Isotropic =	29.0159	Anisotropy =	8.0767
17 H	Isotropic =	28.6114	Anisotropy =	6.8578
18 H	Isotropic =	28.9420	Anisotropy =	10.2100
19 H	Isotropic =	28.9463	Anisotropy =	10.1908
20 H	Isotropic =	28.8141	Anisotropy =	9.7616
21 H	Isotropic =	28.8255	Anisotropy =	8.2469

3-methylbutan-1-amine _neutral

Conformer_1

C	-0.726853097945	0.074555993560	-1.771295722564
C	-0.076455545235	-0.333099065023	-0.450766489081
C	-0.486837532893	0.632928742477	0.660824792238
C	1.444896691913	-0.416478432390	-0.613407095630
C	2.180968450055	-1.030077611187	0.570142110218
N	3.622342540896	-1.092396136901	0.302891422014
H	-0.378276993609	1.066126151802	-2.085494627076
H	-0.486105840320	-0.632801488858	-2.571925003553
H	-1.817353393783	0.119536797648	-1.680162815315
H	-0.442864849864	-1.335144813416	-0.185473196539
H	-1.577423021820	0.702055428836	0.736216497215
H	-0.109772205496	0.323677365334	1.640062209249
H	-0.102767651976	1.640358008659	0.456587901884
H	1.680842882798	-1.009526786648	-1.506162789780
H	1.838412813288	0.594736108611	-0.796881815307
H	1.955235603334	-0.466549097305	1.486278462127
H	1.821643147577	-2.053735648496	0.727884009120
H	3.995459315606	-0.150037234834	0.234528430029
H	4.100808687475	-1.526728281870	1.085353720753

SCF Done: E(RwB97X) = -253.127585405

Zero-point correction=	0.178689
Thermal correction to Energy=	0.186923
Thermal correction to Enthalpy=	0.187868
Thermal correction to Gibbs Free Energy=	0.146534

Sum of electronic and zero-point Energies=	-252.948897
Sum of electronic and thermal Energies=	-252.940662
Sum of electronic and thermal Enthalpies=	-252.939718
Sum of electronic and thermal Free Energies=	-252.981051

1 C	Isotropic =	166.7806	Anisotropy =	41.5293
2 C	Isotropic =	162.1996	Anisotropy =	10.4013
3 C	Isotropic =	169.8194	Anisotropy =	34.9824
4 C	Isotropic =	147.3705	Anisotropy =	43.7499
5 C	Isotropic =	148.2281	Anisotropy =	36.3715
6 N	Isotropic =	235.8841	Anisotropy =	37.3018
7 H	Isotropic =	31.1048	Anisotropy =	7.6679
8 H	Isotropic =	30.7968	Anisotropy =	9.7719
9 H	Isotropic =	30.8387	Anisotropy =	10.0772
10 H	Isotropic =	30.4706	Anisotropy =	7.3547
11 H	Isotropic =	30.9199	Anisotropy =	9.9483
12 H	Isotropic =	30.6257	Anisotropy =	8.7309
13 H	Isotropic =	31.3695	Anisotropy =	7.9028
14 H	Isotropic =	30.3669	Anisotropy =	5.6426
15 H	Isotropic =	30.8902	Anisotropy =	3.8948
16 H	Isotropic =	28.8148	Anisotropy =	6.9729
17 H	Isotropic =	29.5343	Anisotropy =	5.8513
18 H	Isotropic =	31.2921	Anisotropy =	12.9024
19 H	Isotropic =	30.7599	Anisotropy =	16.0040

Conformer_2

C	-0.642551775736	0.244261597068	0.735261603666
C	0.162369830897	0.262666199156	-0.564357703719
C	-0.755399848646	0.003789582220	-1.757534255864
C	1.310222081847	-0.752280726165	-0.549305121754
C	2.410942084336	-0.456545108163	0.460661319420
N	3.472780009950	-1.465421740219	0.373987257499
H	-1.062384588135	-0.753704330156	0.913982860362
H	-0.034326366819	0.511514967651	1.604374863726
H	-1.477008249680	0.952325284184	0.688700472386
H	0.599427861993	1.264635735928	-0.681698912902
H	-1.204778019185	-0.994792451474	-1.691726549808
H	-1.571507591334	0.733126328342	-1.796976205715
H	-0.207994796860	0.061494540210	-2.704286943027
H	0.897303037112	-1.752497121869	-0.348967572351
H	1.765877868668	-0.797174720702	-1.546678415125
H	2.853948074987	0.520892026402	0.236530014115
H	1.985509973222	-0.391206225758	1.471879385251
H	3.105782046518	-2.369054108072	0.658048077926

H 4.213788366863 -1.245129728584 1.031405825916

SCF Done: E(RwB97X) = -253.127585409

Zero-point correction= 0.178689
Thermal correction to Energy= 0.186924
Thermal correction to Enthalpy= 0.187868
Thermal correction to Gibbs Free Energy= 0.146533
Sum of electronic and zero-point Energies= -252.948897
Sum of electronic and thermal Energies= -252.940662
Sum of electronic and thermal Enthalpies= -252.939717
Sum of electronic and thermal Free Energies= -252.981052

1 C	Isotropic =	169.8202	Anisotropy =	34.9794
2 C	Isotropic =	162.2003	Anisotropy =	10.3992
3 C	Isotropic =	166.7803	Anisotropy =	41.5303
4 C	Isotropic =	147.3697	Anisotropy =	43.7505
5 C	Isotropic =	148.2292	Anisotropy =	36.3693
6 N	Isotropic =	235.8841	Anisotropy =	37.2970
7 H	Isotropic =	31.3695	Anisotropy =	7.9027
8 H	Isotropic =	30.6257	Anisotropy =	8.7311
9 H	Isotropic =	30.9200	Anisotropy =	9.9480
10 H	Isotropic =	30.4706	Anisotropy =	7.3551
11 H	Isotropic =	31.1048	Anisotropy =	7.6679
12 H	Isotropic =	30.8387	Anisotropy =	10.0773
13 H	Isotropic =	30.7968	Anisotropy =	9.7718
14 H	Isotropic =	30.8903	Anisotropy =	3.8947
15 H	Isotropic =	30.3668	Anisotropy =	5.6429
16 H	Isotropic =	29.5343	Anisotropy =	5.8513
17 H	Isotropic =	28.8149	Anisotropy =	6.9736
18 H	Isotropic =	31.2920	Anisotropy =	12.9029
19 H	Isotropic =	30.7598	Anisotropy =	16.0038

Conformer_3

C	-0.612657746052	0.482164328180	0.729734812528
C	0.108279373848	0.388101462815	-0.615082960239
C	-0.567353602430	-0.639941102441	-1.523718200347
C	1.612766128115	0.127336173549	-0.450403859928
C	1.983259992597	-1.178794448784	0.242435218464
N	3.442898307929	-1.315283260576	0.311159677166
H	-1.654407948073	0.791543561507	0.593627351505
H	-0.623821860961	-0.483249418311	1.248129221602
H	-0.131211888875	1.210844857380	1.391338972850
H	0.019035183356	1.365978964395	-1.106273531790

H	-1.600820660755	-0.348672373613	-1.739683127936
H	-0.040848927668	-0.733686942049	-2.479989546735
H	-0.598083998174	-1.631524069890	-1.058914522590
H	2.082213259749	0.135757816209	-1.444161475119
H	2.061645096617	0.955470433424	0.113034457853
H	1.599109261190	-1.182200833134	1.267937075634
H	1.512734763647	-2.023927605525	-0.280258315540
H	3.689209075786	-2.185420864048	0.771488847198
H	3.821056190155	-1.377596679091	-0.629600094576

SCF Done: E(RwB97X) = -253.126610021

Zero-point correction=	0.178898
Thermal correction to Energy=	0.187130
Thermal correction to Enthalpy=	0.188074
Thermal correction to Gibbs Free Energy=	0.146494
Sum of electronic and zero-point Energies=	-252.947712
Sum of electronic and thermal Energies=	-252.939480
Sum of electronic and thermal Enthalpies=	-252.938536
Sum of electronic and thermal Free Energies=	-252.980116

1 C	Isotropic =	170.6745	Anisotropy =	34.1929
2 C	Isotropic =	163.2090	Anisotropy =	6.9889
3 C	Isotropic =	170.3156	Anisotropy =	35.1353
4 C	Isotropic =	149.8349	Anisotropy =	33.3745
5 C	Isotropic =	153.6335	Anisotropy =	36.6720
6 N	Isotropic =	236.4247	Anisotropy =	36.8273
7 H	Isotropic =	30.8599	Anisotropy =	9.9396
8 H	Isotropic =	31.0166	Anisotropy =	6.6275
9 H	Isotropic =	30.8868	Anisotropy =	9.8406
10 H	Isotropic =	30.0962	Anisotropy =	8.8704
11 H	Isotropic =	30.8629	Anisotropy =	9.9446
12 H	Isotropic =	30.9247	Anisotropy =	9.7103
13 H	Isotropic =	30.9631	Anisotropy =	6.6755
14 H	Isotropic =	30.4812	Anisotropy =	6.0586
15 H	Isotropic =	30.3050	Anisotropy =	6.4375
16 H	Isotropic =	29.3971	Anisotropy =	6.1784
17 H	Isotropic =	28.9950	Anisotropy =	7.2216
18 H	Isotropic =	30.7561	Anisotropy =	15.9113
19 H	Isotropic =	31.3730	Anisotropy =	13.2369

Conformer_4

C	-0.655161134554	0.104095420770	-1.752627112954
C	0.391465003013	0.146582903337	-0.641546896030

C	-0.238344465802	0.603553009557	0.673414293955
C	1.072121992961	-1.221889501163	-0.511491850072
C	2.144926277446	-1.319493999535	0.566912016135
N	3.237492314820	-0.369940630170	0.329183095679
H	-1.119419430514	1.084844351497	-1.900971777870
H	-0.213008045014	-0.204633629685	-2.706154131121
H	-1.452408984769	-0.608886159168	-1.508511645859
H	1.153139455718	0.884534638810	-0.929741383433
H	0.509963558684	0.751322509948	1.458749916208
H	-0.769700239325	1.552221958344	0.542418889942
H	-0.962317730898	-0.136839210211	1.036399200854
H	1.520873181181	-1.486920579382	-1.477708431837
H	0.301631438015	-1.976763719139	-0.301262556320
H	1.686403187201	-1.187058113578	1.558141161280
H	2.569109335313	-2.328512335825	0.550731734355
H	2.911293637933	0.579847245918	0.480474267835
H	3.977340648591	-0.521264160325	1.006891209252

SCF Done: E(RwB97X) = -253.128134063

Zero-point correction=	0.179195
Thermal correction to Energy=	0.187146
Thermal correction to Enthalpy=	0.188090
Thermal correction to Gibbs Free Energy=	0.147638
Sum of electronic and zero-point Energies=	-252.948939
Sum of electronic and thermal Energies=	-252.940988
Sum of electronic and thermal Enthalpies=	-252.940044
Sum of electronic and thermal Free Energies=	-252.980496

1 C	Isotropic =	167.1861	Anisotropy =	41.4038
2 C	Isotropic =	166.1074	Anisotropy =	7.8991
3 C	Isotropic =	172.1283	Anisotropy =	31.1077
4 C	Isotropic =	149.7141	Anisotropy =	23.3585
5 C	Isotropic =	151.6238	Anisotropy =	32.3927
6 N	Isotropic =	239.6059	Anisotropy =	32.4197
7 H	Isotropic =	30.7470	Anisotropy =	10.2381
8 H	Isotropic =	30.8537	Anisotropy =	9.9867
9 H	Isotropic =	31.1723	Anisotropy =	8.0864
10 H	Isotropic =	30.2639	Anisotropy =	6.6146
11 H	Isotropic =	30.5396	Anisotropy =	8.5548
12 H	Isotropic =	30.9334	Anisotropy =	9.9136
13 H	Isotropic =	31.4528	Anisotropy =	8.6708
14 H	Isotropic =	30.3409	Anisotropy =	7.6033
15 H	Isotropic =	30.8802	Anisotropy =	6.7253
16 H	Isotropic =	28.8744	Anisotropy =	6.6017
17 H	Isotropic =	29.3660	Anisotropy =	8.9178

18 H Isotropic = 30.9869 Anisotropy = 11.1385
 19 H Isotropic = 30.8509 Anisotropy = 16.5793

Conformer_5

C	-0.722475423963	-0.056396984481	-1.718695184073
C	0.154562381168	-0.418349932738	-0.522234570110
C	-0.416945684280	0.177569130423	0.763400569405
C	1.598364996540	0.033009964548	-0.776456540083
C	2.585575036222	-0.268724118254	0.345038422793
N	2.676349714772	-1.708355559515	0.611693688513
H	-1.748460433706	-0.415109539358	-1.584187373043
H	-0.333967187357	-0.493006752272	-2.645228080644
H	-0.764544523953	1.031373324767	-1.854815576622
H	0.147775137679	-1.512876608362	-0.423505760413
H	0.128051251790	-0.159446337349	1.651068915729
H	-1.466160605512	-0.108449630866	0.893078911723
H	-0.370667715334	1.273620285379	0.738694591346
H	1.599172768971	1.117424077333	-0.954599671768
H	1.959716647377	-0.440427969731	-1.698670471484
H	3.578551796865	0.078799379908	0.042485435917
H	2.311945305445	0.304694151185	1.243169404308
H	1.813386654065	-2.038625018664	1.033131146681
H	3.405269883211	-1.885621861953	1.294932141825

SCF Done: E(RwB97X) = -253.128134060

Zero-point correction=	0.179195
Thermal correction to Energy=	0.187146
Thermal correction to Enthalpy=	0.188091
Thermal correction to Gibbs Free Energy=	0.147639
Sum of electronic and zero-point Energies=	-252.948939
Sum of electronic and thermal Energies=	-252.940988
Sum of electronic and thermal Enthalpies=	-252.940043
Sum of electronic and thermal Free Energies=	-252.980495

1 C	Isotropic = 167.1855	Anisotropy = 41.4040
2 C	Isotropic = 166.1076	Anisotropy = 7.8994
3 C	Isotropic = 172.1274	Anisotropy = 31.1075
4 C	Isotropic = 149.7131	Anisotropy = 23.3587
5 C	Isotropic = 151.6234	Anisotropy = 32.3925
6 N	Isotropic = 239.6050	Anisotropy = 32.4217
7 H	Isotropic = 30.7470	Anisotropy = 10.2382
8 H	Isotropic = 30.8537	Anisotropy = 9.9866
9 H	Isotropic = 31.1722	Anisotropy = 8.0863

10	H	Isotropic =	30.2639	Anisotropy =	6.6148
11	H	Isotropic =	30.5395	Anisotropy =	8.5550
12	H	Isotropic =	30.9334	Anisotropy =	9.9133
13	H	Isotropic =	31.4527	Anisotropy =	8.6706
14	H	Isotropic =	30.8801	Anisotropy =	6.7253
15	H	Isotropic =	30.3408	Anisotropy =	7.6030
16	H	Isotropic =	29.3661	Anisotropy =	8.9179
17	H	Isotropic =	28.8744	Anisotropy =	6.6011
18	H	Isotropic =	30.9868	Anisotropy =	11.1383
19	H	Isotropic =	30.8508	Anisotropy =	16.5793

Conformer_6

C	-0.817435441350	0.219125803475	-1.626580303260
C	-0.028965990130	-0.377518252357	-0.462348192197
C	-0.019410067038	0.587264631297	0.722711090199
C	1.376287781430	-0.774156608315	-0.933681472846
C	2.293089294835	-1.398989538064	0.119767233923
N	3.076004243500	-0.400704095879	0.861409652528
H	-1.851405965695	0.435896467249	-1.338354134999
H	-0.361311500480	1.158659745523	-1.962289950190
H	-0.844113212260	-0.463284205609	-2.483022964679
H	-0.540709095534	-1.296332794371	-0.142409884017
H	0.396721790346	0.127208955464	1.624873916893
H	0.566890051711	1.485987630441	0.494365414096
H	-1.037492903199	0.908644022802	0.967836238739
H	1.259905047368	-1.488446201223	-1.757836944536
H	1.881037700130	0.106100613889	-1.356155296661
H	3.012788370997	-2.052771004589	-0.382158376843
H	1.694133959036	-2.042780952406	0.783577482784
H	3.728312534339	-0.872128264536	1.479575888855
H	2.474973401992	0.154524047211	1.460720602211

SCF Done: E(RwB97X) = -253.125501006

Zero-point correction=	0.179170
Thermal correction to Energy=	0.187146
Thermal correction to Enthalpy=	0.188090
Thermal correction to Gibbs Free Energy=	0.147606
Sum of electronic and zero-point Energies=	-252.946331
Sum of electronic and thermal Energies=	-252.938355
Sum of electronic and thermal Enthalpies=	-252.937411
Sum of electronic and thermal Free Energies=	-252.977895

1	C	Isotropic =	166.9061	Anisotropy =	41.4618

2 C	Isotropic =	158.8760	Anisotropy =	14.6387
3 C	Isotropic =	169.5727	Anisotropy =	29.8973
4 C	Isotropic =	148.4817	Anisotropy =	27.7076
5 C	Isotropic =	148.2115	Anisotropy =	25.1635
6 N	Isotropic =	232.4901	Anisotropy =	44.6429
7 H	Isotropic =	30.8539	Anisotropy =	10.1780
8 H	Isotropic =	31.1338	Anisotropy =	7.5912
9 H	Isotropic =	30.8520	Anisotropy =	9.7913
10 H	Isotropic =	30.3883	Anisotropy =	7.6042
11 H	Isotropic =	30.5651	Anisotropy =	7.9647
12 H	Isotropic =	31.2027	Anisotropy =	6.9286
13 H	Isotropic =	30.8551	Anisotropy =	9.8217
14 H	Isotropic =	30.0503	Anisotropy =	7.2694
15 H	Isotropic =	30.9508	Anisotropy =	4.9041
16 H	Isotropic =	29.2073	Anisotropy =	8.5967
17 H	Isotropic =	29.0084	Anisotropy =	6.4890
18 H	Isotropic =	30.8742	Anisotropy =	16.5855
19 H	Isotropic =	30.7131	Anisotropy =	11.1524

Conformer_7

C	-0.957296987113	-0.092187710267	-1.530499803651
C	0.247915809786	0.239194248290	-0.652576411159
C	-0.160401042470	0.273185299219	0.819624709153
C	1.390164176685	-0.743132229831	-0.943281801409
C	2.679529559287	-0.538249772635	-0.145621966587
N	2.685922361285	-1.269386004554	1.129113760514
H	-1.365382197618	-1.077266686202	-1.272508595468
H	-1.758275177890	0.643447067165	-1.402307151481
H	-0.686075877576	-0.111109610266	-2.591617242893
H	0.599956135542	1.244055896735	-0.926040841185
H	-0.427557815087	-0.728841281159	1.177625344799
H	-1.032089257201	0.920571697645	0.964241924191
H	0.637705436783	0.663686254650	1.459353482069
H	1.038023358114	-1.771033621094	-0.777377347670
H	1.628707724761	-0.667104947960	-2.011131421380
H	3.521055556199	-0.920702705558	-0.731188372664
H	2.854430110600	0.541427963071	-0.013079679008
H	3.593824369736	-1.171440434132	1.571830429897
H	2.015143756176	-0.869413423118	1.776240983932

SCF Done: E(RwB97X) = -253.125501019

Zero-point correction=	0.179173
Thermal correction to Energy=	0.187147

Thermal correction to Enthalpy=	0.188092
Thermal correction to Gibbs Free Energy=	0.147612
Sum of electronic and zero-point Energies=	-252.946328
Sum of electronic and thermal Energies=	-252.938354
Sum of electronic and thermal Enthalpies=	-252.937409
Sum of electronic and thermal Free Energies=	-252.977889

1	C	Isotropic =	166.9072	Anisotropy =	41.4601
2	C	Isotropic =	158.8783	Anisotropy =	14.6367
3	C	Isotropic =	169.5748	Anisotropy =	29.8932
4	C	Isotropic =	148.4830	Anisotropy =	27.7114
5	C	Isotropic =	148.2141	Anisotropy =	25.1650
6	N	Isotropic =	232.4907	Anisotropy =	44.6537
7	H	Isotropic =	31.1339	Anisotropy =	7.5912
8	H	Isotropic =	30.8539	Anisotropy =	10.1783
9	H	Isotropic =	30.8520	Anisotropy =	9.7914
10	H	Isotropic =	30.3883	Anisotropy =	7.6050
11	H	Isotropic =	31.2028	Anisotropy =	6.9284
12	H	Isotropic =	30.8551	Anisotropy =	9.8218
13	H	Isotropic =	30.5651	Anisotropy =	7.9649
14	H	Isotropic =	30.9511	Anisotropy =	4.9038
15	H	Isotropic =	30.0501	Anisotropy =	7.2699
16	H	Isotropic =	29.2074	Anisotropy =	8.5970
17	H	Isotropic =	29.0085	Anisotropy =	6.4885
18	H	Isotropic =	30.8744	Anisotropy =	16.5859
19	H	Isotropic =	30.7133	Anisotropy =	11.1515

Conformer_8

C	-0.242672312398	0.339851262466	-1.698149553255
C	-0.152960382301	-0.381976108835	-0.353950003677
C	-0.098502875481	0.630729195738	0.791355339816
C	0.981944428993	-1.420220730067	-0.327566710333
C	2.417335071965	-0.910810189334	-0.458113445289
N	2.958095605732	-0.377070754827	0.800064531455
H	-1.119032723682	0.996203214046	-1.728157947165
H	-0.326604402425	-0.368244435586	-2.529889494927
H	0.638971870473	0.965319893616	-1.879068204365
H	-1.080843408524	-0.956634095061	-0.231371471926
H	0.045248645956	0.142721855862	1.761210742028
H	-1.031337994999	1.202864577275	0.841035403575
H	0.709916556814	1.357608030568	0.650656861863
H	0.802413067121	-2.120310671695	-1.153382409118
H	0.913525102759	-2.006622121906	0.597860158678
H	3.051509413188	-1.757715944069	-0.738179031973

H	2.484518427812	-0.186637571858	-1.283548960077
H	2.549776979595	0.526411351574	1.011964607557
H	3.954198929403	-0.213666757907	0.695229587135

SCF Done: E(RwB97X) = -253.124592954

Zero-point correction=	0.179568
Thermal correction to Energy=	0.187472
Thermal correction to Enthalpy=	0.188416
Thermal correction to Gibbs Free Energy=	0.147701
Sum of electronic and zero-point Energies=	-252.945025
Sum of electronic and thermal Energies=	-252.937121
Sum of electronic and thermal Enthalpies=	-252.936177
Sum of electronic and thermal Free Energies=	-252.976892

1 C	Isotropic = 170.7614	Anisotropy = 35.8633
2 C	Isotropic = 161.8512	Anisotropy = 9.6445
3 C	Isotropic = 168.6281	Anisotropy = 31.5362
4 C	Isotropic = 150.4141	Anisotropy = 13.5455
5 C	Isotropic = 152.8947	Anisotropy = 38.0462
6 N	Isotropic = 231.0545	Anisotropy = 37.8809
7 H	Isotropic = 30.8498	Anisotropy = 9.7187
8 H	Isotropic = 31.0587	Anisotropy = 10.4746
9 H	Isotropic = 30.7830	Anisotropy = 6.5857
10 H	Isotropic = 30.0899	Anisotropy = 8.9942
11 H	Isotropic = 30.6984	Anisotropy = 8.6153
12 H	Isotropic = 30.7666	Anisotropy = 10.1404
13 H	Isotropic = 31.0386	Anisotropy = 5.8509
14 H	Isotropic = 30.2758	Anisotropy = 8.2430
15 H	Isotropic = 30.3265	Anisotropy = 7.6083
16 H	Isotropic = 29.4717	Anisotropy = 9.1640
17 H	Isotropic = 28.6873	Anisotropy = 6.0508
18 H	Isotropic = 30.8798	Anisotropy = 11.3827
19 H	Isotropic = 30.7882	Anisotropy = 16.3495

Conformer_9

C	-0.709338080082	-0.679364998803	-1.318219922537
C	0.182945945044	0.351469682520	-0.627449012981
C	-0.177313688848	0.458683848174	0.855447065957
C	1.676661306104	0.096747313277	-0.893133165407
C	2.286692898671	-1.196161104307	-0.351712650907
N	2.615317209460	-1.125533403593	1.079136523227
H	-0.572419185647	-1.680120867779	-0.892802767983
H	-1.766488196879	-0.417794350420	-1.201086046517

H	-0.496860010015	-0.740295932882	-2.391241821584
H	-0.035112639955	1.326834191161	-1.082793625029
H	-1.196009440721	0.843335677208	0.974989297112
H	0.498660559970	1.132935652562	1.391990056214
H	-0.149536943147	-0.519082520610	1.350312681251
H	1.819330273806	0.100175305258	-1.981233750385
H	2.262009956687	0.938023789531	-0.499962058810
H	1.632254838261	-2.047848489284	-0.589667917885
H	3.227888585585	-1.372661468019	-0.881676460243
H	3.164151520540	-1.938827401911	1.338456457559
H	1.774065091164	-1.167414922083	1.643447118947

SCF Done: E(RwB97X) = -253.124592946

Zero-point correction=	0.179568
Thermal correction to Energy=	0.187472
Thermal correction to Enthalpy=	0.188416
Thermal correction to Gibbs Free Energy=	0.147701
Sum of electronic and zero-point Energies=	-252.945025
Sum of electronic and thermal Energies=	-252.937121
Sum of electronic and thermal Enthalpies=	-252.936177
Sum of electronic and thermal Free Energies=	-252.976892

1 C	Isotropic =	170.7616	Anisotropy =	35.8629
2 C	Isotropic =	161.8512	Anisotropy =	9.6445
3 C	Isotropic =	168.6279	Anisotropy =	31.5367
4 C	Isotropic =	150.4141	Anisotropy =	13.5451
5 C	Isotropic =	152.8946	Anisotropy =	38.0464
6 N	Isotropic =	231.0547	Anisotropy =	37.8803
7 H	Isotropic =	30.7831	Anisotropy =	6.5857
8 H	Isotropic =	30.8498	Anisotropy =	9.7187
9 H	Isotropic =	31.0586	Anisotropy =	10.4746
10 H	Isotropic =	30.0899	Anisotropy =	8.9942
11 H	Isotropic =	30.7666	Anisotropy =	10.1404
12 H	Isotropic =	30.6984	Anisotropy =	8.6153
13 H	Isotropic =	31.0386	Anisotropy =	5.8509
14 H	Isotropic =	30.2758	Anisotropy =	8.2431
15 H	Isotropic =	30.3265	Anisotropy =	7.6083
16 H	Isotropic =	28.6873	Anisotropy =	6.0507
17 H	Isotropic =	29.4717	Anisotropy =	9.1640
18 H	Isotropic =	30.7882	Anisotropy =	16.3495
19 H	Isotropic =	30.8798	Anisotropy =	11.3827

3-methylbutan-1-amine_protonated

Conformer_1

C	-1.289828176183	-0.875091175481	-0.268780052597
C	0.012928020236	-0.270370636300	0.248490081395
C	-0.051218784196	1.255947783347	0.215216892432
C	1.193195885780	-0.818555904255	-0.559807735325
C	2.539982315928	-0.325136393603	-0.063081521635
N	3.642849995039	-1.023919223520	-0.787533690743
H	-2.143095154070	-0.540994793111	0.329881172340
H	-1.472035020033	-0.573374082306	-1.307205491657
H	-1.263852185905	-1.969291921857	-0.236981640492
H	0.147684772382	-0.585979654312	1.292032344130
H	-0.107628796344	1.619715260418	-0.818216486139
H	-0.939467820033	1.616185976597	0.744195539800
H	0.820343720324	1.718547878227	0.688695304499
H	1.180666378399	-1.914314117648	-0.507386017640
H	1.071616133343	-0.543270925282	-1.616039683541
H	2.680200286097	-0.535094626045	0.998856162629
H	2.684712964211	0.741432968593	-0.235856653684
H	4.560341121448	-0.718051605753	-0.458150170464
H	3.600435443887	-0.843709579204	-1.793204067315
H	3.588068899689	-2.036175228504	-0.655124285994

SCF Done: E(RwB97X) = -253.599521800

Zero-point correction=	0.194229
Thermal correction to Energy=	0.202523
Thermal correction to Enthalpy=	0.203468
Thermal correction to Gibbs Free Energy=	0.162049
Sum of electronic and zero-point Energies=	-253.405293
Sum of electronic and thermal Energies=	-253.396998
Sum of electronic and thermal Enthalpies=	-253.396054
Sum of electronic and thermal Free Energies=	-253.437472

1 C	Isotropic =	167.4282	Anisotropy =	40.9303
2 C	Isotropic =	162.5481	Anisotropy =	9.5693
3 C	Isotropic =	170.7384	Anisotropy =	32.6498
4 C	Isotropic =	152.9436	Anisotropy =	39.2862
5 C	Isotropic =	146.8693	Anisotropy =	40.4204
6 N	Isotropic =	219.6193	Anisotropy =	25.6059
7 H	Isotropic =	30.7572	Anisotropy =	10.1808
8 H	Isotropic =	31.0579	Anisotropy =	7.8151
9 H	Isotropic =	30.7686	Anisotropy =	9.8366
10 H	Isotropic =	30.2714	Anisotropy =	7.6446
11 H	Isotropic =	31.2854	Anisotropy =	8.0465
12 H	Isotropic =	30.8571	Anisotropy =	9.9886

13	H	Isotropic =	30.7141	Anisotropy =	8.7752
14	H	Isotropic =	30.1723	Anisotropy =	6.3920
15	H	Isotropic =	30.4751	Anisotropy =	4.9312
16	H	Isotropic =	28.7845	Anisotropy =	6.3954
17	H	Isotropic =	28.5134	Anisotropy =	5.8498
18	H	Isotropic =	27.0111	Anisotropy =	17.3373
19	H	Isotropic =	27.3111	Anisotropy =	14.3554
20	H	Isotropic =	27.3231	Anisotropy =	14.3908

Conformer_2

C	-1.276105660025	-0.924882510003	-0.101590823360
C	-0.039881521740	-0.078664399015	-0.395008404123
C	-0.030124281614	1.179409477843	0.472185250426
C	1.222514227538	-0.924960433767	-0.202590289355
C	2.500337174989	-0.181218156725	-0.546173621949
N	3.666999113614	-1.111567248851	-0.493297540502
H	-2.193667082674	-0.357408603422	-0.286346277847
H	-1.304055164437	-1.823353668960	-0.726834336416
H	-1.287012506767	-1.244942318874	0.947219295232
H	-0.077228257763	0.230419262887	-1.448488956846
H	0.085238590300	0.919676740091	1.531771764001
H	0.780427233670	1.863469602588	0.202241131968
H	-0.970629214513	1.729331419668	0.364423523447
H	1.272976977311	-1.274149721908	0.837462447051
H	1.153373172031	-1.815238332518	-0.839940876040
H	2.470343176395	0.226651403977	-1.558200295898
H	2.716784721364	0.625042891045	0.154869865834
H	3.547868740248	-1.890251018287	-1.144953048536
H	3.783832459560	-1.509401796220	0.441435012679
H	4.537508102512	-0.635162589551	-0.736383819766

SCF Done: E(RwB97X) = -253.599521801

Zero-point correction=	0.194229
Thermal correction to Energy=	0.202523
Thermal correction to Enthalpy=	0.203468
Thermal correction to Gibbs Free Energy=	0.162049
Sum of electronic and zero-point Energies=	-253.405293
Sum of electronic and thermal Energies=	-253.396998
Sum of electronic and thermal Enthalpies=	-253.396054
Sum of electronic and thermal Free Energies=	-253.437473

1	C	Isotropic =	167.4282	Anisotropy =	40.9303
2	C	Isotropic =	162.5481	Anisotropy =	9.5693

3 C	Isotropic =	170.7384	Anisotropy =	32.6498
4 C	Isotropic =	152.9436	Anisotropy =	39.2862
5 C	Isotropic =	146.8693	Anisotropy =	40.4204
6 N	Isotropic =	219.6193	Anisotropy =	25.6059
7 H	Isotropic =	30.7572	Anisotropy =	10.1808
8 H	Isotropic =	30.7686	Anisotropy =	9.8366
9 H	Isotropic =	31.0579	Anisotropy =	7.8151
10 H	Isotropic =	30.2714	Anisotropy =	7.6446
11 H	Isotropic =	31.2854	Anisotropy =	8.0465
12 H	Isotropic =	30.7141	Anisotropy =	8.7752
13 H	Isotropic =	30.8571	Anisotropy =	9.9886
14 H	Isotropic =	30.4751	Anisotropy =	4.9312
15 H	Isotropic =	30.1723	Anisotropy =	6.3920
16 H	Isotropic =	28.7845	Anisotropy =	6.3954
17 H	Isotropic =	28.5134	Anisotropy =	5.8498
18 H	Isotropic =	27.3231	Anisotropy =	14.3908
19 H	Isotropic =	27.3111	Anisotropy =	14.3554
20 H	Isotropic =	27.0111	Anisotropy =	17.3373

Conformer_3

C	-0.794881959378	-1.135333471155	0.338935872585
C	-0.142510420642	-0.011539071380	-0.466231393485
C	-0.095963049664	1.286295535003	0.340152655795
C	1.239250558268	-0.410065716952	-1.005436573707
C	2.260738348219	-0.705476609415	0.080122327252
N	3.565567399954	-1.081692412540	-0.539887411749
H	-1.827746552160	-0.877796489355	0.594100506768
H	-0.813658919442	-2.073267463823	-0.226437218464
H	-0.263829827153	-1.319219002461	1.279743909076
H	-0.765905458230	0.168827139537	-1.350400362833
H	0.451160777559	1.158066432215	1.280983489526
H	0.388061311329	2.090519602237	-0.224350213211
H	-1.107281599578	1.618478086101	0.595364663465
H	1.134901177425	-1.298472461799	-1.640663015307
H	1.624530041664	0.397937595153	-1.639754396593
H	2.457404984229	0.161448054252	0.711448129629
H	1.965063632314	-1.544542340492	0.710481889524
H	3.469935604908	-1.911671069549	-1.129526587026
H	3.927044475148	-0.327762509255	-1.128621915741
H	4.272219475229	-1.286033826325	0.169175644496

SCF Done: E(RwB97X) = -253.598559062

Zero-point correction= 0.194823

Thermal correction to Energy=	0.202916
Thermal correction to Enthalpy=	0.203860
Thermal correction to Gibbs Free Energy=	0.163019
Sum of electronic and zero-point Energies=	-253.403736
Sum of electronic and thermal Energies=	-253.395643
Sum of electronic and thermal Enthalpies=	-253.394699
Sum of electronic and thermal Free Energies=	-253.435540

1 C	Isotropic =	170.9608	Anisotropy =	34.6125
2 C	Isotropic =	163.8260	Anisotropy =	6.3186
3 C	Isotropic =	170.9608	Anisotropy =	34.6137
4 C	Isotropic =	154.5252	Anisotropy =	31.8321
5 C	Isotropic =	150.7540	Anisotropy =	42.5249
6 N	Isotropic =	220.3089	Anisotropy =	24.5574
7 H	Isotropic =	30.7789	Anisotropy =	10.0580
8 H	Isotropic =	30.8587	Anisotropy =	9.9605
9 H	Isotropic =	30.9710	Anisotropy =	6.7091
10 H	Isotropic =	29.9532	Anisotropy =	9.0442
11 H	Isotropic =	30.9709	Anisotropy =	6.7092
12 H	Isotropic =	30.8587	Anisotropy =	9.9605
13 H	Isotropic =	30.7789	Anisotropy =	10.0580
14 H	Isotropic =	30.0912	Anisotropy =	7.0985
15 H	Isotropic =	30.0913	Anisotropy =	7.0984
16 H	Isotropic =	28.6268	Anisotropy =	6.1432
17 H	Isotropic =	28.6268	Anisotropy =	6.1432
18 H	Isotropic =	27.3659	Anisotropy =	14.6809
19 H	Isotropic =	27.3659	Anisotropy =	14.6808
20 H	Isotropic =	27.0043	Anisotropy =	17.2326

Conformer_4

C	-1.200834960544	-0.919351552805	-0.060224315170
C	0.209327023863	-0.379705222058	0.166484727042
C	0.176414825509	1.122756333729	0.439087288622
C	1.087252321824	-0.731073890516	-1.041544437405
C	2.535820629951	-0.280763997778	-0.974464382808
N	3.246284697365	-0.898080946734	0.187673012157
H	-1.191229588918	-1.999900653180	-0.237446019625
H	-1.841127726974	-0.726832947886	0.806367636330
H	-1.663059548402	-0.440813758490	-0.931841778267
H	0.614580475850	-0.882827725664	1.056186882602
H	-0.497715547417	1.349162547357	1.271188387778
H	1.162498642629	1.520304157631	0.700214374549
H	-0.183644194631	1.668240441865	-0.441641241670
H	1.064646834983	-1.815904995908	-1.203752746028

H	0.657895487507	-0.272296281339	-1.940485540794
H	2.637122936913	0.799220156379	-0.862849654614
H	3.079207794591	-0.590834938464	-1.867062137334
H	4.244268627620	-0.680016459359	0.168340644816
H	2.881029061344	-0.561602183277	1.081203790733
H	3.153262206936	-1.916778083502	0.179065509085

SCF Done: E(RwB97X) = -253.599608439

Zero-point correction=	0.194526
Thermal correction to Energy=	0.202685
Thermal correction to Enthalpy=	0.203629
Thermal correction to Gibbs Free Energy=	0.162632
Sum of electronic and zero-point Energies=	-253.405082
Sum of electronic and thermal Energies=	-253.396923
Sum of electronic and thermal Enthalpies=	-253.395979
Sum of electronic and thermal Free Energies=	-253.436977

1 C	Isotropic = 167.6035	Anisotropy = 40.5970
2 C	Isotropic = 166.2513	Anisotropy = 8.0911
3 C	Isotropic = 172.2991	Anisotropy = 31.1303
4 C	Isotropic = 154.3361	Anisotropy = 24.4262
5 C	Isotropic = 149.2643	Anisotropy = 38.5776
6 N	Isotropic = 223.5988	Anisotropy = 16.6843
7 H	Isotropic = 30.8159	Anisotropy = 10.0733
8 H	Isotropic = 30.6868	Anisotropy = 10.2657
9 H	Isotropic = 31.0922	Anisotropy = 8.1560
10 H	Isotropic = 30.2168	Anisotropy = 6.9069
11 H	Isotropic = 30.8263	Anisotropy = 10.0581
12 H	Isotropic = 30.5283	Anisotropy = 8.6251
13 H	Isotropic = 31.3544	Anisotropy = 8.7599
14 H	Isotropic = 30.0403	Anisotropy = 7.6840
15 H	Isotropic = 30.5402	Anisotropy = 7.2486
16 H	Isotropic = 28.4711	Anisotropy = 6.3965
17 H	Isotropic = 28.6092	Anisotropy = 9.5222
18 H	Isotropic = 27.0780	Anisotropy = 17.7513
19 H	Isotropic = 27.0496	Anisotropy = 12.6762
20 H	Isotropic = 27.5371	Anisotropy = 14.7714

Conformer_5

C	-1.219637591735	-0.853818241928	-0.305335122158
C	0.163404028039	-0.219586263721	-0.432290068914
C	0.149252010722	1.217459336412	0.084900081464
C	1.190335105228	-1.090631315658	0.302720437861

C	2.630686255305	-0.611663248832	0.262637872490
N	3.144456597049	-0.542985833017	-1.140118762733
H	-1.534515281136	-0.889159337956	0.744412518171
H	-1.968974021050	-0.280996594246	-0.860663962612
H	-1.226052548975	-1.878506736025	-0.691416084912
H	0.418422883133	-0.198758556603	-1.501618897086
H	-0.627352341185	1.801254418178	-0.419255386552
H	-0.060730201166	1.239544066874	1.161142562205
H	1.102534930648	1.729403771145	-0.081705701916
H	0.911101356481	-1.155420995448	1.361375324830
H	1.149762105990	-2.112806665615	-0.093754590327
H	3.283399541626	-1.303028419277	0.795670691316
H	2.756114577570	0.384185477476	0.688829091962
H	3.014885356526	-1.434228798968	-1.625266598030
H	4.142601430646	-0.325483749451	-1.157366699014
H	2.668805806285	0.178527686660	-1.686196706046

SCF Done: E(RwB97X) = -253.599608438

Zero-point correction=	0.194526
Thermal correction to Energy=	0.202685
Thermal correction to Enthalpy=	0.203629
Thermal correction to Gibbs Free Energy=	0.162632
Sum of electronic and zero-point Energies=	-253.405082
Sum of electronic and thermal Energies=	-253.396923
Sum of electronic and thermal Enthalpies=	-253.395979
Sum of electronic and thermal Free Energies=	-253.436977

1 C	Isotropic =	167.6035	Anisotropy =	40.5970
2 C	Isotropic =	166.2513	Anisotropy =	8.0910
3 C	Isotropic =	172.2991	Anisotropy =	31.1303
4 C	Isotropic =	154.3361	Anisotropy =	24.4263
5 C	Isotropic =	149.2643	Anisotropy =	38.5776
6 N	Isotropic =	223.5988	Anisotropy =	16.6844
7 H	Isotropic =	31.0922	Anisotropy =	8.1560
8 H	Isotropic =	30.6868	Anisotropy =	10.2657
9 H	Isotropic =	30.8159	Anisotropy =	10.0733
10 H	Isotropic =	30.2168	Anisotropy =	6.9069
11 H	Isotropic =	30.8263	Anisotropy =	10.0581
12 H	Isotropic =	31.3544	Anisotropy =	8.7599
13 H	Isotropic =	30.5283	Anisotropy =	8.6251
14 H	Isotropic =	30.5402	Anisotropy =	7.2486
15 H	Isotropic =	30.0402	Anisotropy =	7.6840
16 H	Isotropic =	28.6092	Anisotropy =	9.5222
17 H	Isotropic =	28.4711	Anisotropy =	6.3965
18 H	Isotropic =	27.5371	Anisotropy =	14.7714

19 H Isotropic = 27.0780 Anisotropy = 17.7513
 20 H Isotropic = 27.0496 Anisotropy = 12.6762

Conformer_6

C	0.374407689057	1.174985472963	0.036564346498
C	0.073081746769	-0.305835245253	0.259758963975
C	-1.328148474703	-0.649638038793	-0.239660892804
C	1.095564647073	-1.234631984377	-0.405759090653
C	2.546046397167	-1.048792281712	0.022239651776
N	3.265327735597	-0.051185260078	-0.831367143912
H	0.462339301786	1.403113874268	-1.033241079631
H	-0.429674112429	1.797585760028	0.441531936050
H	1.296170985932	1.491506054199	0.537732593559
H	0.108571198819	-0.499345110725	1.340377017002
H	-2.087892635730	-0.053447931061	0.275404724976
H	-1.417386326862	-0.448616004599	-1.314138342314
H	-1.562008634453	-1.706813252215	-0.075823744074
H	0.823622512670	-2.269240250883	-0.174103399453
H	1.027809456206	-1.140758468298	-1.498673200431
H	3.108626574495	-1.976476128354	-0.078245033932
H	2.631333094043	-0.700744028684	1.053441964270
H	3.233026679143	-0.323092950201	-1.816572133280
H	4.248907776597	0.017008971077	-0.563291616850
H	2.865074388821	0.886916802700	-0.760775520772

SCF Done: E(RwB97X) = -253.597478146

Zero-point correction=	0.194661
Thermal correction to Energy=	0.202760
Thermal correction to Enthalpy=	0.203704
Thermal correction to Gibbs Free Energy=	0.162852
Sum of electronic and zero-point Energies=	-253.402817
Sum of electronic and thermal Energies=	-253.394718
Sum of electronic and thermal Enthalpies=	-253.393774
Sum of electronic and thermal Free Energies=	-253.434626

1 C	Isotropic =	170.4505	Anisotropy =	31.0469
2 C	Isotropic =	160.1194	Anisotropy =	14.2284
3 C	Isotropic =	167.5549	Anisotropy =	40.5085
4 C	Isotropic =	154.2507	Anisotropy =	25.9995
5 C	Isotropic =	146.8337	Anisotropy =	31.1166
6 N	Isotropic =	217.2788	Anisotropy =	26.2714
7 H	Isotropic =	31.1753	Anisotropy =	7.2228
8 H	Isotropic =	30.7071	Anisotropy =	10.0119

9	H	Isotropic =	30.6089	Anisotropy =	8.0719
10	H	Isotropic =	30.2161	Anisotropy =	7.7811
11	H	Isotropic =	30.7950	Anisotropy =	10.2719
12	H	Isotropic =	31.0973	Anisotropy =	7.7393
13	H	Isotropic =	30.8129	Anisotropy =	9.9493
14	H	Isotropic =	29.8809	Anisotropy =	8.1849
15	H	Isotropic =	30.6764	Anisotropy =	5.2570
16	H	Isotropic =	28.4968	Anisotropy =	9.2486
17	H	Isotropic =	28.6468	Anisotropy =	6.5525
18	H	Isotropic =	27.4115	Anisotropy =	14.3328
19	H	Isotropic =	27.1201	Anisotropy =	17.7454
20	H	Isotropic =	26.9471	Anisotropy =	12.6782

Conformer_7

C	0.388790563557	1.148432487965	0.188871004125
C	0.006064712652	-0.180608454110	-0.459702091918
C	-1.292739330486	-0.715432871603	0.138749098612
C	1.101804815830	-1.246396371212	-0.339144189919
C	2.456973312106	-0.882787732653	-0.933178384033
N	3.348391842790	-0.206277788142	0.061267549553
H	-0.455011351628	1.845355355182	0.167142531765
H	0.674238623998	1.007551779084	1.239071832174
H	1.215126302305	1.643197850873	-0.333981053860
H	-0.159224954861	0.000452054873	-1.530368897559
H	-1.181112114994	-0.889108461703	1.215898883303
H	-2.113557294603	-0.005076331245	-0.001240366364
H	-1.585310945160	-1.663269842744	-0.325099223855
H	1.234376342554	-1.526463792679	0.715295983776
H	0.760386141467	-2.151441055277	-0.851349344415
H	2.366571076816	-0.207267602952	-1.785991597667
H	2.999306066483	-1.772549735507	-1.251592334980
H	4.269738269650	-0.021974742750	-0.340101929429
H	3.484528675842	-0.792776119463	0.887770185594
H	2.971459245682	0.688541374061	0.381282345098

SCF Done: E(RwB97X) = -253.597478270

Zero-point correction=	0.194665
Thermal correction to Energy=	0.202761
Thermal correction to Enthalpy=	0.203706
Thermal correction to Gibbs Free Energy=	0.162861
Sum of electronic and zero-point Energies=	-253.402813
Sum of electronic and thermal Energies=	-253.394717
Sum of electronic and thermal Enthalpies=	-253.393773

Sum of electronic and thermal Free Energies= -253.434617

1	C	Isotropic =	170.4456	Anisotropy =	31.0431
2	C	Isotropic =	160.1196	Anisotropy =	14.2290
3	C	Isotropic =	167.5536	Anisotropy =	40.5110
4	C	Isotropic =	154.2499	Anisotropy =	25.9929
5	C	Isotropic =	146.8328	Anisotropy =	31.1136
6	N	Isotropic =	217.2755	Anisotropy =	26.2678
7	H	Isotropic =	30.7068	Anisotropy =	10.0118
8	H	Isotropic =	31.1751	Anisotropy =	7.2225
9	H	Isotropic =	30.6095	Anisotropy =	8.0717
10	H	Isotropic =	30.2160	Anisotropy =	7.7812
11	H	Isotropic =	31.0973	Anisotropy =	7.7390
12	H	Isotropic =	30.7950	Anisotropy =	10.2717
13	H	Isotropic =	30.8128	Anisotropy =	9.9495
14	H	Isotropic =	30.6762	Anisotropy =	5.2580
15	H	Isotropic =	29.8810	Anisotropy =	8.1849
16	H	Isotropic =	28.6466	Anisotropy =	6.5549
17	H	Isotropic =	28.4970	Anisotropy =	9.2499
18	H	Isotropic =	27.1200	Anisotropy =	17.7458
19	H	Isotropic =	27.4118	Anisotropy =	14.3292
20	H	Isotropic =	26.9464	Anisotropy =	12.6803

Conformer_8

C	-0.845931073906	-1.064739094927	0.403966755219
C	-0.075742831002	-0.053353115210	-0.443525564628
C	0.350898418762	1.145302102062	0.403730468317
C	1.087515562195	-0.713512594533	-1.200941182580
C	2.246365021644	-1.237324552749	-0.360800870031
N	3.248233275758	-0.168232201873	-0.051709483991
H	-0.224726878299	-1.470044538451	1.211041107868
H	-1.718790682010	-0.595319382681	0.869066005023
H	-1.199834320341	-1.905430557004	-0.201821150114
H	-0.758181600472	0.317692166940	-1.218186388065
H	-0.525822794433	1.680377840614	0.781196784721
H	0.927402645920	0.833562255275	1.284502767611
H	0.951791953035	1.859019546766	-0.171392020090
H	0.691631569332	-1.568761046798	-1.758121370796
H	1.486047082601	-0.020483743086	-1.952720832953
H	2.798027356509	-2.007767585926	-0.898846250395
H	1.923093616781	-1.649562288808	0.596348713861
H	3.620093176435	0.243846511855	-0.910283456269
H	4.037584035447	-0.547894088760	0.474581459901
H	2.848746466046	0.590324367293	0.503914507389

SCF Done: E(RwB97X) = -253.596753360

Zero-point correction=	0.195025
Thermal correction to Energy=	0.202985
Thermal correction to Enthalpy=	0.203930
Thermal correction to Gibbs Free Energy=	0.163238
Sum of electronic and zero-point Energies=	-253.401728
Sum of electronic and thermal Energies=	-253.393768
Sum of electronic and thermal Enthalpies=	-253.392824
Sum of electronic and thermal Free Energies=	-253.433515

1	C	Isotropic =	170.9803	Anisotropy =	36.3355
2	C	Isotropic =	163.0851	Anisotropy =	8.7781
3	C	Isotropic =	170.1969	Anisotropy =	31.2163
4	C	Isotropic =	156.1603	Anisotropy =	15.6901
5	C	Isotropic =	151.0451	Anisotropy =	42.3594
6	N	Isotropic =	216.7501	Anisotropy =	25.3196
7	H	Isotropic =	30.7562	Anisotropy =	6.5981
8	H	Isotropic =	30.7993	Anisotropy =	9.9699
9	H	Isotropic =	30.9856	Anisotropy =	10.6661
10	H	Isotropic =	29.9843	Anisotropy =	9.2262
11	H	Isotropic =	30.6287	Anisotropy =	10.2928
12	H	Isotropic =	31.0293	Anisotropy =	6.0274
13	H	Isotropic =	30.7690	Anisotropy =	9.0598
14	H	Isotropic =	30.0499	Anisotropy =	9.0394
15	H	Isotropic =	30.0561	Anisotropy =	7.9237
16	H	Isotropic =	28.6825	Anisotropy =	9.6626
17	H	Isotropic =	28.3829	Anisotropy =	5.6737
18	H	Isotropic =	27.3951	Anisotropy =	14.6050
19	H	Isotropic =	27.1221	Anisotropy =	17.5656
20	H	Isotropic =	26.9725	Anisotropy =	12.9548

Conformer_9

C	-0.171741085745	1.233218461329	0.464760107202
C	-0.067842835390	-0.008926987434	-0.418786128253
C	-0.330296211871	-1.274246069989	0.397722623137
C	1.257379932566	-0.045579873452	-1.196830452896
C	2.529719319535	-0.238764994702	-0.379980716735
N	2.815994166559	-1.684087911793	-0.113163135367
H	0.581770824478	1.225520561907	1.260790339039
H	-0.035012974460	2.149983850385	-0.118154983038
H	-1.153652436204	1.284976033005	0.946127386859
H	-0.854329617837	0.059596329335	-1.180501205667

H	-1.351627651040	-1.272980321960	0.790507051900
H	0.336587983449	-1.340566070802	1.267286904717
H	-0.208725650173	-2.181688707484	-0.204729173595
H	1.216351000965	-0.823461723441	-1.969783583303
H	1.367641570064	0.904333225873	-1.729863915749
H	3.398144173925	0.136132807250	-0.921037006058
H	2.488351614753	0.256849228004	0.591236562730
H	2.900008179986	-2.207753882743	-0.987152464749
H	2.082959811670	-2.129668833300	0.441479332525
H	3.693919884771	-1.794685119989	0.397872457300

SCF Done: E(RwB97X) = -253.596753373

Zero-point correction=	0.195033
Thermal correction to Energy=	0.202992
Thermal correction to Enthalpy=	0.203937
Thermal correction to Gibbs Free Energy=	0.163254
Sum of electronic and zero-point Energies=	-253.401720
Sum of electronic and thermal Energies=	-253.393761
Sum of electronic and thermal Enthalpies=	-253.392817
Sum of electronic and thermal Free Energies=	-253.433499

1 C	Isotropic = 170.9932	Anisotropy = 36.3214
2 C	Isotropic = 163.0790	Anisotropy = 8.7899
3 C	Isotropic = 170.1920	Anisotropy = 31.2207
4 C	Isotropic = 156.1704	Anisotropy = 15.6882
5 C	Isotropic = 151.0481	Anisotropy = 42.3662
6 N	Isotropic = 216.7851	Anisotropy = 25.2874
7 H	Isotropic = 30.7560	Anisotropy = 6.5988
8 H	Isotropic = 30.9858	Anisotropy = 10.6678
9 H	Isotropic = 30.8000	Anisotropy = 9.9688
10 H	Isotropic = 29.9844	Anisotropy = 9.2246
11 H	Isotropic = 30.6297	Anisotropy = 10.2924
12 H	Isotropic = 31.0299	Anisotropy = 6.0279
13 H	Isotropic = 30.7690	Anisotropy = 9.0613
14 H	Isotropic = 30.0555	Anisotropy = 7.9265
15 H	Isotropic = 30.0511	Anisotropy = 9.0406
16 H	Isotropic = 28.6822	Anisotropy = 9.6629
17 H	Isotropic = 28.3823	Anisotropy = 5.6748
18 H	Isotropic = 27.3958	Anisotropy = 14.6069
19 H	Isotropic = 26.9754	Anisotropy = 12.9614
20 H	Isotropic = 27.1227	Anisotropy = 17.5658

1,2,3,4-tetrahydroisoquinoline_neutral
Conformer_1

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C   -2.994619556366   -2.407127705826   -0.801362832398
C   -1.739363298629   -1.794321660733   -0.820237556630
C   -0.587412397076   -2.580841108528   -0.718180385114
C   -0.720961749939   -3.966990858547   -0.594256748455
C   -1.971225503185   -4.570112871927   -0.572930999499
C   -3.117608154235   -3.784330496529   -0.678235286209
C   -1.639051761245   -0.287001077276   -0.977022775913
N   -0.331907669546    0.277832480623   -0.661038528397
C    0.742878098883   -0.510957021053   -1.260823374135
C    0.784106960289   -1.940920868860   -0.726770015315
H   -3.886783570962   -1.789291237790   -0.881661388631
H    0.175528115994   -4.578389092066   -0.516435825501
H   -2.053933496133   -5.648764444140   -0.476612229143
H   -4.101071257767   -4.244907464034   -0.661622698938
H   -1.885747128945   -0.026790623871   -2.014826635491
H   -2.391401492994    0.196897166688   -0.347561513826
H   -0.208815591387    0.283406621600    0.347437887565
H    1.698431597221   -0.011157857993   -1.079931905706
H    0.581202231918   -0.520284004440   -2.345749306500
H    1.179568120206   -1.929861456740    0.297146538234
H    1.473687503900   -2.550386418557   -1.320424419997

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SCF Done: E(RwB97X) = -404.338966539

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Zero-point correction=          0.184334
Thermal correction to Energy=      0.192045
Thermal correction to Enthalpy=     0.192990
Thermal correction to Gibbs Free Energy=  0.151953
Sum of electronic and zero-point Energies= -404.154633
Sum of electronic and thermal Energies=    -404.146921
Sum of electronic and thermal Enthalpies=   -404.145977
Sum of electronic and thermal Free Energies= -404.187014

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1 C  Isotropic =  58.8890  Anisotropy = 174.5273
2 C  Isotropic =  45.6816  Anisotropy = 201.5494
3 C  Isotropic =  47.7017  Anisotropy = 200.1007
4 C  Isotropic =  55.4305  Anisotropy = 171.5135
5 C  Isotropic =  59.2328  Anisotropy = 185.1635
6 C  Isotropic =  59.3226  Anisotropy = 184.8633
7 C  Isotropic = 141.9650  Anisotropy =  40.1827
8 N  Isotropic = 225.7474  Anisotropy =  54.1815
9 C  Isotropic = 146.3673  Anisotropy =  34.3158
10 C Isotropic = 160.9809  Anisotropy =  14.7962
11 H Isotropic =  24.2961  Anisotropy =   7.1465
12 H Isotropic =  24.2069  Anisotropy =   7.2365

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13	H	Isotropic =	24.2557	Anisotropy =	4.4169
14	H	Isotropic =	24.2580	Anisotropy =	4.3950
15	H	Isotropic =	27.8113	Anisotropy =	7.4098
16	H	Isotropic =	27.8377	Anisotropy =	8.3949
17	H	Isotropic =	30.6560	Anisotropy =	12.8942
18	H	Isotropic =	28.6009	Anisotropy =	9.4400
19	H	Isotropic =	28.9661	Anisotropy =	8.0036
20	H	Isotropic =	29.0394	Anisotropy =	7.8565
21	H	Isotropic =	29.2149	Anisotropy =	8.7349

Conformer_2

C	-2.993592679336	-2.397927852432	-0.678885461203
C	-1.738958310378	-1.790754051659	-0.772631328691
C	-0.587870635299	-2.585116568957	-0.774821856636
C	-0.721722937333	-3.974035722739	-0.687697090521
C	-1.971417985777	-4.572007541416	-0.597905830372
C	-3.116883667735	-3.777894794743	-0.592486735441
C	-1.637947924548	-0.277069749301	-0.844853792303
N	-0.336895321121	0.232496784444	-1.263318541903
C	0.748614654728	-0.458985871538	-0.570054502567
C	0.782807650443	-1.952817141731	-0.884710482500
H	-3.885078196121	-1.773926834667	-0.677246807214
H	0.174120694632	-4.591305609432	-0.687921144937
H	-2.054362736032	-5.652823398450	-0.530345538690
H	-4.099913928749	-4.234552156948	-0.523767386084
H	-2.401176458406	0.108114469022	-1.527147303074
H	-1.867818546214	0.135820656647	0.146249614906
H	-0.230457761124	0.086939939379	-2.263164353702
H	0.604864021862	-0.305651288243	0.506567348903
H	1.700433345442	0.006930665800	-0.839435978473
H	1.482841163730	-2.467435237131	-0.217989829381
H	1.161315557334	-2.095598695907	-1.905133000117

SCF Done: E(RwB97X) = -404.338966539

Zero-point correction=	0.184334
Thermal correction to Energy=	0.192045
Thermal correction to Enthalpy=	0.192990
Thermal correction to Gibbs Free Energy=	0.151953
Sum of electronic and zero-point Energies=	-404.154633
Sum of electronic and thermal Energies=	-404.146921
Sum of electronic and thermal Enthalpies=	-404.145977
Sum of electronic and thermal Free Energies=	-404.187014

1 C	Isotropic =	58.8890	Anisotropy =	174.5273
2 C	Isotropic =	45.6816	Anisotropy =	201.5494
3 C	Isotropic =	47.7017	Anisotropy =	200.1007
4 C	Isotropic =	55.4305	Anisotropy =	171.5135
5 C	Isotropic =	59.2328	Anisotropy =	185.1635
6 C	Isotropic =	59.3226	Anisotropy =	184.8633
7 C	Isotropic =	141.9650	Anisotropy =	40.1827
8 N	Isotropic =	225.7474	Anisotropy =	54.1815
9 C	Isotropic =	146.3673	Anisotropy =	34.3158
10 C	Isotropic =	160.9809	Anisotropy =	14.7962
11 H	Isotropic =	24.2961	Anisotropy =	7.1465
12 H	Isotropic =	24.2069	Anisotropy =	7.2365
13 H	Isotropic =	24.2557	Anisotropy =	4.4169
14 H	Isotropic =	24.2580	Anisotropy =	4.3950
15 H	Isotropic =	27.8377	Anisotropy =	8.3949
16 H	Isotropic =	27.8113	Anisotropy =	7.4098
17 H	Isotropic =	30.6560	Anisotropy =	12.8942
18 H	Isotropic =	28.9661	Anisotropy =	8.0036
19 H	Isotropic =	28.6009	Anisotropy =	9.4400
20 H	Isotropic =	29.2149	Anisotropy =	8.7349
21 H	Isotropic =	29.0394	Anisotropy =	7.8565

Conformer_3

C	-2.997788025412	-2.384322224691	-0.787632355261
C	-1.751290776141	-1.812350592403	-1.020340103868
C	-0.592871488167	-2.595234497065	-0.925401265170
C	-0.699803787928	-3.941083174521	-0.587049475879
C	-1.950757421503	-4.513562431929	-0.364010797260
C	-3.100457650826	-3.737002737319	-0.468325054276
C	-1.536992410736	-0.345305258429	-1.302757725212
N	-0.471627138025	0.198340866903	-0.452921506555
C	0.813829931645	-0.505848570068	-0.601431881888
C	0.709056875639	-1.910478498040	-1.239035199532
H	-3.892667189250	-1.769382290977	-0.851379885039
H	0.199026172676	-4.547591152557	-0.503998555357
H	-2.027199068364	-5.565817859986	-0.105693244500
H	-4.075584527129	-4.181184912659	-0.290716435339
H	-1.255012450555	-0.193099692809	-2.352229230887
H	-2.456002936150	0.220505798719	-1.129047708170
H	-0.778218340191	0.103668540311	0.508534550570
H	1.493046433734	0.097953953372	-1.213495886166
H	1.264563579207	-0.583508935145	0.391870522342
H	1.560628638442	-2.525172537249	-0.935151981071
H	0.774821579031	-1.801323793455	-2.328586781483

SCF Done: E(RwB97X) = -404.334084282

Zero-point correction= 0.184431
Thermal correction to Energy= 0.192241
Thermal correction to Enthalpy= 0.193186
Thermal correction to Gibbs Free Energy= 0.151782
Sum of electronic and zero-point Energies= -404.149654
Sum of electronic and thermal Energies= -404.141843
Sum of electronic and thermal Enthalpies= -404.140899
Sum of electronic and thermal Free Energies= -404.182302

1	C	Isotropic =	60.3611	Anisotropy =	168.0604
2	C	Isotropic =	40.2271	Anisotropy =	208.1111
3	C	Isotropic =	45.6429	Anisotropy =	203.7841
4	C	Isotropic =	57.2200	Anisotropy =	168.3495
5	C	Isotropic =	58.1424	Anisotropy =	186.4963
6	C	Isotropic =	59.4532	Anisotropy =	184.9190
7	C	Isotropic =	143.4152	Anisotropy =	27.3091
8	N	Isotropic =	228.3689	Anisotropy =	56.1454
9	C	Isotropic =	149.5193	Anisotropy =	39.6897
10	C	Isotropic =	163.0858	Anisotropy =	16.8658
11	H	Isotropic =	24.1816	Anisotropy =	6.4582
12	H	Isotropic =	24.0972	Anisotropy =	6.8451
13	H	Isotropic =	24.1425	Anisotropy =	4.5688
14	H	Isotropic =	24.2001	Anisotropy =	4.4031
15	H	Isotropic =	28.2529	Anisotropy =	8.1352
16	H	Isotropic =	28.1365	Anisotropy =	8.9430
17	H	Isotropic =	31.0145	Anisotropy =	14.3439
18	H	Isotropic =	28.6092	Anisotropy =	9.6829
19	H	Isotropic =	29.0349	Anisotropy =	9.8205
20	H	Isotropic =	29.0622	Anisotropy =	8.8692
21	H	Isotropic =	29.2169	Anisotropy =	9.2962

Conformer_4

C	-2.962941346597	-2.361643765760	-0.689758395055
C	-1.712307882561	-1.741058009435	-0.737210743416
C	-0.553322384279	-2.522540638681	-0.692078746544
C	-0.675214849723	-3.911931758669	-0.595533153159
C	-1.920836478419	-4.522966470781	-0.545683655501
C	-3.074319810516	-3.742000732312	-0.593958453678
C	-1.624871024261	-0.230188036286	-0.862911225940
N	-0.310883134422	0.335744572563	-0.578959271618
C	0.746985600204	-0.432838176319	-1.232275313962

C	0.813730821444	-1.874066255288	-0.731985573940
H	-3.860577457906	-1.747562430068	-0.725678886996
H	0.226623600580	-4.519499893552	-0.562231290870
H	-1.994484496605	-5.604017943832	-0.471438760944
H	-4.054173202199	-4.208842725104	-0.554513324113
H	-1.908452172042	0.052260353262	-1.885380358198
H	-2.357870993572	0.234547484203	-0.197229927706
H	-0.153893175951	0.320253626048	0.424675524478
H	0.548503384690	-0.419238591839	-2.311027414865
H	1.705397265218	0.068772779502	-1.072843390655
H	1.243276738597	-1.883323402966	0.278130685521
H	1.486330998319	-2.465959984686	-1.361808322838

SCF Done: E(RwB97X) = -404.338966314

Zero-point correction=	0.184334
Thermal correction to Energy=	0.192046
Thermal correction to Enthalpy=	0.192990
Thermal correction to Gibbs Free Energy=	0.151951
Sum of electronic and zero-point Energies=	-404.154633
Sum of electronic and thermal Energies=	-404.146921
Sum of electronic and thermal Enthalpies=	-404.145976
Sum of electronic and thermal Free Energies=	-404.187015

1 C	Isotropic =	58.9099	Anisotropy =	174.5124
2 C	Isotropic =	45.6937	Anisotropy =	201.5684
3 C	Isotropic =	47.6966	Anisotropy =	200.0998
4 C	Isotropic =	55.4280	Anisotropy =	171.5171
5 C	Isotropic =	59.2344	Anisotropy =	185.1559
6 C	Isotropic =	59.3183	Anisotropy =	184.8763
7 C	Isotropic =	141.9794	Anisotropy =	40.1788
8 N	Isotropic =	225.7710	Anisotropy =	54.1253
9 C	Isotropic =	146.3802	Anisotropy =	34.2756
10 C	Isotropic =	160.9683	Anisotropy =	14.7923
11 H	Isotropic =	24.2962	Anisotropy =	7.1439
12 H	Isotropic =	24.2072	Anisotropy =	7.2357
13 H	Isotropic =	24.2557	Anisotropy =	4.4170
14 H	Isotropic =	24.2576	Anisotropy =	4.3948
15 H	Isotropic =	27.8113	Anisotropy =	7.4145
16 H	Isotropic =	27.8383	Anisotropy =	8.3948
17 H	Isotropic =	30.6550	Anisotropy =	12.8995
18 H	Isotropic =	28.9659	Anisotropy =	8.0022
19 H	Isotropic =	28.6009	Anisotropy =	9.4406
20 H	Isotropic =	29.0402	Anisotropy =	7.8566
21 H	Isotropic =	29.2149	Anisotropy =	8.7352

1,2,3,4-tetrahydroisoquinoline_protonated

Conformer_1

C	-0.065131578875	-0.153621342570	0.228531819337
C	1.124091512379	-0.884556964716	0.287805439338
C	2.339587676306	-0.197818828862	0.269201167114
C	2.352431392837	1.196094746020	0.189240011153
C	1.166006100371	1.910723922132	0.125401923174
C	-0.050429415417	1.230779139815	0.146215143971
C	1.080973016408	-2.391612855759	0.404806908676
C	2.401851958167	-3.040735381808	0.042701560387
N	3.502554345847	-2.330276346618	0.758977377101
C	3.662280885524	-0.923900999721	0.297765932906
H	-1.012425371107	-0.686757433080	0.244270103532
H	3.304856157051	1.720107164347	0.178270583490
H	1.187271284194	2.994253336786	0.062903787107
H	-0.984891714187	1.781388920391	0.097604062454
H	0.808745561496	-2.668522216948	1.429952075698
H	0.304499003070	-2.797407198644	-0.247959034635
H	2.437572193154	-4.088356003231	0.338652276111
H	2.622765097301	-2.958058988550	-1.023089745172
H	3.317591482626	-2.347077997803	1.766174465461
H	4.384810990332	-2.827620753914	0.622944946631
H	4.104630076169	-0.972318269023	-0.699838258605
H	4.369959346352	-0.436105648243	0.968667454769

SCF Done: E(RwB97X) = -404.809221624

Zero-point correction= 0.199906
Thermal correction to Energy= 0.207702
Thermal correction to Enthalpy= 0.208646
Thermal correction to Gibbs Free Energy= 0.167336
Sum of electronic and zero-point Energies= -404.609316
Sum of electronic and thermal Energies= -404.601520
Sum of electronic and thermal Enthalpies= -404.600575
Sum of electronic and thermal Free Energies= -404.641886

1 C Isotropic = 55.6219 Anisotropy = 175.2158
2 C Isotropic = 51.5745 Anisotropy = 196.4637
3 C Isotropic = 55.6266 Anisotropy = 180.5613
4 C Isotropic = 57.7212 Anisotropy = 178.8317
5 C Isotropic = 57.9010 Anisotropy = 189.3117
6 C Isotropic = 56.4708 Anisotropy = 190.1434
7 C Isotropic = 163.7641 Anisotropy = 15.3118

8	C	Isotropic =	145.0818	Anisotropy =	40.3912
9	N	Isotropic =	211.3164	Anisotropy =	11.4613
10	C	Isotropic =	142.5161	Anisotropy =	39.7732
11	H	Isotropic =	24.0479	Anisotropy =	7.3710
12	H	Isotropic =	24.1402	Anisotropy =	7.2445
13	H	Isotropic =	24.0904	Anisotropy =	4.4335
14	H	Isotropic =	24.0494	Anisotropy =	4.5138
15	H	Isotropic =	28.5463	Anisotropy =	8.4551
16	H	Isotropic =	28.7362	Anisotropy =	9.4215
17	H	Isotropic =	28.0466	Anisotropy =	9.8779
18	H	Isotropic =	28.3354	Anisotropy =	8.2716
19	H	Isotropic =	26.8151	Anisotropy =	13.6536
20	H	Isotropic =	26.4370	Anisotropy =	16.9914
21	H	Isotropic =	27.2882	Anisotropy =	7.6877
22	H	Isotropic =	27.3126	Anisotropy =	9.0926

Conformer_2

C	-0.060718237020	-0.157113015494	0.131302118876
C	1.126616582374	-0.886548108598	0.232260109775
C	2.337673042738	-0.196293347901	0.311486521510
C	2.347755079106	1.199802830989	0.292310645888
C	1.162741111127	1.913309060461	0.197306711343
C	-0.049029163682	1.229669017199	0.115314965093
C	1.089365910310	-2.398245212391	0.220003328282
C	2.369983522123	-3.015490850370	0.745577209111
N	3.533237160215	-2.354545646204	0.082749149241
C	3.655169802578	-0.918255802824	0.454668561888
H	-1.004433232559	-0.693083806412	0.068178147398
H	3.296981591621	1.726348744135	0.351814470042
H	1.181782356664	2.998596187217	0.183760463719
H	-0.982268657689	1.779306382526	0.039705630643
H	0.255741223896	-2.758800517158	0.827254572895
H	0.910043935015	-2.748698786860	-0.803097405442
H	2.493896564511	-2.856028903150	1.818315086702
H	2.428917654637	-4.081484826214	0.529810347917
H	4.397963572023	-2.838008922196	0.333237785583
H	3.440042653456	-2.443991674371	-0.933249740283
H	4.422186712750	-0.477431715041	-0.182686240198
H	4.005350815805	-0.893711087344	1.489077560018

SCF Done: E(RwB97X) = -404.809221624

Zero-point correction=	0.199906
Thermal correction to Energy=	0.207702

Thermal correction to Enthalpy=	0.208646
Thermal correction to Gibbs Free Energy=	0.167336
Sum of electronic and zero-point Energies=	-404.609316
Sum of electronic and thermal Energies=	-404.601520
Sum of electronic and thermal Enthalpies=	-404.600575
Sum of electronic and thermal Free Energies=	-404.641886

1 C	Isotropic =	55.6219	Anisotropy =	175.2158
2 C	Isotropic =	51.5745	Anisotropy =	196.4637
3 C	Isotropic =	55.6266	Anisotropy =	180.5613
4 C	Isotropic =	57.7212	Anisotropy =	178.8317
5 C	Isotropic =	57.9010	Anisotropy =	189.3117
6 C	Isotropic =	56.4708	Anisotropy =	190.1434
7 C	Isotropic =	163.7641	Anisotropy =	15.3118
8 C	Isotropic =	145.0818	Anisotropy =	40.3911
9 N	Isotropic =	211.3164	Anisotropy =	11.4613
10 C	Isotropic =	142.5161	Anisotropy =	39.7732
11 H	Isotropic =	24.0479	Anisotropy =	7.3710
12 H	Isotropic =	24.1402	Anisotropy =	7.2445
13 H	Isotropic =	24.0904	Anisotropy =	4.4335
14 H	Isotropic =	24.0494	Anisotropy =	4.5138
15 H	Isotropic =	28.7362	Anisotropy =	9.4215
16 H	Isotropic =	28.5463	Anisotropy =	8.4551
17 H	Isotropic =	28.3354	Anisotropy =	8.2716
18 H	Isotropic =	28.0466	Anisotropy =	9.8779
19 H	Isotropic =	26.4370	Anisotropy =	16.9914
20 H	Isotropic =	26.8151	Anisotropy =	13.6536
21 H	Isotropic =	27.3126	Anisotropy =	9.0926
22 H	Isotropic =	27.2882	Anisotropy =	7.6877

Conformer_3

C	-0.060428574144	-0.184834738161	0.173837311714
C	1.111967999298	-0.872744608883	0.468124105045
C	2.326711061326	-0.181587210125	0.493724598582
C	2.369915894148	1.182543502843	0.229448682204
C	1.191042317198	1.868154188686	-0.048419034470
C	-0.020891236089	1.184427492758	-0.075958261725
C	1.180329369578	-2.349547284753	0.743470843536
C	2.275995630318	-2.993253903044	-0.097979260350
N	3.586915094288	-2.244227918484	0.024210412633
C	3.547713422067	-0.981124832735	0.839100517578
H	-1.005571679704	-0.720343571777	0.143092526846
H	3.321508445162	1.707010881141	0.244597744419
H	1.218581215481	2.934432361895	-0.250371292695

H	-0.939288184931	1.719059736703	-0.299176679139
H	0.235027710450	-2.842706785201	0.508446041735
H	1.384695644015	-2.521810285873	1.806570372898
H	2.006716649742	-2.973727920225	-1.153438129624
H	2.463728351937	-4.022561926275	0.202926920268
H	3.920714381137	-2.013890645734	-0.912796302044
H	4.294534382750	-2.860264777488	0.427683986601
H	3.530855856151	-1.292672176888	1.885996864853
H	4.474026249820	-0.441629578381	0.645008031134

SCF Done: E(RwB97X) = -404.805384796

Zero-point correction=	0.199865
Thermal correction to Energy=	0.207736
Thermal correction to Enthalpy=	0.208680
Thermal correction to Gibbs Free Energy=	0.167000
Sum of electronic and zero-point Energies=	-404.605520
Sum of electronic and thermal Energies=	-404.597649
Sum of electronic and thermal Enthalpies=	-404.596705
Sum of electronic and thermal Free Energies=	-404.638385

1 C	Isotropic = 57.6771	Anisotropy = 170.9512
2 C	Isotropic = 45.6891	Anisotropy = 205.2676
3 C	Isotropic = 53.3690	Anisotropy = 186.4008
4 C	Isotropic = 57.0589	Anisotropy = 175.3393
5 C	Isotropic = 57.6040	Anisotropy = 189.2808
6 C	Isotropic = 54.8371	Anisotropy = 192.3268
7 C	Isotropic = 163.3929	Anisotropy = 17.3456
8 C	Isotropic = 146.4704	Anisotropy = 43.0107
9 N	Isotropic = 216.0791	Anisotropy = 22.5595
10 C	Isotropic = 144.2410	Anisotropy = 29.0741
11 H	Isotropic = 23.9323	Anisotropy = 6.7541
12 H	Isotropic = 23.9439	Anisotropy = 6.7120
13 H	Isotropic = 24.0202	Anisotropy = 4.5103
14 H	Isotropic = 23.9212	Anisotropy = 4.6459
15 H	Isotropic = 28.7959	Anisotropy = 9.8901
16 H	Isotropic = 28.7388	Anisotropy = 9.0059
17 H	Isotropic = 28.7584	Anisotropy = 9.7422
18 H	Isotropic = 27.9998	Anisotropy = 9.8765
19 H	Isotropic = 26.9120	Anisotropy = 15.9868
20 H	Isotropic = 26.4709	Anisotropy = 16.9416
21 H	Isotropic = 27.5741	Anisotropy = 8.3990
22 H	Isotropic = 27.4153	Anisotropy = 9.3071

Conformer_4

C	-0.060170651028	-0.185026088971	0.168420289367
C	1.133914679409	-0.886700273764	0.041546626863
C	2.347156154427	-0.194593564167	0.095754737766
C	2.367565086095	1.183988706865	0.273523881297
C	1.168708520150	1.882284389919	0.383568860218
C	-0.041912440568	1.197730119907	0.331087240567
C	1.225250615893	-2.378060502156	-0.128517337576
C	2.226692600180	-2.962008913038	0.860946796839
N	3.545649007274	-2.218003624833	0.825526381760
C	3.594479652369	-1.010796361650	-0.069632624003
H	-1.005257658544	-0.720594647723	0.136834276202
H	3.317449700138	1.709543069472	0.321966223039
H	1.178944069887	2.959556278082	0.517289322705
H	-0.976587359014	1.742677630411	0.423473735852
H	0.259181643155	-2.858053105418	0.039864790295
H	1.537076461709	-2.618478924981	-1.151551832750
H	1.850662070682	-2.874951940872	1.879723790353
H	2.441042630041	-4.007992510741	0.648293663349
H	3.782253439150	-1.926012949569	1.774866073314
H	4.288907040756	-2.856622128285	0.537825566123
H	3.684153219055	-1.389936258476	-1.090199812447
H	4.497741518781	-0.456648400010	0.182989350869

SCF Done: E(RwB97X) = -404.805384776

Zero-point correction=	0.199865
Thermal correction to Energy=	0.207736
Thermal correction to Enthalpy=	0.208681
Thermal correction to Gibbs Free Energy=	0.166998
Sum of electronic and zero-point Energies=	-404.605520
Sum of electronic and thermal Energies=	-404.597648
Sum of electronic and thermal Enthalpies=	-404.596704
Sum of electronic and thermal Free Energies=	-404.638387

1 C	Isotropic =	57.6803	Anisotropy =	170.9492
2 C	Isotropic =	45.6961	Anisotropy =	205.2639
3 C	Isotropic =	53.3723	Anisotropy =	186.4019
4 C	Isotropic =	57.0621	Anisotropy =	175.3343
5 C	Isotropic =	57.6072	Anisotropy =	189.2778
6 C	Isotropic =	54.8405	Anisotropy =	192.3231
7 C	Isotropic =	163.3938	Anisotropy =	17.3491
8 C	Isotropic =	146.4741	Anisotropy =	43.0128
9 N	Isotropic =	216.0775	Anisotropy =	22.5546
10 C	Isotropic =	144.2396	Anisotropy =	29.0743
11 H	Isotropic =	23.9324	Anisotropy =	6.7541

12 H	Isotropic =	23.9441	Anisotropy =	6.7121
13 H	Isotropic =	24.0203	Anisotropy =	4.5101
14 H	Isotropic =	23.9213	Anisotropy =	4.6456
15 H	Isotropic =	28.7959	Anisotropy =	9.8900
16 H	Isotropic =	28.7387	Anisotropy =	9.0060
17 H	Isotropic =	28.7581	Anisotropy =	9.7428
18 H	Isotropic =	28.0000	Anisotropy =	9.8762
19 H	Isotropic =	26.9116	Anisotropy =	15.9867
20 H	Isotropic =	26.4703	Anisotropy =	16.9410
21 H	Isotropic =	27.5741	Anisotropy =	8.3991
22 H	Isotropic =	27.4153	Anisotropy =	9.3071

Conformer_5

C	-0.068622985499	-0.203530959511	0.200347440566
C	1.129071755724	-0.893048559283	0.043059857257
C	2.336920717050	-0.190424056733	0.083969302195
C	2.348615823993	1.186271512293	0.275957889208
C	1.145850805621	1.872598207288	0.414687040343
C	-0.059313511179	1.177318250644	0.378964092063
C	1.227810864877	-2.378177331403	-0.173234707854
C	2.256701407502	-3.006925200024	0.762869485435
N	3.528509664674	-2.187346450827	0.834925688836
C	3.587690585599	-1.001133155709	-0.082801385240
H	-1.009612731632	-0.746695089799	0.178430662800
H	3.294789452552	1.719282575217	0.314717770278
H	1.148970405334	2.948498083257	0.559296711329
H	-0.996787800571	1.712753190355	0.495470634744
H	0.267861605779	-2.870030266368	-0.004436093647
H	1.516246561967	-2.573774675162	-1.212307077146
H	1.871154065634	-3.063749172923	1.779989387132
H	2.534702838640	-4.005886944602	0.430909909182
H	3.651251595127	-1.854859121010	1.792803981546
H	4.331665471833	-2.788359133592	0.644107877093
H	3.680603817191	-1.397619810158	-1.096570701658
H	4.488919589784	-0.441861891950	0.166042235536

SCF Done: E(RwB97X) = -404.805371350

Zero-point correction=	0.199860
Thermal correction to Energy=	0.207764
Thermal correction to Enthalpy=	0.208708
Thermal correction to Gibbs Free Energy=	0.166833
Sum of electronic and zero-point Energies=	-404.605512
Sum of electronic and thermal Energies=	-404.597608

Sum of electronic and thermal Enthalpies= -404.596663
 Sum of electronic and thermal Free Energies= -404.638538

1 C	Isotropic =	57.4671	Anisotropy =	171.2713
2 C	Isotropic =	46.4743	Anisotropy =	203.7121
3 C	Isotropic =	52.7778	Anisotropy =	187.4666
4 C	Isotropic =	57.1033	Anisotropy =	175.2632
5 C	Isotropic =	57.6598	Anisotropy =	189.2620
6 C	Isotropic =	54.7068	Anisotropy =	192.4633
7 C	Isotropic =	163.7631	Anisotropy =	17.7031
8 C	Isotropic =	146.9558	Anisotropy =	45.8433
9 N	Isotropic =	214.8938	Anisotropy =	20.9110
10 C	Isotropic =	144.0657	Anisotropy =	28.2102
11 H	Isotropic =	23.9306	Anisotropy =	6.7839
12 H	Isotropic =	23.9352	Anisotropy =	6.6742
13 H	Isotropic =	24.0250	Anisotropy =	4.4960
14 H	Isotropic =	23.9176	Anisotropy =	4.6654
15 H	Isotropic =	28.7814	Anisotropy =	9.8161
16 H	Isotropic =	28.7361	Anisotropy =	9.1242
17 H	Isotropic =	28.6299	Anisotropy =	9.9821
18 H	Isotropic =	28.0132	Anisotropy =	9.8265
19 H	Isotropic =	27.0669	Anisotropy =	15.4656
20 H	Isotropic =	26.4627	Anisotropy =	17.1156
21 H	Isotropic =	27.5602	Anisotropy =	8.3475
22 H	Isotropic =	27.4390	Anisotropy =	9.3635

1-benzylguanidine_neutral
 Conformer_1

C	0.311285473720	0.564257073161	-0.619673781347
N	-0.618827212261	-0.063066832119	-1.426430315352
N	0.072763428868	1.747378260065	-0.161221714400
N	1.429134365275	-0.190178323525	-0.380061264294
C	2.447114180329	0.214023705793	0.574833092572
C	3.662977722747	-0.676651297924	0.471691317599
C	4.314174452638	-0.850591392260	-0.752053296576
C	5.443723070123	-1.654646525519	-0.842466520244
C	5.940512117331	-2.293624088829	0.291977899538
C	5.299085708430	-2.124231773638	1.513192852011
C	4.163565407514	-1.321551642176	1.600115889509
H	-1.316423656667	0.562520882572	-1.803584158133
H	-0.253820691595	-0.715120356096	-2.106962004018
H	0.795290215398	2.038917869507	0.489590491364
H	1.344614348789	-1.183204026076	-0.548144988096
H	2.740712641082	1.246096613175	0.352880692848
H	2.067526074762	0.195946318882	1.604348018290

H	3.931587241397	-0.351473616875	-1.638675345631
H	5.941143351850	-1.781209953296	-1.799608489699
H	6.823664632695	-2.921480980004	0.221298422045
H	5.678334667744	-2.619951145760	2.401883072682
H	3.660762459831	-1.195958769060	2.555570129330

SCF Done: E(RwB97X) = -475.762987523

Zero-point correction=	0.187254
Thermal correction to Energy=	0.197487
Thermal correction to Enthalpy=	0.198431
Thermal correction to Gibbs Free Energy=	0.150466
Sum of electronic and zero-point Energies=	-475.575734
Sum of electronic and thermal Energies=	-475.565501
Sum of electronic and thermal Enthalpies=	-475.564557
Sum of electronic and thermal Free Energies=	-475.612521

1 C	Isotropic = 22.6980	Anisotropy = 133.1247
2 N	Isotropic = 191.6864	Anisotropy = 113.9521
3 N	Isotropic = 120.0274	Anisotropy = 183.9015
4 N	Isotropic = 168.6526	Anisotropy = 123.6093
5 C	Isotropic = 144.2637	Anisotropy = 20.7022
6 C	Isotropic = 44.1723	Anisotropy = 198.4050
7 C	Isotropic = 55.9746	Anisotropy = 187.2992
8 C	Isotropic = 55.4655	Anisotropy = 191.9906
9 C	Isotropic = 56.9474	Anisotropy = 191.5148
10 C	Isotropic = 55.7775	Anisotropy = 190.1874
11 C	Isotropic = 55.2215	Anisotropy = 170.9279
12 H	Isotropic = 27.9778	Anisotropy = 12.0677
13 H	Isotropic = 28.2258	Anisotropy = 10.1344
14 H	Isotropic = 27.0956	Anisotropy = 5.6749
15 H	Isotropic = 27.8934	Anisotropy = 5.6262
16 H	Isotropic = 27.4451	Anisotropy = 4.1493
17 H	Isotropic = 27.9823	Anisotropy = 8.6645
18 H	Isotropic = 23.7620	Anisotropy = 9.0573
19 H	Isotropic = 23.8805	Anisotropy = 5.1698
20 H	Isotropic = 24.0403	Anisotropy = 4.4333
21 H	Isotropic = 23.9944	Anisotropy = 4.8012
22 H	Isotropic = 23.9760	Anisotropy = 7.2930

Conformer_2

C	0.609298681118	0.236128645682	-0.529620105360
N	-0.226865455953	0.704992335378	-1.523357887203
N	0.325411419469	-0.865325006696	0.085168744868

N	1.723548161498	0.999630429144	-0.328494678071
C	2.664347762087	0.761182551283	0.743257753030
C	3.637743952282	-0.378391021387	0.496850033299
C	4.075860462366	-1.156852653915	1.567356024159
C	5.007034614112	-2.172857345841	1.372470805658
C	5.506178309832	-2.425890790439	0.098827295584
C	5.068697718880	-1.656484775913	-0.975901546999
C	4.141299217800	-0.638734901996	-0.777050312072
H	-0.243696824101	1.704282139246	-1.671673041978
H	-1.141465912048	0.277592365872	-1.528051621079
H	1.068102132997	-1.125583960869	0.727103749545
H	1.809992457672	1.856436092943	-0.852133429467
H	2.131122547164	0.579650538625	1.683830476964
H	3.229136668236	1.687287599708	0.878900040573
H	3.681575176296	-0.967746899162	2.563149581257
H	5.336880883223	-2.771715771539	2.216348346854
H	6.228702838122	-3.221312631697	-0.057393600265
H	5.451223295686	-1.849858330232	-1.973928439634
H	3.800071893261	-0.043628608194	-1.619958189664

SCF Done: E(RwB97X) = -475.763841547

Zero-point correction=	0.187662
Thermal correction to Energy=	0.197664
Thermal correction to Enthalpy=	0.198608
Thermal correction to Gibbs Free Energy=	0.151787
Sum of electronic and zero-point Energies=	-475.576180
Sum of electronic and thermal Energies=	-475.566177
Sum of electronic and thermal Enthalpies=	-475.565233
Sum of electronic and thermal Free Energies=	-475.612055

1 C	Isotropic =	23.3779	Anisotropy =	132.0745
2 N	Isotropic =	192.7898	Anisotropy =	113.4343
3 N	Isotropic =	121.5632	Anisotropy =	183.0739
4 N	Isotropic =	177.1764	Anisotropy =	92.0131
5 C	Isotropic =	144.9716	Anisotropy =	31.3505
6 C	Isotropic =	41.6153	Anisotropy =	196.5908
7 C	Isotropic =	57.4621	Anisotropy =	174.4485
8 C	Isotropic =	55.7427	Anisotropy =	190.7874
9 C	Isotropic =	57.9741	Anisotropy =	188.5862
10 C	Isotropic =	55.3599	Anisotropy =	192.0066
11 C	Isotropic =	59.3891	Anisotropy =	189.4363
12 H	Isotropic =	28.2048	Anisotropy =	10.8893
13 H	Isotropic =	28.0987	Anisotropy =	12.2950
14 H	Isotropic =	27.7704	Anisotropy =	3.8801
15 H	Isotropic =	26.8187	Anisotropy =	9.6799

16	H	Isotropic =	27.6258	Anisotropy =	7.1755
17	H	Isotropic =	27.4980	Anisotropy =	7.1341
18	H	Isotropic =	23.9827	Anisotropy =	7.3877
19	H	Isotropic =	23.9808	Anisotropy =	4.7706
20	H	Isotropic =	24.0674	Anisotropy =	4.3829
21	H	Isotropic =	23.9344	Anisotropy =	5.3231
22	H	Isotropic =	23.8250	Anisotropy =	9.2410

Conformer_3

C	0.799468432130	0.639959841005	-0.550299400112
N	-0.107426350044	0.942518702844	-1.546549063549
N	1.461216054108	1.588037243112	0.028515708447
N	0.939554057549	-0.696504607507	-0.307188516373
C	1.739210747279	-1.225299015579	0.775192034127
C	3.235737049781	-1.238823970722	0.516219742228
C	4.121919951315	-1.034865291505	1.573106175319
C	5.497352018671	-1.094350381690	1.368275058469
C	6.002289626659	-1.352678853737	0.097987088796
C	5.123393219140	-1.551417899775	-0.963356927761
C	3.749097351370	-1.495825082675	-0.754438133068
H	-0.881711588421	0.304787184520	-1.667599619119
H	-0.373110785125	1.915904028199	-1.580171817846
H	2.145567158734	1.210642256816	0.677073014066
H	0.337767738487	-1.332975823532	-0.805721304990
H	1.399425733829	-2.250075939023	0.946769075841
H	1.540869722545	-0.671250449384	1.700203368144
H	3.731170606747	-0.824143489165	2.565953202315
H	6.174587519347	-0.931286753281	2.201537470130
H	7.074886467732	-1.394391532598	-0.066159491455
H	5.509772270117	-1.750452103460	-1.958785608354
H	3.067362998051	-1.647708062862	-1.587062055254

SCF Done: E(RwB97X) = -475.763841324

Zero-point correction=	0.187658
Thermal correction to Energy=	0.197663
Thermal correction to Enthalpy=	0.198607
Thermal correction to Gibbs Free Energy=	0.151780
Sum of electronic and zero-point Energies=	-475.576183
Sum of electronic and thermal Energies=	-475.566179
Sum of electronic and thermal Enthalpies=	-475.565235
Sum of electronic and thermal Free Energies=	-475.612062

1	C	Isotropic =	23.3762	Anisotropy =	132.0787

2 N	Isotropic =	192.7882	Anisotropy =	113.4328
3 N	Isotropic =	121.5648	Anisotropy =	183.0620
4 N	Isotropic =	177.1743	Anisotropy =	92.0056
5 C	Isotropic =	144.9711	Anisotropy =	31.3478
6 C	Isotropic =	41.6170	Anisotropy =	196.5933
7 C	Isotropic =	57.4595	Anisotropy =	174.4421
8 C	Isotropic =	55.7439	Anisotropy =	190.7850
9 C	Isotropic =	57.9742	Anisotropy =	188.5879
10 C	Isotropic =	55.3601	Anisotropy =	192.0060
11 C	Isotropic =	59.3875	Anisotropy =	189.4335
12 H	Isotropic =	28.2052	Anisotropy =	10.8889
13 H	Isotropic =	28.0986	Anisotropy =	12.2942
14 H	Isotropic =	27.7708	Anisotropy =	3.8804
15 H	Isotropic =	26.8185	Anisotropy =	9.6791
16 H	Isotropic =	27.4979	Anisotropy =	7.1334
17 H	Isotropic =	27.6259	Anisotropy =	7.1754
18 H	Isotropic =	23.9827	Anisotropy =	7.3878
19 H	Isotropic =	23.9808	Anisotropy =	4.7707
20 H	Isotropic =	24.0673	Anisotropy =	4.3829
21 H	Isotropic =	23.9344	Anisotropy =	5.3228
22 H	Isotropic =	23.8251	Anisotropy =	9.2392

Conformer_4

C	0.847314680920	0.695255395008	-0.514985509706
N	0.004644233098	0.905705769505	-1.590150709520
N	1.511433837559	1.686389515707	-0.017427179633
N	0.909692644420	-0.605594174452	-0.105385130173
C	1.770869003509	-1.072083516490	0.959113798057
C	3.239617641344	-1.195790844620	0.592911916321
C	4.221502702261	-0.824014479602	1.509339151086
C	5.571700391841	-0.980443212149	1.206490592872
C	5.953489830374	-1.507042086969	-0.022690293588
C	4.978127022772	-1.875435120918	-0.946024971875
C	3.630745801496	-1.721471981095	-0.638767839346
H	-0.782967133055	0.279225341592	-1.681919700739
H	-0.232319177866	1.876132137100	-1.737821465253
H	2.148033432838	1.370440296312	0.708077037564
H	0.408692272345	-1.292898830492	-0.646255735757
H	1.393907186552	-2.052662825951	1.261390508456
H	1.669764160645	-0.418340989270	1.832098170733
H	3.927028506980	-0.406443710573	2.469410415362
H	6.325541780003	-0.684400814572	1.930076341007
H	7.005608861954	-1.626953973174	-0.262960212667
H	5.268295653655	-2.285324408660	-1.909065373902

H 2.874676666353 -2.009547486238 -1.364753809298

SCF Done: E(RwB97X) = -475.763903664

Zero-point correction= 0.187222
Thermal correction to Energy= 0.197396
Thermal correction to Enthalpy= 0.198340
Thermal correction to Gibbs Free Energy= 0.151018
Sum of electronic and zero-point Energies= -475.576682
Sum of electronic and thermal Energies= -475.566508
Sum of electronic and thermal Enthalpies= -475.565564
Sum of electronic and thermal Free Energies= -475.612885

1 C	Isotropic =	24.0429	Anisotropy =	130.9078
2 N	Isotropic =	192.3294	Anisotropy =	114.0329
3 N	Isotropic =	123.2517	Anisotropy =	183.6960
4 N	Isotropic =	175.7033	Anisotropy =	89.5513
5 C	Isotropic =	145.7923	Anisotropy =	31.7204
6 C	Isotropic =	41.7474	Anisotropy =	197.7676
7 C	Isotropic =	57.0019	Anisotropy =	173.4001
8 C	Isotropic =	55.9089	Anisotropy =	190.2628
9 C	Isotropic =	57.9016	Anisotropy =	189.2402
10 C	Isotropic =	55.3591	Anisotropy =	192.0648
11 C	Isotropic =	58.6038	Anisotropy =	188.7269
12 H	Isotropic =	28.1987	Anisotropy =	10.9157
13 H	Isotropic =	28.1037	Anisotropy =	12.3419
14 H	Isotropic =	27.6123	Anisotropy =	4.1209
15 H	Isotropic =	26.6625	Anisotropy =	9.2059
16 H	Isotropic =	27.5585	Anisotropy =	7.2564
17 H	Isotropic =	27.6390	Anisotropy =	6.9209
18 H	Isotropic =	23.9740	Anisotropy =	7.3746
19 H	Isotropic =	24.0032	Anisotropy =	4.8341
20 H	Isotropic =	24.0793	Anisotropy =	4.3928
21 H	Isotropic =	23.9218	Anisotropy =	5.2501
22 H	Isotropic =	23.8828	Anisotropy =	9.0272

Conformer_5

C	0.252691802471	0.537973056094	-0.439937310512
N	-0.835231699327	-0.226987688866	-0.812984411810
N	0.078517402179	1.775521565476	-0.111101197914
N	1.432841430690	-0.153601973842	-0.397237412242
C	2.712483809330	0.485609815482	-0.139343550166
C	3.785496335254	-0.548041979132	0.109275659525
C	4.933703075047	-0.580682396818	-0.677939834179

C	5.934001936107	-1.519633806454	-0.434111249758
C	5.789532307269	-2.438697257458	0.598154316637
C	4.641320433644	-2.415125490139	1.387815482206
C	3.647534032283	-1.475194702668	1.145296253005
H	-0.651683022928	-1.024158984876	-1.406185152288
H	-1.638068967182	0.314018397349	-1.099446519301
H	0.952844137442	2.205734279094	0.172035903524
H	1.463827327280	-1.040091979790	-0.881206805081
H	3.014733625873	1.134245168059	-0.971059186392
H	2.617951353228	1.117306022745	0.750522955416
H	5.047279048361	0.134266276682	-1.488755944499
H	6.824909999904	-1.532341668574	-1.054939890135
H	6.567186591969	-3.172193339586	0.788950362917
H	4.523665411771	-3.128984938469	2.197823958679
H	2.754763629338	-1.456738374307	1.765373572369

SCF Done: E(RwB97X) = -475.762534221

Zero-point correction=	0.187525
Thermal correction to Energy=	0.197719
Thermal correction to Enthalpy=	0.198664
Thermal correction to Gibbs Free Energy=	0.151168
Sum of electronic and zero-point Energies=	-475.575009
Sum of electronic and thermal Energies=	-475.564815
Sum of electronic and thermal Enthalpies=	-475.563871
Sum of electronic and thermal Free Energies=	-475.611366

1 C	Isotropic =	23.1239	Anisotropy =	133.0332
2 N	Isotropic =	191.6646	Anisotropy =	114.2451
3 N	Isotropic =	123.2337	Anisotropy =	183.1747
4 N	Isotropic =	168.4460	Anisotropy =	125.1541
5 C	Isotropic =	144.2873	Anisotropy =	20.0267
6 C	Isotropic =	44.2690	Anisotropy =	198.6869
7 C	Isotropic =	55.1164	Anisotropy =	171.0063
8 C	Isotropic =	55.8035	Anisotropy =	190.1583
9 C	Isotropic =	56.8590	Anisotropy =	191.8098
10 C	Isotropic =	55.4513	Anisotropy =	191.9877
11 C	Isotropic =	55.5261	Anisotropy =	186.8385
12 H	Isotropic =	28.3487	Anisotropy =	9.9139
13 H	Isotropic =	28.0087	Anisotropy =	12.2546
14 H	Isotropic =	27.1411	Anisotropy =	5.5519
15 H	Isotropic =	27.9468	Anisotropy =	5.8840
16 H	Isotropic =	27.9920	Anisotropy =	8.6027
17 H	Isotropic =	27.4220	Anisotropy =	4.2207
18 H	Isotropic =	23.9782	Anisotropy =	7.2623
19 H	Isotropic =	23.9911	Anisotropy =	4.8117

20	H	Isotropic =	24.0288	Anisotropy =	4.4321
21	H	Isotropic =	23.8734	Anisotropy =	5.1476
22	H	Isotropic =	23.7676	Anisotropy =	8.9701

Conformer_6

C	0.430672088456	0.877576617703	-0.494477854903
N	-0.529190113403	-0.038588289653	-0.856746576837
N	0.114568402338	2.130371052282	-0.413945026334
N	1.673320264308	0.365858908178	-0.218508228909
C	1.941984472841	-1.047721079442	0.027356551498
C	3.424227098294	-1.271733435379	0.211566753592
C	4.316522769889	-0.966506180793	-0.819174151156
C	5.679868708688	-1.178721219224	-0.657848484254
C	6.169580019195	-1.702131342454	0.537429306517
C	5.288271858708	-2.007940491255	1.567457362071
C	3.921552800177	-1.790470162690	1.404364651669
H	-1.348887087678	0.373723867903	-1.278296911177
H	-0.235777217762	-0.900055172039	-1.292679457094
H	0.900781631586	2.670669312284	-0.062099565572
H	2.292724421277	1.011630088487	0.251568636579
H	1.402656938274	-1.413303772009	0.909396428289
H	1.606007156465	-1.634452185285	-0.833600799450
H	3.936869130643	-0.561213350308	-1.753798302639
H	6.363387917263	-0.940059419369	-1.467368015414
H	7.234926574728	-1.870444711460	0.663185794915
H	5.662324206086	-2.415297899682	2.502023794350
H	3.234507959629	-2.027191135795	2.212694094259

SCF Done: E(RwB97X) = -475.760988432

Zero-point correction=	0.187546
Thermal correction to Energy=	0.197708
Thermal correction to Enthalpy=	0.198652
Thermal correction to Gibbs Free Energy=	0.150705
Sum of electronic and zero-point Energies=	-475.573443
Sum of electronic and thermal Energies=	-475.563281
Sum of electronic and thermal Enthalpies=	-475.562336
Sum of electronic and thermal Free Energies=	-475.610283

1	C	Isotropic =	22.5443	Anisotropy =	135.4952
2	N	Isotropic =	191.9329	Anisotropy =	85.6917
3	N	Isotropic =	124.0574	Anisotropy =	128.9386
4	N	Isotropic =	165.9685	Anisotropy =	135.3396
5	C	Isotropic =	142.1532	Anisotropy =	23.3383

6 C	Isotropic =	44.4534	Anisotropy =	199.2216
7 C	Isotropic =	55.2172	Anisotropy =	186.3609
8 C	Isotropic =	55.4321	Anisotropy =	191.9636
9 C	Isotropic =	56.6740	Anisotropy =	192.0344
10 C	Isotropic =	55.7797	Anisotropy =	190.3167
11 C	Isotropic =	55.1434	Anisotropy =	171.1444
12 H	Isotropic =	27.7604	Anisotropy =	11.9503
13 H	Isotropic =	27.8262	Anisotropy =	8.7797
14 H	Isotropic =	27.5626	Anisotropy =	6.0823
15 H	Isotropic =	28.1787	Anisotropy =	5.0926
16 H	Isotropic =	27.8826	Anisotropy =	7.8289
17 H	Isotropic =	27.5271	Anisotropy =	4.1915
18 H	Isotropic =	23.7601	Anisotropy =	8.7305
19 H	Isotropic =	23.8764	Anisotropy =	5.1291
20 H	Isotropic =	24.0164	Anisotropy =	4.4594
21 H	Isotropic =	23.9873	Anisotropy =	4.8226
22 H	Isotropic =	23.9989	Anisotropy =	7.2663

Conformer_7

C	0.544885223019	0.353393583265	-0.308630250272
N	0.870411232055	-0.359784840311	-1.442128395749
N	-0.697747145168	0.493827519000	0.026070462158
N	1.604831672059	0.893998286433	0.366178771067
C	2.969836682696	0.943623759349	-0.126976677188
C	3.766993102982	-0.332821263962	0.079929050626
C	4.652299362816	-0.769076627532	-0.904721782613
C	5.420777034931	-1.914564398214	-0.712516836747
C	5.306909218192	-2.639552329286	0.468553905495
C	4.421721321722	-2.212217149343	1.455490854884
C	3.658167392957	-1.066700574922	1.261919018772
H	0.104560674210	-0.906764032599	-1.808390577733
H	1.753867277137	-0.850372103903	-1.453544040869
H	-0.776858805822	1.115459717924	0.826982930552
H	1.371096788694	1.496491900260	1.139502105477
H	3.464627342833	1.759358931253	0.406387991033
H	2.984346939567	1.209296526753	-1.189277323860
H	4.737947933288	-0.210171491972	-1.833726191839
H	6.103502132100	-2.243719632001	-1.490376263470
H	5.900869166728	-3.536164955390	0.618364868014
H	4.326068524811	-2.773806546174	2.380255289977
H	2.964886928194	-0.741034278628	2.032853092285

SCF Done: E(RwB97X) = -475.762319527

Zero-point correction=	0.187657
Thermal correction to Energy=	0.197679
Thermal correction to Enthalpy=	0.198623
Thermal correction to Gibbs Free Energy=	0.151277
Sum of electronic and zero-point Energies=	-475.574663
Sum of electronic and thermal Energies=	-475.564640
Sum of electronic and thermal Enthalpies=	-475.563696
Sum of electronic and thermal Free Energies=	-475.611043

1 C	Isotropic =	22.5728	Anisotropy =	132.8312
2 N	Isotropic =	191.0006	Anisotropy =	80.5077
3 N	Isotropic =	125.7185	Anisotropy =	126.9224
4 N	Isotropic =	172.8342	Anisotropy =	91.8671
5 C	Isotropic =	143.7814	Anisotropy =	29.7317
6 C	Isotropic =	41.4694	Anisotropy =	198.1640
7 C	Isotropic =	57.1953	Anisotropy =	173.5882
8 C	Isotropic =	55.7535	Anisotropy =	190.5183
9 C	Isotropic =	57.6146	Anisotropy =	189.5405
10 C	Isotropic =	55.2890	Anisotropy =	192.2704
11 C	Isotropic =	57.6166	Anisotropy =	190.4853
12 H	Isotropic =	28.1326	Anisotropy =	12.0987
13 H	Isotropic =	28.7380	Anisotropy =	11.9044
14 H	Isotropic =	27.5298	Anisotropy =	6.5786
15 H	Isotropic =	26.9742	Anisotropy =	10.5200
16 H	Isotropic =	27.6230	Anisotropy =	6.9381
17 H	Isotropic =	27.6755	Anisotropy =	6.5400
18 H	Isotropic =	23.9873	Anisotropy =	7.2743
19 H	Isotropic =	23.9778	Anisotropy =	4.8613
20 H	Isotropic =	24.0427	Anisotropy =	4.3971
21 H	Isotropic =	23.8772	Anisotropy =	5.2207
22 H	Isotropic =	23.7874	Anisotropy =	8.9601

Conformer_8

C	0.626241021255	0.432860047959	-0.556107395269
N	0.417754370377	-0.872616173891	-0.166781823003
N	-0.216396158487	1.006629310725	-1.354037944300
N	1.730337113179	1.034197654886	-0.017218222754
C	2.540894883375	0.482938495614	1.054235712407
C	3.578486335620	-0.532813623885	0.607877127393
C	4.309710815744	-0.347477361653	-0.566199385210
C	5.283676294482	-1.264520458632	-0.944482510893
C	5.540991177055	-2.380675012998	-0.151892991393
C	4.816297281252	-2.573291601640	1.019089079313
C	3.839134595197	-1.654398282922	1.393816384969

H	-0.278219306757	-1.352145335021	-0.719527373979
H	1.229135470574	-1.440162087107	0.035311788749
H	0.025980230174	1.987002091023	-1.473500543784
H	1.837378471296	2.015759333323	-0.219060298127
H	3.052252493591	1.326945419808	1.524211726854
H	1.904658498026	0.033639235155	1.824059468777
H	4.108975685957	0.518532899382	-1.191318503566
H	5.844527622499	-1.107743291561	-1.861317545165
H	6.299424148384	-3.098721204459	-0.449102441956
H	5.005405900691	-3.444012343114	1.640056722534
H	3.268453056516	-1.813727710992	2.305788968403

SCF Done: E(RwB97X) = -475.762319162

Zero-point correction=	0.187654
Thermal correction to Energy=	0.197679
Thermal correction to Enthalpy=	0.198623
Thermal correction to Gibbs Free Energy=	0.151254
Sum of electronic and zero-point Energies=	-475.574665
Sum of electronic and thermal Energies=	-475.564641
Sum of electronic and thermal Enthalpies=	-475.563696
Sum of electronic and thermal Free Energies=	-475.611065

1 C	Isotropic =	22.5683	Anisotropy =	132.8427
2 N	Isotropic =	190.9988	Anisotropy =	80.5141
3 N	Isotropic =	125.7267	Anisotropy =	126.8838
4 N	Isotropic =	172.8280	Anisotropy =	91.8409
5 C	Isotropic =	143.7788	Anisotropy =	29.7138
6 C	Isotropic =	41.4720	Anisotropy =	198.1695
7 C	Isotropic =	57.6135	Anisotropy =	190.4837
8 C	Isotropic =	55.2895	Anisotropy =	192.2711
9 C	Isotropic =	57.6138	Anisotropy =	189.5425
10 C	Isotropic =	55.7557	Anisotropy =	190.5174
11 C	Isotropic =	57.1928	Anisotropy =	173.5820
12 H	Isotropic =	28.1321	Anisotropy =	12.0985
13 H	Isotropic =	28.7379	Anisotropy =	11.9099
14 H	Isotropic =	27.5307	Anisotropy =	6.5790
15 H	Isotropic =	26.9742	Anisotropy =	10.5199
16 H	Isotropic =	27.6229	Anisotropy =	6.9375
17 H	Isotropic =	27.6757	Anisotropy =	6.5402
18 H	Isotropic =	23.7874	Anisotropy =	8.9586
19 H	Isotropic =	23.8772	Anisotropy =	5.2203
20 H	Isotropic =	24.0427	Anisotropy =	4.3970
21 H	Isotropic =	23.9779	Anisotropy =	4.8611
22 H	Isotropic =	23.9873	Anisotropy =	7.2736

1-benzylguanidine_protonated

Conformer_1

C	-0.388978419061	3.237622468873	-1.542530276081
C	-0.489811170707	1.849970600030	-1.481174655716
C	-0.459903771780	1.191936253703	-0.253661886468
C	-0.324624288386	1.941388177252	0.915730445588
C	-0.216492299588	3.325658050377	0.855991694877
C	-0.250212011228	3.978120653799	-0.374162458447
C	-0.621497167074	-0.314752737366	-0.200578665429
N	0.275425805156	-0.985597012236	0.731550916173
C	1.553399746006	-1.271978470183	0.488104352527
N	2.267627308688	-1.931309999508	1.399532632073
N	2.124078946742	-0.897043420497	-0.653388942517
H	-0.412308740650	3.738242280865	-2.505850822860
H	-0.591221757362	1.273147926335	-2.397245447080
H	-0.298334814536	1.439482798729	1.879515146304
H	-0.108111671326	3.897621383665	1.772753155220
H	-0.165717098144	5.059654095563	-0.420500849535
H	-1.633422768721	-0.565671354457	0.123518919678
H	-0.500408166636	-0.742590370906	-1.200116044937
H	-0.100160974739	-1.276309148991	1.622944931324
H	3.233017353129	-2.164507264382	1.222679326510
H	1.834774019990	-2.269757381658	2.245427547097
H	3.079844870848	-1.153815873989	-0.851035234180
H	1.617137069379	-0.378611655017	-1.354003784121

SCF Done: E(RwB97X) = -476.244407071

Zero-point correction= 0.200451
Thermal correction to Energy= 0.211150
Thermal correction to Enthalpy= 0.212095
Thermal correction to Gibbs Free Energy= 0.164203
Sum of electronic and zero-point Energies= -476.043956
Sum of electronic and thermal Energies= -476.033257
Sum of electronic and thermal Enthalpies= -476.032313
Sum of electronic and thermal Free Energies= -476.080204

1 C Isotropic = 55.6487 Anisotropy = 191.0526
2 C Isotropic = 56.6670 Anisotropy = 173.7471
3 C Isotropic = 45.3256 Anisotropy = 192.5318
4 C Isotropic = 57.7619 Anisotropy = 188.5536
5 C Isotropic = 55.1538 Anisotropy = 193.0163
6 C Isotropic = 56.7154 Anisotropy = 191.6270
7 C Isotropic = 144.8324 Anisotropy = 30.1570

8	N	Isotropic =	168.1316	Anisotropy =	62.3366
9	C	Isotropic =	29.4135	Anisotropy =	141.3021
10	N	Isotropic =	186.3600	Anisotropy =	88.3711
11	N	Isotropic =	184.5807	Anisotropy =	59.1902
12	H	Isotropic =	23.9566	Anisotropy =	4.8686
13	H	Isotropic =	23.9328	Anisotropy =	7.3664
14	H	Isotropic =	23.8462	Anisotropy =	8.9952
15	H	Isotropic =	23.8606	Anisotropy =	5.2434
16	H	Isotropic =	23.9801	Anisotropy =	4.3980
17	H	Isotropic =	27.2593	Anisotropy =	7.1990
18	H	Isotropic =	27.5857	Anisotropy =	6.7199
19	H	Isotropic =	25.9019	Anisotropy =	10.2465
20	H	Isotropic =	26.7992	Anisotropy =	12.8260
21	H	Isotropic =	26.7516	Anisotropy =	11.8967
22	H	Isotropic =	26.7668	Anisotropy =	12.8842
23	H	Isotropic =	26.7880	Anisotropy =	10.9109

Conformer_2

C	-0.184352981924	2.751871703524	-1.834634428996
C	-0.297876290114	1.463078848912	-1.327099126545
C	-0.463617183218	1.255035962454	0.042833750331
C	-0.518462368425	2.356317961301	0.894221061774
C	-0.412269434747	3.648824182044	0.386614825694
C	-0.243094125495	3.849123301886	-0.978646864044
C	-0.631233385327	-0.143119228521	0.605088779593
N	0.283921522324	-1.131174368641	0.048634873240
C	1.554539162643	-1.286771995544	0.417228735499
N	2.286664840631	-2.256790677034	-0.129253717654
N	2.100318469406	-0.475754608132	1.319244443269
H	-0.052157188910	2.900744505331	-2.902202419493
H	-0.251950157450	0.611898159957	-2.001533161531
H	-0.643689244606	2.202758699744	1.963300673718
H	-0.455255476743	4.498670886659	1.061198772256
H	-0.154387218484	4.855924894047	-1.375489243167
H	-0.535581825035	-0.125570847384	1.694734705399
H	-1.636524192986	-0.509557019875	0.388047114824
H	-0.072295002147	-1.762130648060	-0.655034925534
H	1.871852621772	-2.913311317070	-0.772962391902
H	3.246334897587	-2.393040346214	0.150230658022
H	3.049799286161	-0.624943197918	1.627001160132
H	1.579315275088	0.280115148537	1.736176725114

SCF Done: E(RwB97X) = -476.244406053

Zero-point correction=	0.200457
Thermal correction to Energy=	0.211153
Thermal correction to Enthalpy=	0.212098
Thermal correction to Gibbs Free Energy=	0.164215
Sum of electronic and zero-point Energies=	-476.043949
Sum of electronic and thermal Energies=	-476.033253
Sum of electronic and thermal Enthalpies=	-476.032308
Sum of electronic and thermal Free Energies=	-476.080191

1 C	Isotropic =	55.1531	Anisotropy =	193.0168
2 C	Isotropic =	57.7577	Anisotropy =	188.5528
3 C	Isotropic =	45.3265	Anisotropy =	192.5328
4 C	Isotropic =	56.6656	Anisotropy =	173.7466
5 C	Isotropic =	55.6492	Anisotropy =	191.0516
6 C	Isotropic =	56.7145	Anisotropy =	191.6283
7 C	Isotropic =	144.8307	Anisotropy =	30.1522
8 N	Isotropic =	168.1237	Anisotropy =	62.3185
9 C	Isotropic =	29.4089	Anisotropy =	141.3052
10 N	Isotropic =	186.3603	Anisotropy =	88.3700
11 N	Isotropic =	184.5763	Anisotropy =	59.1901
12 H	Isotropic =	23.8605	Anisotropy =	5.2433
13 H	Isotropic =	23.8461	Anisotropy =	8.9948
14 H	Isotropic =	23.9328	Anisotropy =	7.3662
15 H	Isotropic =	23.9566	Anisotropy =	4.8686
16 H	Isotropic =	23.9801	Anisotropy =	4.3980
17 H	Isotropic =	27.5859	Anisotropy =	6.7202
18 H	Isotropic =	27.2593	Anisotropy =	7.1988
19 H	Isotropic =	25.9019	Anisotropy =	10.2467
20 H	Isotropic =	26.7517	Anisotropy =	11.8968
21 H	Isotropic =	26.7991	Anisotropy =	12.8265
22 H	Isotropic =	26.7669	Anisotropy =	12.8854
23 H	Isotropic =	26.7874	Anisotropy =	10.9093

Conformer_3

C	-0.432031175040	3.652141949212	0.319062634306
C	-0.521008067473	2.372374541039	0.861109818433
C	-0.472074991871	1.250012412241	0.037347830784
C	-0.329800101823	1.424022045592	-1.339950657854
C	-0.233529193209	2.700078209709	-1.881953528710
C	-0.286214295496	3.818493047665	-1.053403676871
C	-0.620604997564	-0.134418444308	0.637645690474
N	0.292547537371	-1.130078908858	0.091507709467
C	1.569993894037	-1.268165817437	0.443231707728
N	2.124799197458	-0.430881237013	1.315320876284

N	2.299676570740	-2.247327497829	-0.090114322049
H	-0.470146726492	4.518662076487	0.972400864238
H	-0.627997863401	2.245409729503	1.935651066723
H	-0.288718996399	0.556107284228	-1.993057446203
H	-0.119565336359	2.822421873422	-2.954985897184
H	-0.210976209161	4.815364535908	-1.477198590700
H	-1.626592999908	-0.513095088129	0.446335771898
H	-0.507494675275	-0.088447688475	1.724758799838
H	-0.070883962414	-1.781572400905	-0.589371728624
H	3.079988861445	-0.566469477973	1.611558477350
H	1.605590760498	0.332112469198	1.721419259195
H	3.264823197110	-2.369985518543	0.176552957191
H	1.878919573224	-2.922558094735	-0.710167615714

SCF Done: E(RwB97X) = -476.244406015

Zero-point correction=	0.200453
Thermal correction to Energy=	0.211149
Thermal correction to Enthalpy=	0.212093
Thermal correction to Gibbs Free Energy=	0.164213
Sum of electronic and zero-point Energies=	-476.043953
Sum of electronic and thermal Energies=	-476.033257
Sum of electronic and thermal Enthalpies=	-476.032313
Sum of electronic and thermal Free Energies=	-476.080193

1 C	Isotropic =	55.6530	Anisotropy =	191.0456
2 C	Isotropic =	56.6667	Anisotropy =	173.7505
3 C	Isotropic =	45.3218	Anisotropy =	192.5372
4 C	Isotropic =	57.7571	Anisotropy =	188.5507
5 C	Isotropic =	55.1610	Anisotropy =	193.0058
6 C	Isotropic =	56.7194	Anisotropy =	191.6238
7 C	Isotropic =	144.8287	Anisotropy =	30.1487
8 N	Isotropic =	168.1118	Anisotropy =	62.3067
9 C	Isotropic =	29.4000	Anisotropy =	141.3041
10 N	Isotropic =	184.5762	Anisotropy =	59.2001
11 N	Isotropic =	186.3514	Anisotropy =	88.3781
12 H	Isotropic =	23.9565	Anisotropy =	4.8683
13 H	Isotropic =	23.9330	Anisotropy =	7.3654
14 H	Isotropic =	23.8459	Anisotropy =	8.9950
15 H	Isotropic =	23.8608	Anisotropy =	5.2431
16 H	Isotropic =	23.9802	Anisotropy =	4.3976
17 H	Isotropic =	27.2591	Anisotropy =	7.1983
18 H	Isotropic =	27.5865	Anisotropy =	6.7201
19 H	Isotropic =	25.9027	Anisotropy =	10.2465
20 H	Isotropic =	26.7665	Anisotropy =	12.8866
21 H	Isotropic =	26.7871	Anisotropy =	10.9081

22 H Isotropic = 26.7981 Anisotropy = 12.8260
 23 H Isotropic = 26.7514 Anisotropy = 11.8952

Methyl L-tyrosinate_neutral
 Conformer_1

```
-----
C      0.027416998240    1.344651592910   -0.664157465133
C     -0.856071329913    0.639905931974    0.155340101192
C     -1.357104821154    1.194226372527    1.327114806346
C     -0.975506143895    2.480308521325    1.696613745044
C     -0.101328485597    3.205379494761    0.890508297891
C      0.391117077557    2.634297305359   -0.277140603071
O     -1.490026267389    2.988673701672    2.852539505979
C      0.610525015577    0.719397728926   -1.907600081024
C      2.016336559464    0.123874762286   -1.709134920419
N      2.474956932746   -0.448839836093   -2.966099703939
C      1.965521937317   -0.903763536176   -0.583100361533
O      2.434573010538   -0.422457912541    0.568010100822
O      1.534431908944   -2.026867036137   -0.711585717492
C      2.317787962492   -1.283664941695    1.711684822497
H     -1.165557767178   -0.363547835220   -0.127461694245
H     -2.045318684184    0.639063579876    1.957133851869
H      0.190200736541    4.213589181947    1.175368206771
H      1.072314395933    3.209693053436   -0.899490516720
H     -1.147274863785    3.878482734572    2.992441992536
H      0.690818591556    1.463559880702   -2.705180158418
H     -0.048598548549   -0.078191550865   -2.268983464465
H      2.704791276562    0.919507827944   -1.412516220531
H      1.892823925917   -1.245483871493   -3.209607871951
H      3.422502249612   -0.799881525283   -2.868237192951
H      2.871596839547   -2.210762658502    1.553397214820
H      2.745032837975   -0.728327143820    2.544788951951
H      1.267638655129   -1.509923822394    1.908654374172
```

SCF Done: E(RwB97X) = -669.364544277

```
Zero-point correction=          0.224177
Thermal correction to Energy=      0.237870
Thermal correction to Enthalpy=     0.238814
Thermal correction to Gibbs Free Energy= 0.182879
Sum of electronic and zero-point Energies= -669.140367
Sum of electronic and thermal Energies= -669.126675
Sum of electronic and thermal Enthalpies= -669.125730
Sum of electronic and thermal Free Energies= -669.181666
```

1 C Isotropic = 53.9959 Anisotropy = 191.2991

2 C	Isotropic =	53.4564	Anisotropy =	173.3919
3 C	Isotropic =	71.7920	Anisotropy =	151.5125
4 C	Isotropic =	28.6542	Anisotropy =	146.7901
5 C	Isotropic =	71.7796	Anisotropy =	141.4901
6 C	Isotropic =	52.8319	Anisotropy =	176.9904
7 O	Isotropic =	229.4842	Anisotropy =	67.9292
8 C	Isotropic =	147.7648	Anisotropy =	34.4813
9 C	Isotropic =	131.0031	Anisotropy =	23.8286
10 N	Isotropic =	226.1719	Anisotropy =	50.7903
11 C	Isotropic =	3.4987	Anisotropy =	114.5757
12 O	Isotropic =	145.6723	Anisotropy =	139.1656
13 O	Isotropic =	-43.7033	Anisotropy =	592.1377
14 C	Isotropic =	138.4943	Anisotropy =	72.0653
15 H	Isotropic =	24.4653	Anisotropy =	7.1675
16 H	Isotropic =	24.6413	Anisotropy =	5.0791
17 H	Isotropic =	24.6749	Anisotropy =	4.8227
18 H	Isotropic =	24.0822	Anisotropy =	7.6893
19 H	Isotropic =	27.3600	Anisotropy =	14.3699
20 H	Isotropic =	28.8581	Anisotropy =	6.3669
21 H	Isotropic =	29.3787	Anisotropy =	4.4602
22 H	Isotropic =	28.5242	Anisotropy =	3.9197
23 H	Isotropic =	30.2642	Anisotropy =	11.8416
24 H	Isotropic =	30.4791	Anisotropy =	15.9355
25 H	Isotropic =	28.3052	Anisotropy =	9.7673
26 H	Isotropic =	28.6602	Anisotropy =	8.2296
27 H	Isotropic =	28.6904	Anisotropy =	6.9996

Conformer_10

C	0.252529616819	1.526191738758	-0.766277583387
C	-1.138966694613	1.487270036856	-0.649273102447
C	-1.788729923903	2.006983014283	0.463424312752
C	-1.044497441430	2.580550157740	1.489990456681
C	0.343392198067	2.637727165315	1.393652666861
C	0.976728563093	2.114177006331	0.272180841881
O	-1.721556559039	3.078928959306	2.563299303362
C	0.956776805397	0.921150772235	-1.957740567511
C	1.357820217614	-0.554996535198	-1.756298987749
N	0.185388412387	-1.396851738002	-1.596280971144
C	2.397272416331	-0.632343891343	-0.638582877849
O	1.933640593016	-1.192716446136	0.477313138371
O	3.525392589280	-0.208363621694	-0.752181625431
C	2.837211673605	-1.233985334453	1.592476704715
H	-1.730579625589	1.047326146005	-1.448172265876
H	-2.871022697285	1.974715577219	0.542111457447

H	0.926054245846	3.095432023090	2.189517850133
H	2.060635094375	2.174722459488	0.205937569537
H	-1.094605105622	3.443591847508	3.198010765695
H	1.858925178809	1.494681264586	-2.187457063361
H	0.306635274662	0.960894215664	-2.835832263067
H	1.887137755100	-0.872185793086	-2.659723529583
H	-0.301908716810	-1.168530930510	-0.735182006364
H	0.459803641065	-2.370691911159	-1.522432951469
H	3.726895943425	-1.814257410032	1.342006062686
H	3.126011389656	-0.222603699351	1.885507719206
H	2.288715155747	-1.716715073419	2.399506945912

SCF Done: E(RwB97X) = -669.363783824

Zero-point correction=	0.224296
Thermal correction to Energy=	0.237893
Thermal correction to Enthalpy=	0.238837
Thermal correction to Gibbs Free Energy=	0.182944
Sum of electronic and zero-point Energies=	-669.139488
Sum of electronic and thermal Energies=	-669.125891
Sum of electronic and thermal Enthalpies=	-669.124946
Sum of electronic and thermal Free Energies=	-669.180840

1 C	Isotropic =	56.1577	Anisotropy =	189.7067
2 C	Isotropic =	51.6259	Anisotropy =	175.0169
3 C	Isotropic =	71.8006	Anisotropy =	150.7168
4 C	Isotropic =	28.3011	Anisotropy =	147.1017
5 C	Isotropic =	72.1742	Anisotropy =	141.6364
6 C	Isotropic =	53.7186	Anisotropy =	174.5023
7 O	Isotropic =	229.3591	Anisotropy =	67.0710
8 C	Isotropic =	150.1579	Anisotropy =	11.9901
9 C	Isotropic =	132.7220	Anisotropy =	30.9912
10 N	Isotropic =	230.2363	Anisotropy =	24.8545
11 C	Isotropic =	6.3984	Anisotropy =	114.6092
12 O	Isotropic =	145.9420	Anisotropy =	177.7751
13 O	Isotropic =	-53.2081	Anisotropy =	569.9526
14 C	Isotropic =	138.0615	Anisotropy =	72.4997
15 H	Isotropic =	24.1343	Anisotropy =	7.6523
16 H	Isotropic =	24.5310	Anisotropy =	4.9584
17 H	Isotropic =	24.7197	Anisotropy =	5.3496
18 H	Isotropic =	24.5098	Anisotropy =	7.5524
19 H	Isotropic =	27.3878	Anisotropy =	14.0532
20 H	Isotropic =	28.7207	Anisotropy =	6.9700
21 H	Isotropic =	29.0672	Anisotropy =	7.7719
22 H	Isotropic =	28.2650	Anisotropy =	6.9104
23 H	Isotropic =	30.8929	Anisotropy =	9.6851

24	H	Isotropic =	30.5636	Anisotropy =	15.9008
25	H	Isotropic =	28.1843	Anisotropy =	9.9424
26	H	Isotropic =	28.3253	Anisotropy =	7.6557
27	H	Isotropic =	28.3634	Anisotropy =	8.3631

Conformer_11

C	0.280770404687	1.448636874829	-0.734223746373
C	-1.102219741504	1.388695244778	-0.546548677905
C	-1.695932095215	1.839679578606	0.625851423753
C	-0.902637499332	2.363849169568	1.642040983024
C	0.477707016707	2.440833029146	1.476168556412
C	1.054585559002	1.986315982192	0.295680369983
O	-1.525523751564	2.795414959732	2.775420171650
C	0.925395811479	0.917425001102	-1.992755640658
C	1.347917939373	-0.563201480074	-1.894749084388
N	0.192185926116	-1.425004116692	-1.720084169803
C	2.445949800167	-0.690843851016	-0.839375778285
O	2.046839706983	-1.317201342966	0.266329226839
O	3.563013652009	-0.248921079630	-0.988403446828
C	3.008877981919	-1.410723654476	1.328150714817
H	-1.732040357013	0.987046510010	-1.336358644604
H	-2.772242677532	1.791742844564	0.759441645546
H	1.098301940231	2.860278126257	2.264401137310
H	2.132956685471	2.061814783283	0.175998457633
H	-0.868561403791	3.131263798553	3.395498317151
H	1.809634768026	1.512250410567	-2.237455554590
H	0.229276045546	0.998448515071	-2.831896546006
H	1.830866552220	-0.824691686683	-2.840978812053
H	0.477684242986	-2.398444787738	-1.714927458458
H	-0.250309353573	-1.249593649885	-0.823142546781
H	2.507993576371	-1.943517291749	2.134635839772
H	3.888429888441	-1.966572560686	0.998888857632
H	3.304979381788	-0.414179326667	1.661894405213

SCF Done: E(RwB97X) = -669.363783998

Zero-point correction=	0.224294
Thermal correction to Energy=	0.237893
Thermal correction to Enthalpy=	0.238837
Thermal correction to Gibbs Free Energy=	0.182930
Sum of electronic and zero-point Energies=	-669.139490
Sum of electronic and thermal Energies=	-669.125891
Sum of electronic and thermal Enthalpies=	-669.124947
Sum of electronic and thermal Free Energies=	-669.180854

1 C	Isotropic =	56.1563	Anisotropy =	189.7060
2 C	Isotropic =	51.6260	Anisotropy =	175.0180
3 C	Isotropic =	71.8002	Anisotropy =	150.7186
4 C	Isotropic =	28.3012	Anisotropy =	147.1006
5 C	Isotropic =	72.1725	Anisotropy =	141.6380
6 C	Isotropic =	53.7175	Anisotropy =	174.4988
7 O	Isotropic =	229.3616	Anisotropy =	67.0717
8 C	Isotropic =	150.1608	Anisotropy =	11.9940
9 C	Isotropic =	132.7213	Anisotropy =	30.9923
10 N	Isotropic =	230.2353	Anisotropy =	24.8423
11 C	Isotropic =	6.3975	Anisotropy =	114.6046
12 O	Isotropic =	145.9339	Anisotropy =	177.7731
13 O	Isotropic =	-53.2009	Anisotropy =	569.9675
14 C	Isotropic =	138.0608	Anisotropy =	72.5063
15 H	Isotropic =	24.1343	Anisotropy =	7.6523
16 H	Isotropic =	24.5311	Anisotropy =	4.9584
17 H	Isotropic =	24.7197	Anisotropy =	5.3498
18 H	Isotropic =	24.5097	Anisotropy =	7.5540
19 H	Isotropic =	27.3880	Anisotropy =	14.0536
20 H	Isotropic =	28.7203	Anisotropy =	6.9699
21 H	Isotropic =	29.0673	Anisotropy =	7.7716
22 H	Isotropic =	28.2650	Anisotropy =	6.9097
23 H	Isotropic =	30.5636	Anisotropy =	15.8997
24 H	Isotropic =	30.8933	Anisotropy =	9.6840
25 H	Isotropic =	28.3629	Anisotropy =	8.3637
26 H	Isotropic =	28.1843	Anisotropy =	9.9420
27 H	Isotropic =	28.3251	Anisotropy =	7.6578

Conformer_12

C	0.335093278113	1.469441609222	-0.692976916983
C	-1.028702762356	1.467836754197	-0.400928995336
C	-1.513509134418	1.968452682472	0.803665869249
C	-0.625360911329	2.482667023487	1.743325938419
C	0.740188251744	2.502863681574	1.470495116070
C	1.205929297637	2.000899389444	0.263112719776
O	-1.041108299899	2.984720784545	2.940771962619
C	0.863238063341	0.884018679386	-1.981317909025
C	1.228370643491	-0.611553394673	-1.877771562478
N	0.051564652517	-1.417902382427	-1.605717317096
C	2.389047481428	-0.765947047305	-0.895582495263
O	2.038041891610	-1.346683612918	0.250629443731
O	3.512143149121	-0.380275427341	-1.130503853960
C	3.064128888113	-1.458001963661	1.248871623541

H	-1.733067787833	1.074196673946	-1.129321533122
H	-2.581092093323	1.961541814727	1.010511897501
H	1.425618218098	2.916790568431	2.203540380762
H	2.273687305820	2.031546365023	0.058262405143
H	-2.000413127287	2.914702380956	3.002281779282
H	1.751995811515	1.434015623028	-2.302591276212
H	0.112429110939	0.977598767011	-2.770509998146
H	1.633921930279	-0.913124041251	-2.848073339248
H	-0.320194136341	-1.205509700726	-0.684985802783
H	0.294890251461	-2.402719525692	-1.597945512878
H	3.894304463903	-2.061381876006	0.877770152112
H	3.425403938459	-0.468070734494	1.534652796294
H	2.595551625198	-1.947323090955	2.101034428031

SCF Done: E(RwB97X) = -669.363833641

Zero-point correction=	0.224315
Thermal correction to Energy=	0.237914
Thermal correction to Enthalpy=	0.238858
Thermal correction to Gibbs Free Energy=	0.183060
Sum of electronic and zero-point Energies=	-669.139519
Sum of electronic and thermal Energies=	-669.125920
Sum of electronic and thermal Enthalpies=	-669.124976
Sum of electronic and thermal Free Energies=	-669.180773

1 C	Isotropic =	56.2035	Anisotropy =	189.7077
2 C	Isotropic =	52.3416	Anisotropy =	173.7360
3 C	Isotropic =	72.6525	Anisotropy =	139.9985
4 C	Isotropic =	28.2824	Anisotropy =	147.2891
5 C	Isotropic =	71.3336	Anisotropy =	152.3930
6 C	Isotropic =	53.0391	Anisotropy =	175.6638
7 O	Isotropic =	229.3190	Anisotropy =	66.7404
8 C	Isotropic =	150.1273	Anisotropy =	11.9321
9 C	Isotropic =	132.7848	Anisotropy =	31.0338
10 N	Isotropic =	230.2145	Anisotropy =	25.0069
11 C	Isotropic =	6.4370	Anisotropy =	114.6008
12 O	Isotropic =	146.0413	Anisotropy =	177.7221
13 O	Isotropic =	-53.3219	Anisotropy =	570.0404
14 C	Isotropic =	138.0563	Anisotropy =	72.4923
15 H	Isotropic =	24.2052	Anisotropy =	7.7048
16 H	Isotropic =	24.6695	Anisotropy =	5.0656
17 H	Isotropic =	24.5642	Anisotropy =	5.2383
18 H	Isotropic =	24.4436	Anisotropy =	7.4770
19 H	Isotropic =	27.3677	Anisotropy =	14.2459
20 H	Isotropic =	28.7234	Anisotropy =	7.0170
21 H	Isotropic =	29.0727	Anisotropy =	7.7305

22	H	Isotropic =	28.2701	Anisotropy =	6.9266
23	H	Isotropic =	30.8858	Anisotropy =	9.7548
24	H	Isotropic =	30.5683	Anisotropy =	15.8999
25	H	Isotropic =	28.1837	Anisotropy =	9.9653
26	H	Isotropic =	28.3200	Anisotropy =	7.6066
27	H	Isotropic =	28.3660	Anisotropy =	8.3602

Conformer_13

C	-0.091312353994	1.115466489675	0.165969879246
C	-0.228356237312	1.092474530727	1.556391520179
C	-0.782664798743	2.160676728545	2.247661122102
C	-1.217572785788	3.282911088059	1.546138114265
C	-1.094588363715	3.326991272080	0.161380613501
C	-0.533354086448	2.247164893084	-0.514736255876
O	-1.759334370238	4.308561962154	2.263958535605
C	0.529073255738	-0.050908970594	-0.562115500045
C	2.062587426435	-0.099272853288	-0.424687622597
N	2.672705114240	1.050282732337	-1.063834156347
C	2.557675546236	-1.430386699295	-0.983507500975
O	2.259518970916	-2.444484787982	-0.168558671389
O	3.133724523503	-1.568403616885	-2.036936486679
C	2.626855270670	-3.758248852149	-0.617547399965
H	0.103335319021	0.218541211394	2.112634146969
H	-0.888437208668	2.133101361722	3.327824501214
H	-1.436473548337	4.201290434053	-0.387393824204
H	-0.441079166383	2.291379215553	-1.596903532654
H	-2.019239326085	5.017190270400	1.664760239273
H	0.280594264655	0.000597372142	-1.628720293078
H	0.113774804537	-0.986445682881	-0.176567191409
H	2.316808991102	-0.085508624743	0.640297591568
H	3.677168098002	1.039846425874	-0.921469732846
H	2.523360102306	1.005203084674	-2.067698035016
H	2.306878979386	-4.439337207014	0.169097839365
H	2.117222862429	-3.997166226550	-1.552755224962
H	3.707128716533	-3.827815551091	-0.756982675246

SCF Done: E(RwB97X) = -669.364200345

Zero-point correction=	0.223981
Thermal correction to Energy=	0.237837
Thermal correction to Enthalpy=	0.238782
Thermal correction to Gibbs Free Energy=	0.181731
Sum of electronic and zero-point Energies=	-669.140220
Sum of electronic and thermal Energies=	-669.126363

Sum of electronic and thermal Enthalpies= -669.125419
Sum of electronic and thermal Free Energies= -669.182469

1 C	Isotropic =	52.1601	Anisotropy =	190.3001
2 C	Isotropic =	53.6366	Anisotropy =	178.5797
3 C	Isotropic =	71.1291	Anisotropy =	151.6033
4 C	Isotropic =	28.9652	Anisotropy =	145.6045
5 C	Isotropic =	73.2300	Anisotropy =	138.6479
6 C	Isotropic =	51.7540	Anisotropy =	169.0260
7 O	Isotropic =	230.0813	Anisotropy =	67.6645
8 C	Isotropic =	149.4609	Anisotropy =	21.4297
9 C	Isotropic =	131.3714	Anisotropy =	24.1391
10 N	Isotropic =	233.6432	Anisotropy =	31.5897
11 C	Isotropic =	4.3991	Anisotropy =	107.1795
12 O	Isotropic =	158.5406	Anisotropy =	142.5739
13 O	Isotropic =	-50.5122	Anisotropy =	598.5008
14 C	Isotropic =	137.6342	Anisotropy =	73.3828
15 H	Isotropic =	24.0168	Anisotropy =	8.2354
16 H	Isotropic =	24.5109	Anisotropy =	5.1446
17 H	Isotropic =	24.7866	Anisotropy =	5.0622
18 H	Isotropic =	24.3024	Anisotropy =	7.8173
19 H	Isotropic =	27.3814	Anisotropy =	14.2153
20 H	Isotropic =	29.6195	Anisotropy =	5.1683
21 H	Isotropic =	28.8025	Anisotropy =	6.3766
22 H	Isotropic =	28.5317	Anisotropy =	5.4458
23 H	Isotropic =	30.8725	Anisotropy =	16.4133
24 H	Isotropic =	30.7695	Anisotropy =	12.7089
25 H	Isotropic =	27.9833	Anisotropy =	8.1832
26 H	Isotropic =	28.1002	Anisotropy =	8.7754
27 H	Isotropic =	28.0180	Anisotropy =	9.0829

Conformer_14

C	-0.118910719684	1.123043862516	0.099600434904
C	-0.183516856113	1.248263291953	1.487400273841
C	-0.733819351141	2.374506096031	2.088702648006
C	-1.235932521491	3.402537741571	1.294448905458
C	-1.185962944225	3.296827474352	-0.091965879871
C	-0.629731476133	2.164608596361	-0.675181286741
O	-1.789491129882	4.529988036152	1.826729259961
C	0.501219610334	-0.098530852804	-0.531691120174
C	2.041299517466	-0.071223965621	-0.506215914157
N	2.549605428780	1.012673694094	-1.324062134613
C	2.559155313787	-1.441268075847	-0.935258062339
O	2.360777972735	-2.358691084364	0.013681622551

O	3.071853687961	-1.685445053830	-2.002049234539
C	2.756353070170	-3.703030852674	-0.300614581120
H	0.201685683278	0.449628993065	2.117392085406
H	-0.778556685241	2.452872466061	3.172496665305
H	-1.582855451789	4.101583339534	-0.703149209019
H	-0.593916475199	2.090431594699	-1.759096433193
H	-1.760771960394	4.478438296736	2.788645415183
H	0.176236567947	-0.185442839252	-1.575184836782
H	0.158325410354	-0.995608089771	-0.008446911082
H	2.368615025777	0.084636549794	0.527078667442
H	2.330646396850	0.838369269431	-2.300672746485
H	3.561112901026	1.057392966550	-1.259547883586
H	2.517824986471	-4.294823705802	0.581407525350
H	2.198890058839	-4.071774399847	-1.163565356473
H	3.827463939515	-3.749863349087	-0.505081913234

SCF Done: E(RwB97X) = -669.364168329

Zero-point correction=	0.224048
Thermal correction to Energy=	0.237877
Thermal correction to Enthalpy=	0.238821
Thermal correction to Gibbs Free Energy=	0.182030
Sum of electronic and zero-point Energies=	-669.140121
Sum of electronic and thermal Energies=	-669.126291
Sum of electronic and thermal Enthalpies=	-669.125347
Sum of electronic and thermal Free Energies=	-669.182138

1 C	Isotropic =	52.1305	Anisotropy =	190.4401
2 C	Isotropic =	54.2116	Anisotropy =	176.6082
3 C	Isotropic =	71.9911	Anisotropy =	140.6163
4 C	Isotropic =	28.9608	Anisotropy =	145.6296
5 C	Isotropic =	72.3738	Anisotropy =	149.3448
6 C	Isotropic =	50.9613	Anisotropy =	170.8805
7 O	Isotropic =	230.1324	Anisotropy =	68.4887
8 C	Isotropic =	149.4894	Anisotropy =	21.2415
9 C	Isotropic =	131.2403	Anisotropy =	23.8882
10 N	Isotropic =	233.6147	Anisotropy =	31.5842
11 C	Isotropic =	4.4276	Anisotropy =	107.0558
12 O	Isotropic =	158.6285	Anisotropy =	142.7081
13 O	Isotropic =	-50.7925	Anisotropy =	598.6988
14 C	Isotropic =	137.6331	Anisotropy =	73.3696
15 H	Isotropic =	24.0936	Anisotropy =	8.2555
16 H	Isotropic =	24.6471	Anisotropy =	5.2553
17 H	Isotropic =	24.6220	Anisotropy =	5.0116
18 H	Isotropic =	24.2198	Anisotropy =	7.8065
19 H	Isotropic =	27.4143	Anisotropy =	14.2111

20	H	Isotropic =	29.6176	Anisotropy =	5.1628
21	H	Isotropic =	28.8063	Anisotropy =	6.3250
22	H	Isotropic =	28.5708	Anisotropy =	5.4153
23	H	Isotropic =	30.7645	Anisotropy =	12.7059
24	H	Isotropic =	30.8708	Anisotropy =	16.4149
25	H	Isotropic =	27.9863	Anisotropy =	8.1704
26	H	Isotropic =	28.1002	Anisotropy =	8.7754
27	H	Isotropic =	28.0194	Anisotropy =	9.0850

Conformer_15

C	-0.017353528746	1.293437404841	-0.593861812370
C	0.198983595649	2.674048063975	-0.596692699078
C	-0.169838290158	3.467582368743	0.480288299733
C	-0.768371329771	2.882320814828	1.593729862414
C	-0.995999153614	1.510099836931	1.619216897910
C	-0.619838366632	0.729479315588	0.529841030505
O	-1.116667646517	3.698769070822	2.628682480370
C	0.425689374944	0.441376249297	-1.757940545090
C	1.918662961938	0.086239807552	-1.711806277232
N	2.260538495029	-0.730911493623	-2.873951379853
C	2.255888341423	-0.660166597654	-0.426842162754
O	1.574624301609	-1.796682369396	-0.294258737652
O	3.044503795730	-0.258353678233	0.398139025402
C	1.795398507162	-2.533539492889	0.916772759956
H	0.661128629700	3.140923342313	-1.463302366747
H	-0.001774880284	4.539981614972	0.466297672299
H	-1.468647391397	1.052248008744	2.484857892813
H	-0.807692238986	-0.341121018606	0.559670603641
H	-1.519848612433	3.174360831115	3.329667095628
H	0.250472280700	0.975999140402	-2.697786358992
H	-0.151643918211	-0.486785026293	-1.794906595071
H	2.498292300027	1.016743633123	-1.659639821517
H	3.263776590437	-0.884925855179	-2.911555427171
H	2.019508600587	-0.216836503890	-3.716264832598
H	2.838676639147	-2.846546740421	0.989949706577
H	1.532479608093	-1.928085131501	1.786608257906
H	1.146151334573	-3.405255595561	0.854787430971

SCF Done: E(RwB97X) = -669.361098656

Zero-point correction=	0.224042
Thermal correction to Energy=	0.237822
Thermal correction to Enthalpy=	0.238766
Thermal correction to Gibbs Free Energy=	0.182684

Sum of electronic and zero-point Energies=	-669.137057
Sum of electronic and thermal Energies=	-669.123277
Sum of electronic and thermal Enthalpies=	-669.122333
Sum of electronic and thermal Free Energies=	-669.178415

1 C	Isotropic =	54.6792	Anisotropy =	189.4847
2 C	Isotropic =	52.3157	Anisotropy =	177.1160
3 C	Isotropic =	70.9510	Anisotropy =	151.7017
4 C	Isotropic =	28.6597	Anisotropy =	146.6631
5 C	Isotropic =	72.5845	Anisotropy =	140.5234
6 C	Isotropic =	54.1640	Anisotropy =	172.0411
7 O	Isotropic =	229.2571	Anisotropy =	67.2680
8 C	Isotropic =	149.0348	Anisotropy =	31.4684
9 C	Isotropic =	126.7161	Anisotropy =	8.9163
10 N	Isotropic =	225.2397	Anisotropy =	46.8485
11 C	Isotropic =	8.0387	Anisotropy =	114.5588
12 O	Isotropic =	156.3741	Anisotropy =	156.2033
13 O	Isotropic =	-80.2733	Anisotropy =	576.8873
14 C	Isotropic =	137.9656	Anisotropy =	71.9511
15 H	Isotropic =	24.1045	Anisotropy =	7.8905
16 H	Isotropic =	24.5339	Anisotropy =	4.8966
17 H	Isotropic =	24.7888	Anisotropy =	5.5682
18 H	Isotropic =	24.3776	Anisotropy =	7.4094
19 H	Isotropic =	27.4251	Anisotropy =	13.9637
20 H	Isotropic =	29.1042	Anisotropy =	6.3110
21 H	Isotropic =	29.0331	Anisotropy =	4.2147
22 H	Isotropic =	28.2219	Anisotropy =	4.4251
23 H	Isotropic =	30.4285	Anisotropy =	15.2103
24 H	Isotropic =	30.6095	Anisotropy =	13.6889
25 H	Isotropic =	28.1561	Anisotropy =	9.8032
26 H	Isotropic =	28.2135	Anisotropy =	8.0299
27 H	Isotropic =	27.9632	Anisotropy =	8.2721

Conformer_16

C	-0.027073701160	1.263670741010	-0.547258183925
C	0.165625899676	2.640888435600	-0.435101406183
C	-0.260550502074	3.343402018456	0.686053372440
C	-0.893220531050	2.664634790980	1.724713940256
C	-1.098131049465	1.291235444038	1.634050274484
C	-0.665710870900	0.605075181991	0.505666988450
O	-1.335222693259	3.299874854504	2.847274883607
C	0.476050125450	0.509524957384	-1.753768560280
C	1.970286911203	0.165985548890	-1.671846389437
N	2.369240076627	-0.558350960596	-2.876531931042

C	2.264468497835	-0.671110575604	-0.433008574789
O	1.595154437614	-1.822176705988	-0.414794255857
O	3.011613229399	-0.323054680784	0.452795713018
C	1.773808212770	-2.643916184633	0.747622387911
H	0.653990734459	3.181678514065	-1.242214758552
H	-0.104682537367	4.417636617253	0.752388024389
H	-1.597599145038	0.770834232895	2.445437616840
H	-0.836418789096	-0.467042862372	0.443082150605
H	-1.132708325849	4.240133479611	2.785518042047
H	0.333548730545	1.113871998103	-2.656109720254
H	-0.087168243381	-0.418501146642	-1.887125279200
H	2.535464349944	1.095498317440	-1.526521031498
H	3.375111572694	-0.698929184679	-2.884478731764
H	2.155217823772	0.014671465341	-3.687514736769
H	1.139450807896	-3.515238769358	0.593871068643
H	2.817078979050	-2.950837114061	0.843173296296
H	1.465875999705	-2.106758412843	1.647025800562

SCF Done: E(RwB97X) = -669.361048342

Zero-point correction=	0.223941
Thermal correction to Energy=	0.237748
Thermal correction to Enthalpy=	0.238693
Thermal correction to Gibbs Free Energy=	0.182485
Sum of electronic and zero-point Energies=	-669.137108
Sum of electronic and thermal Energies=	-669.123300
Sum of electronic and thermal Enthalpies=	-669.122356
Sum of electronic and thermal Free Energies=	-669.178563

1 C	Isotropic =	54.7281	Anisotropy =	189.5013
2 C	Isotropic =	52.9167	Anisotropy =	175.6674
3 C	Isotropic =	71.8491	Anisotropy =	141.0508
4 C	Isotropic =	28.6692	Anisotropy =	146.6660
5 C	Isotropic =	71.6611	Anisotropy =	151.1979
6 C	Isotropic =	53.4889	Anisotropy =	173.5232
7 O	Isotropic =	229.4912	Anisotropy =	67.7084
8 C	Isotropic =	149.0613	Anisotropy =	31.4843
9 C	Isotropic =	126.6760	Anisotropy =	8.7555
10 N	Isotropic =	225.2284	Anisotropy =	46.8926
11 C	Isotropic =	8.0384	Anisotropy =	114.5573
12 O	Isotropic =	156.2947	Anisotropy =	156.4590
13 O	Isotropic =	-80.3149	Anisotropy =	576.9023
14 C	Isotropic =	137.9522	Anisotropy =	71.9507
15 H	Isotropic =	24.1706	Anisotropy =	7.9526
16 H	Isotropic =	24.6706	Anisotropy =	4.9895
17 H	Isotropic =	24.6203	Anisotropy =	5.5045

18	H	Isotropic =	24.3103	Anisotropy =	7.3550
19	H	Isotropic =	27.4097	Anisotropy =	14.3266
20	H	Isotropic =	29.1080	Anisotropy =	6.2798
21	H	Isotropic =	29.0360	Anisotropy =	4.2569
22	H	Isotropic =	28.2332	Anisotropy =	4.4559
23	H	Isotropic =	30.4297	Anisotropy =	15.2112
24	H	Isotropic =	30.6123	Anisotropy =	13.6663
25	H	Isotropic =	27.9533	Anisotropy =	8.2851
26	H	Isotropic =	28.1504	Anisotropy =	9.8182
27	H	Isotropic =	28.1973	Anisotropy =	7.9932

Conformer_18

C	-0.158926400314	1.264147472385	-0.052159490580
C	0.100619369915	2.621624297229	-0.231645762853
C	-0.506019069225	3.588173622477	0.566157717322
C	-1.390154772250	3.198874332722	1.566785693646
C	-1.667348250959	1.847522149870	1.762337255554
C	-1.053718238199	0.898114810517	0.957752409851
O	-2.015110532999	4.098609180227	2.379159302537
C	0.521815957734	0.211360894047	-0.893638225524
C	1.722933537676	-0.414262677548	-0.181502370775
N	2.770799828024	0.580643533023	0.042549911235
C	2.271518177223	-1.588478432540	-0.977060750458
O	3.505982737538	-1.912262800291	-0.587229764304
O	1.663783278992	-2.197904707036	-1.824938319333
C	4.110203318054	-3.037564671265	-1.244569359868
H	0.787330186916	2.937821279519	-1.012916607946
H	-0.292592451561	4.642585374359	0.408158378208
H	-2.364403459516	1.552661170812	2.540712759253
H	-1.281304303523	-0.153588117090	1.115368138868
H	-1.741325691777	4.991236900603	2.140139541334
H	0.863239695489	0.648682964950	-1.837569532646
H	-0.187459811823	-0.583148918919	-1.136835904985
H	1.366537638918	-0.862991644684	0.761608599606
H	2.408097282888	1.313169779604	0.645425965744
H	3.551152872896	0.160950299565	0.536206645727
H	3.515899567255	-3.938469636895	-1.081980046168
H	4.205439727227	-2.844687275608	-2.314634936842
H	5.094609805401	-3.148119180033	-0.793481246604

SCF Done: E(RwB97X) = -669.362112766

Zero-point correction=	0.224014
Thermal correction to Energy=	0.237781

Thermal correction to Enthalpy=	0.238725
Thermal correction to Gibbs Free Energy=	0.181894
Sum of electronic and zero-point Energies=	-669.138099
Sum of electronic and thermal Energies=	-669.124332
Sum of electronic and thermal Enthalpies=	-669.123388
Sum of electronic and thermal Free Energies=	-669.180219

1 C	Isotropic =	53.3617	Anisotropy =	190.8262
2 C	Isotropic =	52.2210	Anisotropy =	171.1755
3 C	Isotropic =	72.6940	Anisotropy =	139.4278
4 C	Isotropic =	28.6727	Anisotropy =	146.2874
5 C	Isotropic =	70.7310	Anisotropy =	152.3045
6 C	Isotropic =	52.8962	Anisotropy =	177.5172
7 O	Isotropic =	229.6793	Anisotropy =	67.2000
8 C	Isotropic =	151.4603	Anisotropy =	19.6138
9 C	Isotropic =	133.1502	Anisotropy =	19.4506
10 N	Isotropic =	232.1258	Anisotropy =	30.0226
11 C	Isotropic =	9.5082	Anisotropy =	103.4320
12 O	Isotropic =	156.0362	Anisotropy =	153.0819
13 O	Isotropic =	-53.2990	Anisotropy =	582.9906
14 C	Isotropic =	137.4670	Anisotropy =	73.3796
15 H	Isotropic =	24.2403	Anisotropy =	7.8282
16 H	Isotropic =	24.7046	Anisotropy =	5.1648
17 H	Isotropic =	24.4880	Anisotropy =	5.0735
18 H	Isotropic =	24.1224	Anisotropy =	8.2498
19 H	Isotropic =	27.3696	Anisotropy =	14.1192
20 H	Isotropic =	29.4773	Anisotropy =	5.4776
21 H	Isotropic =	28.5590	Anisotropy =	6.5858
22 H	Isotropic =	28.2202	Anisotropy =	5.7883
23 H	Isotropic =	31.0931	Anisotropy =	13.1683
24 H	Isotropic =	30.3126	Anisotropy =	15.3468
25 H	Isotropic =	28.0280	Anisotropy =	8.9887
26 H	Isotropic =	28.0648	Anisotropy =	8.9394
27 H	Isotropic =	28.0182	Anisotropy =	8.3068

Conformer_19

C	0.384693966302	1.164569731569	0.884837189636
C	-0.971991850067	0.920537653157	1.104060276394
C	-1.864565369372	1.956955625527	1.351105966248
C	-1.403263750121	3.269099858664	1.380839128990
C	-0.053351321850	3.537185327168	1.165410605455
C	0.824912267839	2.488428331570	0.919336404045
O	-2.310539849891	4.256364182292	1.628643669271
C	1.342910032491	0.041952709705	0.577718505655

C	1.586776930495	-0.118687398327	-0.941343914316
N	0.408832525426	-0.472155255638	-1.724848381915
C	2.685641725561	-1.146089360372	-1.135483494386
O	2.215410791479	-2.393653216244	-1.111149016765
O	3.858608477972	-0.877052606011	-1.252936886407
C	3.182500475410	-3.446967236645	-1.246502359829
H	-1.340890715989	-0.102044158402	1.088407566975
H	-2.917356217068	1.756798290084	1.524373205024
H	0.309429715209	4.562037673567	1.194251011864
H	1.877130313573	2.708365412501	0.755139682817
H	-1.864741331498	5.110849772954	1.624230126547
H	0.949742175975	-0.902374189036	0.970145362009
H	2.304185231420	0.230520977887	1.068551716627
H	1.985031791529	0.822701301249	-1.329143742046
H	-0.281944849407	0.267428400106	-1.639862022586
H	-0.018350105843	-1.314755880846	-1.351074882356
H	3.732861813948	-3.340923194266	-2.182675829773
H	3.876889638070	-3.434897145267	-0.404289575222
H	2.611837488406	-4.373995606948	-1.249340311953

SCF Done: E(RwB97X) = -669.362674934

Zero-point correction=	0.223827
Thermal correction to Energy=	0.237731
Thermal correction to Enthalpy=	0.238675
Thermal correction to Gibbs Free Energy=	0.181782
Sum of electronic and zero-point Energies=	-669.138848
Sum of electronic and thermal Energies=	-669.124944
Sum of electronic and thermal Enthalpies=	-669.124000
Sum of electronic and thermal Free Energies=	-669.180893

1 C	Isotropic =	54.2170	Anisotropy =	188.9758
2 C	Isotropic =	51.2938	Anisotropy =	172.1695
3 C	Isotropic =	72.2175	Anisotropy =	149.8196
4 C	Isotropic =	28.6510	Anisotropy =	146.3742
5 C	Isotropic =	71.5682	Anisotropy =	141.2842
6 C	Isotropic =	53.3223	Anisotropy =	176.2280
7 O	Isotropic =	229.5727	Anisotropy =	67.7943
8 C	Isotropic =	146.3388	Anisotropy =	18.6346
9 C	Isotropic =	128.6745	Anisotropy =	17.8646
10 N	Isotropic =	234.7768	Anisotropy =	38.4141
11 C	Isotropic =	8.1948	Anisotropy =	109.3545
12 O	Isotropic =	158.2229	Anisotropy =	151.5750
13 O	Isotropic =	-56.7008	Anisotropy =	548.2178
14 C	Isotropic =	137.4815	Anisotropy =	73.6002
15 H	Isotropic =	24.1705	Anisotropy =	7.7389

16	H	Isotropic =	24.5681	Anisotropy =	5.1590
17	H	Isotropic =	24.6366	Anisotropy =	5.1952
18	H	Isotropic =	24.1898	Anisotropy =	8.1367
19	H	Isotropic =	27.3716	Anisotropy =	14.2751
20	H	Isotropic =	29.4976	Anisotropy =	5.1548
21	H	Isotropic =	28.8786	Anisotropy =	5.6967
22	H	Isotropic =	28.6870	Anisotropy =	6.0561
23	H	Isotropic =	30.9056	Anisotropy =	12.6583
24	H	Isotropic =	31.0324	Anisotropy =	12.3213
25	H	Isotropic =	28.0018	Anisotropy =	9.1923
26	H	Isotropic =	28.0980	Anisotropy =	8.8843
27	H	Isotropic =	27.9499	Anisotropy =	8.3003

Conformer_2

C	0.587966122418	1.669298260463	-0.496965882032
C	1.116359994882	1.830914816233	0.787302698477
C	0.335282333316	2.285087057897	1.841322577082
C	-1.006045480858	2.588730375452	1.623355312784
C	-1.554222825999	2.441447045362	0.352694830954
C	-0.756734257333	1.984869610191	-0.691848465665
O	-1.735762088910	3.032930745976	2.685825357791
C	1.439543645645	1.145563659748	-1.629378419047
C	1.444615917506	-0.392455836364	-1.739536966181
N	0.115530811619	-0.898116808571	-2.027791000351
C	2.065392355868	-1.019436026981	-0.492176341586
O	3.338861202408	-0.647829144870	-0.339815055600
O	1.493861496358	-1.764481725790	0.267840367837
C	4.017433796389	-1.149553287650	0.821665783664
H	2.165578697764	1.608251960314	0.969650270569
H	0.756347060645	2.412794920561	2.833777734737
H	-2.599260192273	2.686455642889	0.178096371214
H	-1.192266514257	1.879389847606	-1.682217172216
H	-2.640224283127	3.209351242998	2.403403789251
H	2.469244913995	1.491415447064	-1.511051922381
H	1.068361765843	1.533407334402	-2.581780114782
H	2.102594604954	-0.656965529959	-2.573927422965
H	-0.501493076510	-0.727315872421	-1.238760578228
H	0.145424660198	-1.904968141158	-2.149362394647
H	4.090774609148	-2.238077078507	0.781307946821
H	5.011171252819	-0.705748948891	0.798205830199
H	3.491763477491	-0.850259565993	1.730462864304

SCF Done: E(RwB97X) = -669.365245414

Zero-point correction=	0.224365
Thermal correction to Energy=	0.237995
Thermal correction to Enthalpy=	0.238939
Thermal correction to Gibbs Free Energy=	0.183099
Sum of electronic and zero-point Energies=	-669.140880
Sum of electronic and thermal Energies=	-669.127251
Sum of electronic and thermal Enthalpies=	-669.126307
Sum of electronic and thermal Free Energies=	-669.182147

1 C	Isotropic =	56.1904	Anisotropy =	188.4734
2 C	Isotropic =	53.4189	Anisotropy =	175.5580
3 C	Isotropic =	71.1320	Anisotropy =	151.8340
4 C	Isotropic =	28.4308	Anisotropy =	147.1563
5 C	Isotropic =	72.7203	Anisotropy =	140.0894
6 C	Isotropic =	51.8273	Anisotropy =	173.5850
7 O	Isotropic =	229.4041	Anisotropy =	67.2006
8 C	Isotropic =	150.9585	Anisotropy =	13.2084
9 C	Isotropic =	134.6385	Anisotropy =	34.9019
10 N	Isotropic =	231.8128	Anisotropy =	24.7116
11 C	Isotropic =	5.2609	Anisotropy =	108.9633
12 O	Isotropic =	158.1075	Anisotropy =	147.8369
13 O	Isotropic =	-65.6243	Anisotropy =	619.3839
14 C	Isotropic =	138.0452	Anisotropy =	72.1701
15 H	Isotropic =	24.4514	Anisotropy =	7.7243
16 H	Isotropic =	24.5895	Anisotropy =	5.6273
17 H	Isotropic =	24.7096	Anisotropy =	5.0331
18 H	Isotropic =	24.2119	Anisotropy =	7.8740
19 H	Isotropic =	27.3497	Anisotropy =	14.3760
20 H	Isotropic =	28.5665	Anisotropy =	6.4322
21 H	Isotropic =	29.0073	Anisotropy =	7.6602
22 H	Isotropic =	28.2485	Anisotropy =	6.8729
23 H	Isotropic =	31.0075	Anisotropy =	10.3740
24 H	Isotropic =	30.6499	Anisotropy =	16.3451
25 H	Isotropic =	28.0980	Anisotropy =	9.6860
26 H	Isotropic =	27.9571	Anisotropy =	8.3345
27 H	Isotropic =	27.9885	Anisotropy =	8.1004

Conformer_20

C	-0.011261777432	0.919961591643	0.669194534013
C	-1.303870978342	1.119748210132	0.181931199637
C	-2.013530588666	2.281436898897	0.462706332183
C	-1.428428126598	3.272099587139	1.244508088175
C	-0.139052992189	3.095191057370	1.741984554451
C	0.555722745746	1.927157141506	1.451385298236

O	-2.158228946535	4.395461257138	1.498535887256
C	0.769042326141	-0.324325436274	0.328599307644
C	1.761629222025	-0.091142238502	-0.836612282942
N	1.150924518804	0.306628604191	-2.095899311225
C	2.533980591205	-1.377524674621	-1.053100015377
O	3.555364352769	-1.491488091825	-0.203594640010
O	2.241094350342	-2.222828038862	-1.865649997702
C	4.313717343873	-2.709876923880	-0.275907708996
H	-1.770458865853	0.348634808477	-0.426056583849
H	-3.020004839679	2.425472183827	0.082069300400
H	0.316883664707	3.867757055020	2.356553633175
H	1.560506912391	1.798848458000	1.847237990608
H	-1.643123548161	4.996044702547	2.048862369523
H	0.080708128763	-1.127393001425	0.041719676562
H	1.328614706883	-0.664276330742	1.206246739190
H	2.473647909730	0.682398394861	-0.533876042054
H	0.529003889081	-0.427264671536	-2.423391385538
H	0.581040942987	1.134198438149	-1.949656496215
H	4.792437081296	-2.801475446707	-1.252476311346
H	5.067231380756	-2.633712175494	0.506007999475
H	3.670410595956	-3.573031359030	-0.096322135273

SCF Done: E(RwB97X) = -669.363780063

Zero-point correction=	0.224214
Thermal correction to Energy=	0.237924
Thermal correction to Enthalpy=	0.238868
Thermal correction to Gibbs Free Energy=	0.182701
Sum of electronic and zero-point Energies=	-669.139566
Sum of electronic and thermal Energies=	-669.125856
Sum of electronic and thermal Enthalpies=	-669.124912
Sum of electronic and thermal Free Energies=	-669.181079

1 C	Isotropic =	54.1596	Anisotropy =	189.0206
2 C	Isotropic =	51.0454	Anisotropy =	171.7164
3 C	Isotropic =	72.1535	Anisotropy =	149.8843
4 C	Isotropic =	28.5739	Anisotropy =	146.3253
5 C	Isotropic =	71.4638	Anisotropy =	141.3915
6 C	Isotropic =	53.5331	Anisotropy =	177.3184
7 O	Isotropic =	229.5722	Anisotropy =	67.6190
8 C	Isotropic =	146.2411	Anisotropy =	18.2588
9 C	Isotropic =	131.6100	Anisotropy =	17.7006
10 N	Isotropic =	235.3724	Anisotropy =	33.6886
11 C	Isotropic =	6.8087	Anisotropy =	106.7606
12 O	Isotropic =	153.8051	Anisotropy =	144.6385
13 O	Isotropic =	-46.7928	Anisotropy =	586.3528

14	C	Isotropic =	137.4249	Anisotropy =	73.5455
15	H	Isotropic =	24.1777	Anisotropy =	7.7556
16	H	Isotropic =	24.5632	Anisotropy =	5.0811
17	H	Isotropic =	24.6356	Anisotropy =	5.2524
18	H	Isotropic =	24.1755	Anisotropy =	8.1368
19	H	Isotropic =	27.3855	Anisotropy =	14.2083
20	H	Isotropic =	29.6454	Anisotropy =	4.8828
21	H	Isotropic =	28.8066	Anisotropy =	5.7809
22	H	Isotropic =	28.5242	Anisotropy =	6.2016
23	H	Isotropic =	30.9578	Anisotropy =	13.1984
24	H	Isotropic =	30.9706	Anisotropy =	12.9062
25	H	Isotropic =	28.0386	Anisotropy =	9.1388
26	H	Isotropic =	27.9754	Anisotropy =	8.2021
27	H	Isotropic =	28.0267	Anisotropy =	8.5392

Conformer_21

C	-0.151883423639	1.279130291708	-0.073803871114
C	0.043838258136	2.603565408461	-0.469491400905
C	-0.501819059224	3.663235214297	0.245907441013
C	-1.260536218637	3.406791977315	1.383465068702
C	-1.470619846825	2.093519539093	1.797371811592
C	-0.917751914910	1.046550639171	1.069607758201
O	-1.780838872260	4.473305672306	2.055472734000
C	0.464327090316	0.128392100988	-0.832858582726
C	1.765004962598	-0.361593976349	-0.192816370139
N	2.794439973147	0.675231898687	-0.247408585796
C	2.255884695605	-1.630894358358	-0.871682515717
O	3.542278457421	-1.865518119717	-0.605819476018
O	1.569894230659	-2.375135741766	-1.531445621429
C	4.102331441486	-3.064994261105	-1.163475721469
H	0.631528863475	2.814115333849	-1.359675512196
H	-0.346122802232	4.689319129734	-0.072721179483
H	-2.068753114283	1.891696774497	2.682809210326
H	-1.094227045421	0.025284648196	1.398875582114
H	-2.285445436610	4.159666466145	2.814311214981
H	0.673690396632	0.428959297377	-1.864715384713
H	-0.237892023425	-0.707529247017	-0.869967505346
H	1.541419217059	-0.672284789634	0.842263754566
H	2.480723964335	1.481681095460	0.284386899630
H	3.644149533053	0.348140234055	0.199561397432
H	3.570723621513	-3.942853168747	-0.791981971448
H	4.051748828200	-3.035299463776	-2.253371931735
H	5.140106223831	-3.085382594870	-0.835797242321

SCF Done: E(RwB97X) = -669.362059188

Zero-point correction=	0.224007
Thermal correction to Energy=	0.237767
Thermal correction to Enthalpy=	0.238711
Thermal correction to Gibbs Free Energy=	0.181983
Sum of electronic and zero-point Energies=	-669.138052
Sum of electronic and thermal Energies=	-669.124292
Sum of electronic and thermal Enthalpies=	-669.123348
Sum of electronic and thermal Free Energies=	-669.180076

1	C	Isotropic =	53.3376	Anisotropy =	190.8394
2	C	Isotropic =	51.5360	Anisotropy =	172.7805
3	C	Isotropic =	71.8695	Anisotropy =	150.3351
4	C	Isotropic =	28.7121	Anisotropy =	146.3759
5	C	Isotropic =	71.5983	Anisotropy =	141.3934
6	C	Isotropic =	53.4767	Anisotropy =	175.9036
7	O	Isotropic =	229.7862	Anisotropy =	67.9290
8	C	Isotropic =	151.4444	Anisotropy =	19.5578
9	C	Isotropic =	133.0259	Anisotropy =	19.3587
10	N	Isotropic =	232.1562	Anisotropy =	29.8840
11	C	Isotropic =	9.5181	Anisotropy =	103.4052
12	O	Isotropic =	155.9958	Anisotropy =	153.1556
13	O	Isotropic =	-53.1913	Anisotropy =	582.8221
14	C	Isotropic =	137.4700	Anisotropy =	73.3735
15	H	Isotropic =	24.1670	Anisotropy =	7.8131
16	H	Isotropic =	24.5688	Anisotropy =	5.0545
17	H	Isotropic =	24.6406	Anisotropy =	5.1699
18	H	Isotropic =	24.1862	Anisotropy =	8.3051
19	H	Isotropic =	27.3694	Anisotropy =	14.2359
20	H	Isotropic =	29.4713	Anisotropy =	5.5105
21	H	Isotropic =	28.5555	Anisotropy =	6.5491
22	H	Isotropic =	28.2313	Anisotropy =	5.7782
23	H	Isotropic =	31.0654	Anisotropy =	13.1521
24	H	Isotropic =	30.3015	Anisotropy =	15.3472
25	H	Isotropic =	28.0296	Anisotropy =	8.9802
26	H	Isotropic =	28.0626	Anisotropy =	8.9497
27	H	Isotropic =	28.0165	Anisotropy =	8.3072

Conformer_22

C	0.001429905151	1.383255744696	-0.558650256780
C	-0.966650154327	0.750977799952	0.223057357960
C	-1.522966853047	1.374509656947	1.333586615838
C	-1.109162651843	2.656089579378	1.682861627230

C	-0.144243399256	3.307227419321	0.918541403209
C	0.399617915348	2.669174657493	-0.190212981780
O	-1.680328577020	3.233444747108	2.778568167435
C	0.615114976721	0.703459917715	-1.759808702041
C	2.025219315479	0.177417792754	-1.500195271309
N	2.613743913148	-0.317820789732	-2.750493505966
C	2.014421309672	-1.000971619059	-0.534248038872
O	3.196339295628	-1.126360233183	0.075187395530
O	1.093267016673	-1.761711357996	-0.360841232488
C	3.345068784041	-2.252717512112	0.954398168214
H	-1.292788663489	-0.251048263088	-0.040891842794
H	-2.278469752114	0.875325104750	1.932650590993
H	0.176514571110	4.310912838082	1.187379862673
H	1.147402074077	3.190810456353	-0.783126749599
H	-1.310021166951	4.113887837695	2.906783901394
H	0.683266265166	1.417893776341	-2.587769435370
H	-0.017255822351	-0.124254234621	-2.092186713404
H	2.627131844738	0.974299700303	-1.043484801226
H	3.597946475012	-0.527970991911	-2.614071735468
H	2.575038808969	0.420225804992	-3.447272094868
H	3.194175415669	-3.185644710057	0.408249007003
H	4.364686217287	-2.199550632968	1.331996598370
H	2.634402936508	-2.187162489154	1.780192666116

SCF Done: E(RwB97X) = -669.360764183

Zero-point correction=	0.223933
Thermal correction to Energy=	0.237819
Thermal correction to Enthalpy=	0.238763
Thermal correction to Gibbs Free Energy=	0.181017
Sum of electronic and zero-point Energies=	-669.136831
Sum of electronic and thermal Energies=	-669.122945
Sum of electronic and thermal Enthalpies=	-669.122001
Sum of electronic and thermal Free Energies=	-669.179748

1 C	Isotropic =	54.1690	Anisotropy =	189.3358
2 C	Isotropic =	50.9768	Anisotropy =	174.5855
3 C	Isotropic =	72.4939	Anisotropy =	149.9800
4 C	Isotropic =	28.9876	Anisotropy =	145.9225
5 C	Isotropic =	72.4692	Anisotropy =	140.2279
6 C	Isotropic =	52.6473	Anisotropy =	177.2886
7 O	Isotropic =	229.9095	Anisotropy =	68.1947
8 C	Isotropic =	151.6474	Anisotropy =	33.3813
9 C	Isotropic =	130.5399	Anisotropy =	17.4285
10 N	Isotropic =	225.0337	Anisotropy =	48.5612
11 C	Isotropic =	9.0745	Anisotropy =	104.2928

12	O	Isotropic =	147.3994	Anisotropy =	148.2560
13	O	Isotropic =	-53.8235	Anisotropy =	586.3386
14	C	Isotropic =	137.8014	Anisotropy =	73.2799
15	H	Isotropic =	24.0847	Anisotropy =	7.8424
16	H	Isotropic =	24.6614	Anisotropy =	5.1464
17	H	Isotropic =	24.7394	Anisotropy =	5.0587
18	H	Isotropic =	24.1921	Anisotropy =	8.2654
19	H	Isotropic =	27.4058	Anisotropy =	14.3153
20	H	Isotropic =	29.2819	Anisotropy =	6.2673
21	H	Isotropic =	28.8938	Anisotropy =	4.7972
22	H	Isotropic =	28.1899	Anisotropy =	4.4166
23	H	Isotropic =	30.4097	Anisotropy =	14.4435
24	H	Isotropic =	30.5737	Anisotropy =	13.4751
25	H	Isotropic =	28.1956	Anisotropy =	9.1201
26	H	Isotropic =	28.2092	Anisotropy =	8.5775
27	H	Isotropic =	28.3290	Anisotropy =	8.2750

Conformer_23

C	0.118419727939	0.981620409481	0.761243818044
C	-1.214782092701	1.173701652340	0.404346003869
C	-1.883541761543	2.356815482027	0.707384497728
C	-1.211838010313	3.373385259391	1.377783822888
C	0.121935318476	3.203282470002	1.744106570524
C	0.772279723641	2.017507029781	1.434825188667
O	-1.811518084874	4.553669295182	1.703558950453
C	0.852414067171	-0.283982323460	0.397313108747
C	1.733429847279	-0.105241269214	-0.863185371757
N	1.009269247567	0.247227967835	-2.074941432147
C	2.477617474932	-1.404747775931	-1.098651542331
O	3.572750677407	-1.492401701055	-0.343118343607
O	2.107949280914	-2.279219217390	-1.846457437007
C	4.317300286372	-2.717815365923	-0.436399344061
H	-1.749115129850	0.383372689177	-0.116883589794
H	-2.925622090834	2.486415015406	0.424603688122
H	0.635825904435	4.001211641893	2.271180043335
H	1.812454513352	1.893385498265	1.727344370446
H	-2.725867790603	4.544467025216	1.398885653292
H	0.133674596001	-1.088959755852	0.206559397770
H	1.488699777330	-0.597576768329	1.231492730505
H	2.473662454798	0.674144542041	-0.659215771204
H	0.357701160958	-0.495035033736	-2.314028357957
H	0.457395120130	1.083162430962	-1.908432775525
H	4.703625600256	-2.850995006793	-1.448462267514
H	5.140027592932	-2.616032000253	0.269114602812

H 3.690652588827 -3.568862191061 -0.164066214298

SCF Done: E(RwB97X) = -669.363796937

Zero-point correction= 0.224112
Thermal correction to Energy= 0.237849
Thermal correction to Enthalpy= 0.238793
Thermal correction to Gibbs Free Energy= 0.182506
Sum of electronic and zero-point Energies= -669.139685
Sum of electronic and thermal Energies= -669.125948
Sum of electronic and thermal Enthalpies= -669.125004
Sum of electronic and thermal Free Energies= -669.181291

1 C	Isotropic =	54.1408	Anisotropy =	188.9492
2 C	Isotropic =	51.7671	Anisotropy =	170.1064
3 C	Isotropic =	73.0958	Anisotropy =	139.2385
4 C	Isotropic =	28.5670	Anisotropy =	146.3163
5 C	Isotropic =	70.6423	Anisotropy =	152.2376
6 C	Isotropic =	52.8908	Anisotropy =	178.9454
7 O	Isotropic =	229.4718	Anisotropy =	66.8290
8 C	Isotropic =	146.1662	Anisotropy =	18.1927
9 C	Isotropic =	131.6561	Anisotropy =	17.7569
10 N	Isotropic =	235.4070	Anisotropy =	33.5760
11 C	Isotropic =	6.8163	Anisotropy =	106.7571
12 O	Isotropic =	153.8253	Anisotropy =	144.6506
13 O	Isotropic =	-46.8114	Anisotropy =	586.4768
14 C	Isotropic =	137.4302	Anisotropy =	73.5458
15 H	Isotropic =	24.2509	Anisotropy =	7.7841
16 H	Isotropic =	24.7326	Anisotropy =	5.1231
17 H	Isotropic =	24.5056	Anisotropy =	5.1487
18 H	Isotropic =	24.0998	Anisotropy =	8.1021
19 H	Isotropic =	27.3378	Anisotropy =	14.1806
20 H	Isotropic =	29.6476	Anisotropy =	4.8670
21 H	Isotropic =	28.7990	Anisotropy =	5.8128
22 H	Isotropic =	28.5107	Anisotropy =	6.1973
23 H	Isotropic =	30.9704	Anisotropy =	13.2035
24 H	Isotropic =	30.9766	Anisotropy =	12.9260
25 H	Isotropic =	28.0371	Anisotropy =	9.1415
26 H	Isotropic =	27.9712	Anisotropy =	8.2143
27 H	Isotropic =	28.0249	Anisotropy =	8.5394

Conformer_24

C	0.458446272356	1.263888549868	0.847486554914
C	-0.862342900876	1.037146601881	1.227586929656

C	-1.745200877538	2.090726983542	1.445346282814
C	-1.307245733444	3.400842381691	1.280307748356
C	0.009708018014	3.651383547858	0.902513571738
C	0.876649941026	2.587700875337	0.691667472314
O	-2.125309733785	4.473920001517	1.480037596270
C	1.410798986637	0.122966125431	0.590605631554
C	1.573704866683	-0.198690384209	-0.907567989901
N	0.325272195779	-0.685521680228	-1.467889264809
C	2.767939879875	-1.136604040086	-1.054529409185
O	2.424057968398	-2.422871934988	-0.982511214769
O	3.909630299957	-0.758842756316	-1.186637280711
C	3.492370492912	-3.378080072064	-1.076738663431
H	-1.214393874677	0.017278631045	1.359481372553
H	-2.772000329291	1.892994447007	1.743371194262
H	0.345040117550	4.677023873255	0.782836178890
H	1.904431845773	2.793949690778	0.401562679412
H	-3.001328833092	4.166035632466	1.738000637012
H	1.057455889851	-0.779158388315	1.103174138464
H	2.395162098396	0.367286814586	1.002996906559
H	1.857854575008	0.718364863960	-1.432549537994
H	0.424962780345	-0.856971680258	-2.462946909623
H	0.068160957493	-1.569522944876	-1.039658286669
H	4.016765578361	-3.269925473611	-2.027819042327
H	4.193439611905	-3.249750721363	-0.249862819338
H	3.018769906383	-4.356768943907	-1.020064476010

SCF Done: E(RwB97X) = -669.362993784

Zero-point correction=	0.224464
Thermal correction to Energy=	0.238109
Thermal correction to Enthalpy=	0.239053
Thermal correction to Gibbs Free Energy=	0.182844
Sum of electronic and zero-point Energies=	-669.138530
Sum of electronic and thermal Energies=	-669.124885
Sum of electronic and thermal Enthalpies=	-669.123941
Sum of electronic and thermal Free Energies=	-669.180149

1 C	Isotropic =	52.5940	Anisotropy =	189.6843
2 C	Isotropic =	51.3271	Anisotropy =	170.7155
3 C	Isotropic =	73.4106	Anisotropy =	138.7297
4 C	Isotropic =	29.0199	Anisotropy =	145.6321
5 C	Isotropic =	71.2167	Anisotropy =	151.3290
6 C	Isotropic =	53.2776	Anisotropy =	177.3666
7 O	Isotropic =	229.9464	Anisotropy =	67.5239
8 C	Isotropic =	149.1840	Anisotropy =	22.1677
9 C	Isotropic =	128.7203	Anisotropy =	25.2317

10	N	Isotropic =	231.6422	Anisotropy =	29.4252
11	C	Isotropic =	5.7354	Anisotropy =	112.3360
12	O	Isotropic =	156.6569	Anisotropy =	165.2803
13	O	Isotropic =	-53.8522	Anisotropy =	554.4715
14	C	Isotropic =	137.5253	Anisotropy =	73.4189
15	H	Isotropic =	24.2772	Anisotropy =	7.8635
16	H	Isotropic =	24.7864	Anisotropy =	5.1288
17	H	Isotropic =	24.5425	Anisotropy =	5.0850
18	H	Isotropic =	24.0485	Anisotropy =	8.1269
19	H	Isotropic =	27.3588	Anisotropy =	14.2299
20	H	Isotropic =	29.4692	Anisotropy =	4.8311
21	H	Isotropic =	28.9647	Anisotropy =	5.6047
22	H	Isotropic =	28.6416	Anisotropy =	5.5763
23	H	Isotropic =	30.6980	Anisotropy =	15.9447
24	H	Isotropic =	30.7177	Anisotropy =	11.9972
25	H	Isotropic =	28.0547	Anisotropy =	9.2216
26	H	Isotropic =	28.0840	Anisotropy =	8.7763
27	H	Isotropic =	27.9459	Anisotropy =	8.2469

Conformer_25

C	0.278987839213	1.538200916464	-0.747020474062
C	-1.105615685569	1.457737759220	-0.578738960600
C	-1.730724697004	1.967917875893	0.552314134453
C	-0.968148018272	2.575282691903	1.545486665942
C	0.412844605103	2.674709283168	1.397905540290
C	1.021222687218	2.158966623655	0.258999044372
O	-1.621455910228	3.064644607218	2.637653309729
C	0.956849693201	0.939385009509	-1.954268099795
C	1.350283732090	-0.551812279832	-1.786274510820
N	0.235514125608	-1.471824821638	-1.612542607044
C	2.361944154518	-0.666139686090	-0.659420549328
O	1.844558024745	-1.151505731951	0.467149004379
O	3.513603728448	-0.308919768608	-0.763364368206
C	2.723555667048	-1.196323176247	1.601476063098
H	-1.712484006581	0.993779489734	-1.352188692494
H	-2.807966672722	1.903414597673	0.670594972425
H	1.009326338404	3.158548031462	2.167677751823
H	2.099536018327	2.252223703340	0.152274814897
H	-0.983737012210	3.455022322362	3.245769931264
H	1.859079671426	1.508668725101	-2.198499746414
H	0.292552272933	0.994389042997	-2.822389009732
H	1.890683629316	-0.840540187516	-2.692043581176
H	-0.275569642539	-1.257312092961	-0.761864468371
H	-0.413868339125	-1.350226468464	-2.383644207466

H	3.570120475998	-1.855671170750	1.401822915413
H	3.084431283290	-0.194451094101	1.842345591064
H	2.125776037363	-1.588864201538	2.422189536359

SCF Done: E(RwB97X) = -669.362707686

Zero-point correction=	0.224004
Thermal correction to Energy=	0.237673
Thermal correction to Enthalpy=	0.238617
Thermal correction to Gibbs Free Energy=	0.182682
Sum of electronic and zero-point Energies=	-669.138704
Sum of electronic and thermal Energies=	-669.125034
Sum of electronic and thermal Enthalpies=	-669.124090
Sum of electronic and thermal Free Energies=	-669.180026

1 C	Isotropic = 56.2971	Anisotropy = 190.6637
2 C	Isotropic = 51.3957	Anisotropy = 174.6006
3 C	Isotropic = 72.0123	Anisotropy = 150.3620
4 C	Isotropic = 28.3899	Anisotropy = 147.1837
5 C	Isotropic = 72.2432	Anisotropy = 141.5909
6 C	Isotropic = 53.5037	Anisotropy = 174.0845
7 O	Isotropic = 229.4805	Anisotropy = 67.0454
8 C	Isotropic = 146.8054	Anisotropy = 15.4067
9 C	Isotropic = 131.8498	Anisotropy = 25.5160
10 N	Isotropic = 233.8551	Anisotropy = 53.5416
11 C	Isotropic = 8.8165	Anisotropy = 112.5541
12 O	Isotropic = 147.9159	Anisotropy = 168.8503
13 O	Isotropic = -54.7650	Anisotropy = 561.9654
14 C	Isotropic = 138.2286	Anisotropy = 72.2756
15 H	Isotropic = 24.1716	Anisotropy = 7.6528
16 H	Isotropic = 24.5222	Anisotropy = 4.9722
17 H	Isotropic = 24.7175	Anisotropy = 5.2518
18 H	Isotropic = 24.5070	Anisotropy = 7.3111
19 H	Isotropic = 27.3840	Anisotropy = 14.0689
20 H	Isotropic = 28.7654	Anisotropy = 6.7963
21 H	Isotropic = 29.2417	Anisotropy = 7.4417
22 H	Isotropic = 28.0958	Anisotropy = 6.9537
23 H	Isotropic = 30.6647	Anisotropy = 9.5119
24 H	Isotropic = 31.1189	Anisotropy = 15.3423
25 H	Isotropic = 28.2458	Anisotropy = 10.1442
26 H	Isotropic = 28.3724	Anisotropy = 7.4913
27 H	Isotropic = 28.4595	Anisotropy = 8.3162

Conformer_26

C	0.353783837317	1.574377395371	-0.705085293085
C	-1.016824323054	1.549533735652	-0.447012848215
C	-1.545832820908	2.093532249454	0.719624771228
C	-0.696443350519	2.678578165249	1.653651488258
C	0.674746265977	2.723297527778	1.414083522627
C	1.184779680510	2.175063290246	0.245286252944
O	-1.156895072898	3.229180214155	2.812909534448
C	0.930763794083	0.938405926404	-1.945260674735
C	1.264541372241	-0.568609356773	-1.788067391843
N	0.118757423185	-1.436469331856	-1.556804778999
C	2.321601351080	-0.724626001586	-0.708872382075
O	1.834487890906	-1.177772202958	0.444341440029
O	3.482754614313	-0.423298508981	-0.868716786900
C	2.760690558146	-1.255217398866	1.538690930330
H	-1.692100886583	1.104232388289	-1.173190244488
H	-2.617732022893	2.066449219083	0.901123728810
H	1.329563042969	3.191994634728	2.142155612757
H	2.256343633396	2.223828264936	0.065503445073
H	-2.115217324953	3.135095891961	2.854238216878
H	1.842461781825	1.464262814610	-2.245318526883
H	0.220682719583	1.019159002438	-2.774234811789
H	1.747754322141	-0.884588636221	-2.716736284862
H	-0.341549585744	-1.195510572306	-0.684483868042
H	-0.559822473463	-1.288406232040	-2.297528815418
H	3.566991805574	-1.953515335522	1.307341197065
H	3.176644207311	-0.269164026687	1.754766982829
H	2.183169560459	-1.614813116555	2.388495584059

SCF Done: E(RwB97X) = -669.362742762

Zero-point correction=	0.224086
Thermal correction to Energy=	0.237728
Thermal correction to Enthalpy=	0.238672
Thermal correction to Gibbs Free Energy=	0.182982
Sum of electronic and zero-point Energies=	-669.138656
Sum of electronic and thermal Energies=	-669.125015
Sum of electronic and thermal Enthalpies=	-669.124071
Sum of electronic and thermal Free Energies=	-669.179761

1 C	Isotropic =	56.3149	Anisotropy =	190.7774
2 C	Isotropic =	52.1950	Anisotropy =	173.3340
3 C	Isotropic =	72.8442	Anisotropy =	139.6461
4 C	Isotropic =	28.3789	Anisotropy =	147.3436
5 C	Isotropic =	71.3803	Anisotropy =	152.3081
6 C	Isotropic =	52.7893	Anisotropy =	175.1548
7 O	Isotropic =	229.4468	Anisotropy =	66.7033

8	C	Isotropic =	146.7701	Anisotropy =	15.3878
9	C	Isotropic =	131.8728	Anisotropy =	25.5634
10	N	Isotropic =	233.7774	Anisotropy =	53.7724
11	C	Isotropic =	8.8977	Anisotropy =	112.5250
12	O	Isotropic =	148.0863	Anisotropy =	168.6174
13	O	Isotropic =	-54.8630	Anisotropy =	562.1349
14	C	Isotropic =	138.2232	Anisotropy =	72.2951
15	H	Isotropic =	24.2413	Anisotropy =	7.7001
16	H	Isotropic =	24.6568	Anisotropy =	5.0903
17	H	Isotropic =	24.5543	Anisotropy =	5.1393
18	H	Isotropic =	24.4432	Anisotropy =	7.2348
19	H	Isotropic =	27.3627	Anisotropy =	14.2351
20	H	Isotropic =	28.7656	Anisotropy =	6.8567
21	H	Isotropic =	29.2530	Anisotropy =	7.3999
22	H	Isotropic =	28.0983	Anisotropy =	6.9737
23	H	Isotropic =	30.6356	Anisotropy =	9.6109
24	H	Isotropic =	31.1338	Anisotropy =	15.3297
25	H	Isotropic =	28.2499	Anisotropy =	10.1670
26	H	Isotropic =	28.3853	Anisotropy =	7.4206
27	H	Isotropic =	28.4702	Anisotropy =	8.3113

Conformer_27

C	0.586297168075	1.368296183966	0.804314154104
C	-0.643371589238	1.116538216549	1.409327259463
C	-1.555408015248	2.140246302893	1.651590005168
C	-1.240168572556	3.443754394816	1.282870629056
C	-0.016274546550	3.718667969774	0.676257575644
C	0.880783209892	2.686137641614	0.442815542697
O	-2.090683655527	4.488220227011	1.495320451106
C	1.556566070446	0.253472631917	0.506844212541
C	1.466294587501	-0.222338737667	-0.962183368480
N	0.182455817590	-0.794216934639	-1.350897447645
C	2.588555107867	-1.213170881336	-1.206374022849
O	2.261007237300	-2.446781339212	-0.820279729441
O	3.672230359060	-0.919774786375	-1.655385378855
C	3.270673600369	-3.456836463409	-0.973351940198
H	-0.898067310733	0.102027105139	1.705536800908
H	-2.508187039605	1.924555098510	2.128942885005
H	0.223640851435	4.739799178901	0.396373983199
H	1.834874119454	2.911018963423	-0.028199574890
H	-2.892978079219	4.167537043276	1.922366106876
H	1.356541829549	-0.600404436015	1.163509592049
H	2.580452611493	0.590510331816	0.703579902534
H	1.672159829334	0.629778255602	-1.615393487851

H	-0.539882662649	-0.086879764643	-1.254693968610
H	-0.066117029074	-1.552440611204	-0.721991454237
H	3.580360015531	-3.530959069000	-2.016999005650
H	4.133869232791	-3.228789296987	-0.345294915749
H	2.808276852713	-4.388467224719	-0.651904805894

SCF Done: E(RwB97X) = -669.362688019

Zero-point correction=	0.223810
Thermal correction to Energy=	0.237723
Thermal correction to Enthalpy=	0.238667
Thermal correction to Gibbs Free Energy=	0.181645
Sum of electronic and zero-point Energies=	-669.138878
Sum of electronic and thermal Energies=	-669.124965
Sum of electronic and thermal Enthalpies=	-669.124021
Sum of electronic and thermal Free Energies=	-669.181043

1 C	Isotropic = 54.1793	Anisotropy = 188.8642
2 C	Isotropic = 51.9616	Anisotropy = 170.4513
3 C	Isotropic = 73.1842	Anisotropy = 139.2301
4 C	Isotropic = 28.6692	Anisotropy = 146.2253
5 C	Isotropic = 70.7305	Anisotropy = 152.2752
6 C	Isotropic = 52.7113	Anisotropy = 178.1039
7 O	Isotropic = 229.4598	Anisotropy = 67.0374
8 C	Isotropic = 146.2980	Anisotropy = 18.5979
9 C	Isotropic = 128.7359	Anisotropy = 18.0350
10 N	Isotropic = 234.8130	Anisotropy = 38.3426
11 C	Isotropic = 8.1849	Anisotropy = 109.3569
12 O	Isotropic = 158.2328	Anisotropy = 151.5094
13 O	Isotropic = -56.6904	Anisotropy = 548.2984
14 C	Isotropic = 137.4668	Anisotropy = 73.6312
15 H	Isotropic = 24.2450	Anisotropy = 7.7536
16 H	Isotropic = 24.7459	Anisotropy = 5.2006
17 H	Isotropic = 24.5228	Anisotropy = 5.0698
18 H	Isotropic = 24.1116	Anisotropy = 8.0999
19 H	Isotropic = 27.3159	Anisotropy = 14.1813
20 H	Isotropic = 29.5005	Anisotropy = 5.0968
21 H	Isotropic = 28.8644	Anisotropy = 5.6999
22 H	Isotropic = 28.6600	Anisotropy = 6.0654
23 H	Isotropic = 30.9273	Anisotropy = 12.6350
24 H	Isotropic = 31.0485	Anisotropy = 12.3157
25 H	Isotropic = 28.0039	Anisotropy = 9.1969
26 H	Isotropic = 28.0982	Anisotropy = 8.8798
27 H	Isotropic = 27.9509	Anisotropy = 8.2910

Conformer_28

C	-0.032498409539	0.932229016480	0.611718355649
C	0.519646317719	1.939613955631	1.404669233874
C	-0.185784642893	3.100603493969	1.697063309598
C	-1.473130072026	3.269894985165	1.192144725623
C	-2.044359813930	2.278417965265	0.401110343852
C	-1.323045594602	1.124302347596	0.117128022948
O	-2.214093518117	4.385856919175	1.447945842791
C	0.765424894019	-0.306904378954	0.282562494582
C	1.809841358170	-0.044394450097	-0.814124871755
N	1.160201906890	0.348226826082	-2.056870355739
C	2.682004513673	-1.261517157153	-1.068817197030
O	3.180047186352	-1.759319715152	0.064297916968
O	2.940908030530	-1.708646325458	-2.161212327232
C	4.083291640727	-2.867959517465	-0.068583559741
H	1.521929544541	1.816008223982	1.808298963915
H	0.260515145681	3.872764134249	2.319303897849
H	-3.049588832910	2.416461902408	0.014986533280
H	-1.778969053889	0.354525569101	-0.500353185182
H	-1.707453169560	4.987100262231	2.005280096503
H	0.095684173539	-1.103956194409	-0.057218318882
H	1.279389738092	-0.660619910333	1.179216995294
H	2.504902146008	0.724761255983	-0.439031222732
H	1.843903640901	0.413837240119	-2.803344969374
H	0.752651497742	1.270945075342	-1.945557312004
H	4.355754655799	-3.148691431054	0.947273229458
H	3.593146475876	-3.703838288926	-0.570540220957
H	4.972180241209	-2.569501803774	-0.627646421554

SCF Done: E(RwB97X) = -669.362796843

Zero-point correction= 0.223546
Thermal correction to Energy= 0.237494
Thermal correction to Enthalpy= 0.238439
Thermal correction to Gibbs Free Energy= 0.181006
Sum of electronic and zero-point Energies= -669.139251
Sum of electronic and thermal Energies= -669.125302
Sum of electronic and thermal Enthalpies= -669.124358
Sum of electronic and thermal Free Energies= -669.181791

1 C Isotropic = 53.3028 Anisotropy = 190.1458
2 C Isotropic = 53.4832 Anisotropy = 177.5437
3 C Isotropic = 71.5795 Anisotropy = 141.5641
4 C Isotropic = 28.7069 Anisotropy = 145.9722
5 C Isotropic = 71.9991 Anisotropy = 150.0270

6 C	Isotropic =	51.6791	Anisotropy =	171.4265
7 O	Isotropic =	229.9003	Anisotropy =	68.0759
8 C	Isotropic =	149.5937	Anisotropy =	16.1499
9 C	Isotropic =	133.2306	Anisotropy =	19.8926
10 N	Isotropic =	232.0068	Anisotropy =	23.9900
11 C	Isotropic =	8.5717	Anisotropy =	104.0359
12 O	Isotropic =	158.4995	Anisotropy =	147.9411
13 O	Isotropic =	-53.1220	Anisotropy =	592.8103
14 C	Isotropic =	137.4411	Anisotropy =	73.5797
15 H	Isotropic =	24.1050	Anisotropy =	8.3699
16 H	Isotropic =	24.6341	Anisotropy =	5.2058
17 H	Isotropic =	24.5911	Anisotropy =	5.0079
18 H	Isotropic =	24.1815	Anisotropy =	7.6686
19 H	Isotropic =	27.3732	Anisotropy =	14.2453
20 H	Isotropic =	29.4674	Anisotropy =	5.4034
21 H	Isotropic =	28.5084	Anisotropy =	6.7750
22 H	Isotropic =	28.1837	Anisotropy =	6.2025
23 H	Isotropic =	30.4683	Anisotropy =	15.4649
24 H	Isotropic =	31.2879	Anisotropy =	12.2481
25 H	Isotropic =	27.9954	Anisotropy =	8.1220
26 H	Isotropic =	27.9988	Anisotropy =	8.8609
27 H	Isotropic =	28.1153	Anisotropy =	9.2558

Conformer_29

C	-0.043965323697	1.119811853682	0.086686359151
C	-0.580116384078	0.807454998475	1.339397133824
C	-1.273069271946	1.749918856955	2.085215274693
C	-1.441642038822	3.038466017507	1.581920739661
C	-0.917701665859	3.372704602682	0.337805660561
C	-0.224287716400	2.414259704474	-0.396628659727
O	-2.130653503196	3.931442488125	2.347879961082
C	0.741193663288	0.094986165543	-0.691920561474
C	2.193857396796	-0.043139553639	-0.174524962519
N	2.997507199672	1.166222194278	-0.267101398498
C	2.869183741118	-1.141438433819	-0.971809271031
O	2.579954945554	-2.351365842851	-0.491896156430
O	3.553490538487	-0.954917149637	-1.950332236345
C	3.113635581462	-3.471080795355	-1.217283019776
H	-0.456206039739	-0.196185489641	1.739743663601
H	-1.689918748256	1.497912544946	3.055425000158
H	-1.052024323708	4.376612217763	-0.058190062044
H	0.178646586947	2.683846459753	-1.369654201401
H	-2.178391601676	4.778144929460	1.889880116636
H	0.775547695488	0.378127132635	-1.750037841957

H	0.248092506334	-0.880418586693	-0.624929397578
H	2.158797968981	-0.360153306531	0.872027212810
H	3.091271133639	1.442853409602	-1.240413799634
H	2.523014576508	1.925468265174	0.211925365394
H	2.764527538985	-3.459250807906	-2.251241171036
H	4.204678433132	-3.452438871196	-1.194663441538
H	2.742177110985	-4.357043003787	-0.705380306585

SCF Done: E(RwB97X) = -669.363796778

Zero-point correction=	0.224139
Thermal correction to Energy=	0.237862
Thermal correction to Enthalpy=	0.238806
Thermal correction to Gibbs Free Energy=	0.182570
Sum of electronic and zero-point Energies=	-669.139658
Sum of electronic and thermal Energies=	-669.125935
Sum of electronic and thermal Enthalpies=	-669.124991
Sum of electronic and thermal Free Energies=	-669.181226

1 C	Isotropic = 54.1374	Anisotropy = 188.9531
2 C	Isotropic = 52.8910	Anisotropy = 178.9484
3 C	Isotropic = 70.6427	Anisotropy = 152.2382
4 C	Isotropic = 28.5665	Anisotropy = 146.3164
5 C	Isotropic = 73.0952	Anisotropy = 139.2395
6 C	Isotropic = 51.7684	Anisotropy = 170.1016
7 O	Isotropic = 229.4728	Anisotropy = 66.8269
8 C	Isotropic = 146.1646	Anisotropy = 18.1908
9 C	Isotropic = 131.6532	Anisotropy = 17.7720
10 N	Isotropic = 235.4085	Anisotropy = 33.5659
11 C	Isotropic = 6.8171	Anisotropy = 106.7427
12 O	Isotropic = 153.8330	Anisotropy = 144.6762
13 O	Isotropic = -46.8351	Anisotropy = 586.5252
14 C	Isotropic = 137.4265	Anisotropy = 73.5409
15 H	Isotropic = 24.0998	Anisotropy = 8.1025
16 H	Isotropic = 24.5056	Anisotropy = 5.1487
17 H	Isotropic = 24.7327	Anisotropy = 5.1230
18 H	Isotropic = 24.2511	Anisotropy = 7.7836
19 H	Isotropic = 27.3378	Anisotropy = 14.1806
20 H	Isotropic = 29.6476	Anisotropy = 4.8668
21 H	Isotropic = 28.7985	Anisotropy = 5.8128
22 H	Isotropic = 28.5105	Anisotropy = 6.1955
23 H	Isotropic = 30.9710	Anisotropy = 13.2035
24 H	Isotropic = 30.9769	Anisotropy = 12.9242
25 H	Isotropic = 28.0220	Anisotropy = 8.5309
26 H	Isotropic = 28.0398	Anisotropy = 9.1484
27 H	Isotropic = 27.9711	Anisotropy = 8.2120

Conformer_3

C	0.076715564048	1.403376581861	-0.691937458829
C	-0.793405179478	0.778357554867	0.199506900937
C	-1.227221645832	1.417365524965	1.357337924489
C	-0.789603883086	2.708337255345	1.635236358024
C	0.074370863958	3.354971644038	0.754380808417
C	0.498664625060	2.701361249285	-0.394098153107
O	-1.182366258070	3.385946726739	2.751468245414
C	0.586805838367	0.688808597101	-1.919176037973
C	1.974202116684	0.046045033686	-1.739202221125
N	2.360475057281	-0.611798009569	-2.978692044724
C	1.925298307769	-0.916814092917	-0.557239666061
O	2.455812144603	-0.394158094769	0.548233379917
O	1.445695216918	-2.026378842692	-0.608066352096
C	2.348204540797	-1.187353684336	1.740885059678
H	-1.147826750741	-0.228079660592	-0.010210602419
H	-1.907349933650	0.914504008080	2.040642123910
H	0.403848312598	4.365461964700	0.975661022203
H	1.172440279970	3.214730147098	-1.076077668528
H	-1.774284739310	2.830942536734	3.271631432196
H	0.665963953118	1.385316091237	-2.758802602472
H	-0.116823578690	-0.098677614461	-2.212401283803
H	2.705029719770	0.826548782780	-1.511774699794
H	1.736819294072	-1.394083761833	-3.157399566630
H	3.295604602774	-0.998220003393	-2.895905677638
H	1.298094246735	-1.359632187274	1.986655280183
H	2.859291168869	-2.143433479231	1.614473927456
H	2.827346115465	-0.606144267449	2.526771572374

SCF Done: E(RwB97X) = -669.364624381

Zero-point correction=	0.224294
Thermal correction to Energy=	0.237960
Thermal correction to Enthalpy=	0.238904
Thermal correction to Gibbs Free Energy=	0.183147
Sum of electronic and zero-point Energies=	-669.140330
Sum of electronic and thermal Energies=	-669.126665
Sum of electronic and thermal Enthalpies=	-669.125720
Sum of electronic and thermal Free Energies=	-669.181477

1 C	Isotropic =	54.0412	Anisotropy =	191.2750
2 C	Isotropic =	54.1350	Anisotropy =	172.0838
3 C	Isotropic =	72.6359	Anisotropy =	140.4870

4 C	Isotropic =	28.5333	Anisotropy =	146.7297
5 C	Isotropic =	70.9249	Anisotropy =	152.2511
6 C	Isotropic =	52.2295	Anisotropy =	178.0750
7 O	Isotropic =	229.3821	Anisotropy =	67.3690
8 C	Isotropic =	147.7513	Anisotropy =	34.4835
9 C	Isotropic =	131.0639	Anisotropy =	24.0471
10 N	Isotropic =	226.1619	Anisotropy =	50.8249
11 C	Isotropic =	3.5048	Anisotropy =	114.6092
12 O	Isotropic =	145.6260	Anisotropy =	139.3039
13 O	Isotropic =	-43.7018	Anisotropy =	592.1507
14 C	Isotropic =	138.5226	Anisotropy =	72.0290
15 H	Isotropic =	24.5377	Anisotropy =	7.2348
16 H	Isotropic =	24.7705	Anisotropy =	5.2398
17 H	Isotropic =	24.5186	Anisotropy =	4.7521
18 H	Isotropic =	24.0239	Anisotropy =	7.6281
19 H	Isotropic =	27.3829	Anisotropy =	13.9372
20 H	Isotropic =	28.8592	Anisotropy =	6.4125
21 H	Isotropic =	29.3785	Anisotropy =	4.4233
22 H	Isotropic =	28.5174	Anisotropy =	3.8747
23 H	Isotropic =	30.2661	Anisotropy =	11.8107
24 H	Isotropic =	30.4803	Anisotropy =	15.9501
25 H	Isotropic =	28.6979	Anisotropy =	7.0391
26 H	Isotropic =	28.3073	Anisotropy =	9.7589
27 H	Isotropic =	28.6618	Anisotropy =	8.2252

Conformer_30

C	0.308392492394	1.456889882363	-0.721746401161
C	-1.062421975057	1.337491054567	-0.479818158785
C	-1.626671865842	1.749602700218	0.721059872481
C	-0.815473589897	2.295582928717	1.711349217083
C	0.552677281455	2.432329648762	1.491646143426
C	1.099850563822	2.014913573666	0.283511308704
O	-1.409870308934	2.689253142989	2.873600185245
C	0.922089271544	0.962886900291	-2.008157556082
C	1.346804045415	-0.528877011318	-1.976339559917
N	0.258031538956	-1.480446133929	-1.807844929952
C	2.425306593700	-0.707251791512	-0.922136237759
O	1.983109857108	-1.284780092239	0.192919089363
O	3.563333375726	-0.321249007480	-1.065759981925
C	2.928604899524	-1.396748946929	1.267568033398
H	-1.707257162096	0.921046736957	-1.249582441223
H	-2.693908560714	1.655757736450	0.896570819040
H	1.186625052525	2.868717729342	2.259839640139
H	2.168412607262	2.136597224749	0.121598119547

H	-0.742974365857	3.045270124758	3.471429604742
H	1.799682364920	1.566021489476	-2.260773024371
H	0.206623014759	1.069606877707	-2.829540019619
H	1.836555031948	-0.738990423208	-2.931223325865
H	-0.204881276661	-1.339352863488	-0.915270579292
H	-0.437623438954	-1.314534479929	-2.528694986845
H	2.386608878268	-1.860603684349	2.089805666990
H	3.771538496688	-2.022972159413	0.969939276994
H	3.288237177999	-0.408761157216	1.561750225643

SCF Done: E(RwB97X) = -669.362707708

Zero-point correction=	0.224006
Thermal correction to Energy=	0.237674
Thermal correction to Enthalpy=	0.238618
Thermal correction to Gibbs Free Energy=	0.182684
Sum of electronic and zero-point Energies=	-669.138702
Sum of electronic and thermal Energies=	-669.125033
Sum of electronic and thermal Enthalpies=	-669.124089
Sum of electronic and thermal Free Energies=	-669.180024

1 C	Isotropic =	56.2977	Anisotropy =	190.6648
2 C	Isotropic =	51.3956	Anisotropy =	174.5980
3 C	Isotropic =	72.0125	Anisotropy =	150.3608
4 C	Isotropic =	28.3892	Anisotropy =	147.1844
5 C	Isotropic =	72.2436	Anisotropy =	141.5911
6 C	Isotropic =	53.5039	Anisotropy =	174.0900
7 O	Isotropic =	229.4782	Anisotropy =	67.0454
8 C	Isotropic =	146.8035	Anisotropy =	15.4000
9 C	Isotropic =	131.8508	Anisotropy =	25.5180
10 N	Isotropic =	233.8575	Anisotropy =	53.5326
11 C	Isotropic =	8.8149	Anisotropy =	112.5573
12 O	Isotropic =	147.9122	Anisotropy =	168.8501
13 O	Isotropic =	-54.7649	Anisotropy =	561.9538
14 C	Isotropic =	138.2282	Anisotropy =	72.2753
15 H	Isotropic =	24.1716	Anisotropy =	7.6521
16 H	Isotropic =	24.5221	Anisotropy =	4.9721
17 H	Isotropic =	24.7174	Anisotropy =	5.2517
18 H	Isotropic =	24.5070	Anisotropy =	7.3100
19 H	Isotropic =	27.3838	Anisotropy =	14.0685
20 H	Isotropic =	28.7654	Anisotropy =	6.7964
21 H	Isotropic =	29.2418	Anisotropy =	7.4427
22 H	Isotropic =	28.0960	Anisotropy =	6.9537
23 H	Isotropic =	30.6654	Anisotropy =	9.5139
24 H	Isotropic =	31.1188	Anisotropy =	15.3443
25 H	Isotropic =	28.4597	Anisotropy =	8.3161

26 H Isotropic = 28.2457 Anisotropy = 10.1441
 27 H Isotropic = 28.3725 Anisotropy = 7.4905

Conformer_4

C	0.512641854735	1.646856933509	-0.582292404250
C	-0.834581585062	1.907036083990	-0.845740288951
C	-1.693299464986	2.363764350432	0.145701289596
C	-1.209132713125	2.569244792184	1.434407011462
C	0.130090738202	2.319829457546	1.721760311073
C	0.975777474210	1.863503816763	0.716504509859
O	-2.083920724263	3.022640695692	2.376619519793
C	1.431759741197	1.124687969824	-1.661462801024
C	1.500260120009	-0.414410846370	-1.725240560451
N	0.204658896778	-0.980696097667	-2.050692341232
C	2.093651230749	-0.979280460102	-0.435628188225
O	3.345330592058	-0.554212648439	-0.246242955724
O	1.520664040375	-1.722248622479	0.325297298375
C	3.996174260039	-0.994988395722	0.955068636076
H	-1.219359140464	1.756218865495	-1.851218252409
H	-2.737208261949	2.567470149029	-0.071913673247
H	0.511433104412	2.487851042947	2.726154861667
H	2.022433385077	1.684802510190	0.953701096004
H	-1.625530396138	3.124191053941	3.218339195429
H	2.441540765352	1.513840569000	-1.510609372357
H	1.087382112870	1.470868239935	-2.639647560545
H	2.201541898573	-0.676388771472	-2.524395691534
H	-0.450398361831	-0.813018095214	-1.292258951224
H	0.278471050094	-1.988487873035	-2.141823322205
H	4.110371582736	-2.080711042147	0.951745545378
H	4.973402529344	-0.515335852441	0.955012749661
H	3.425345271007	-0.688327825391	1.833654339004

SCF Done: E(RwB97X) = -669.365223246

Zero-point correction=	0.224427
Thermal correction to Energy=	0.238051
Thermal correction to Enthalpy=	0.238995
Thermal correction to Gibbs Free Energy=	0.182957
Sum of electronic and zero-point Energies=	-669.140796
Sum of electronic and thermal Energies=	-669.127172
Sum of electronic and thermal Enthalpies=	-669.126228
Sum of electronic and thermal Free Energies=	-669.182266

1 C Isotropic = 56.1651 Anisotropy = 188.4840

2	C	Isotropic =	51.1636	Anisotropy =	174.9657
3	C	Isotropic =	71.8217	Anisotropy =	150.8115
4	C	Isotropic =	28.4164	Anisotropy =	147.0761
5	C	Isotropic =	72.0251	Anisotropy =	140.9118
6	C	Isotropic =	54.0414	Anisotropy =	174.2247
7	O	Isotropic =	229.5813	Anisotropy =	67.4419
8	C	Isotropic =	150.9572	Anisotropy =	13.2023
9	C	Isotropic =	134.5615	Anisotropy =	34.8421
10	N	Isotropic =	231.8778	Anisotropy =	24.7364
11	C	Isotropic =	5.2642	Anisotropy =	108.9661
12	O	Isotropic =	158.1365	Anisotropy =	147.9291
13	O	Isotropic =	-65.6014	Anisotropy =	619.5122
14	C	Isotropic =	138.0703	Anisotropy =	72.1650
15	H	Isotropic =	24.1415	Anisotropy =	7.8291
16	H	Isotropic =	24.5675	Anisotropy =	4.9236
17	H	Isotropic =	24.7356	Anisotropy =	5.7441
18	H	Isotropic =	24.5226	Anisotropy =	7.8010
19	H	Isotropic =	27.3806	Anisotropy =	14.0938
20	H	Isotropic =	28.5703	Anisotropy =	6.3993
21	H	Isotropic =	29.0015	Anisotropy =	7.6934
22	H	Isotropic =	28.2441	Anisotropy =	6.8565
23	H	Isotropic =	31.0050	Anisotropy =	10.3067
24	H	Isotropic =	30.6484	Anisotropy =	16.3644
25	H	Isotropic =	28.1039	Anisotropy =	9.6656
26	H	Isotropic =	27.9674	Anisotropy =	8.3167
27	H	Isotropic =	28.0027	Anisotropy =	8.1339

Conformer_5

C	-0.028774305300	1.252653089978	-0.566454025266
C	-0.710418451582	0.577877173230	0.448185989342
C	-1.150394382131	1.237596780357	1.589415622373
C	-0.908659241948	2.600404636679	1.732044728035
C	-0.231177430575	3.294893519201	0.732525897173
C	0.201127367263	2.618900861104	-0.402412354511
O	-1.359351914646	3.210207219769	2.865221230338
C	0.480608864758	0.525828807524	-1.787217588936
C	1.972301163631	0.167050619571	-1.711012050754
N	2.359696551452	-0.554770960655	-2.916923585956
C	2.268517243438	-0.598751558041	-0.424646249202
O	1.664430428018	-1.789628562316	-0.409236869577
O	2.963792777066	-0.193309078326	0.477783248200
C	1.842786535638	-2.586387131957	0.770774807375
H	-0.907982107655	-0.486519815029	0.345023894970
H	-1.683894970281	0.705014412588	2.370622653520

H	-0.045723304853	4.361006423808	0.839932955578
H	0.725694664798	3.171843996820	-1.177922467739
H	-1.129984016999	4.145954384799	2.839678313111
H	0.344717618288	1.142719618714	-2.680413977795
H	-0.089672427187	-0.397074505020	-1.936821305578
H	2.561212466018	1.086219168372	-1.651365956949
H	3.351626345863	-0.770063339305	-2.903225072155
H	1.863572118263	-1.439433612729	-2.970928111688
H	1.288325660464	-3.506320731410	0.593025919827
H	2.899816457900	-2.809131843601	0.927235289588
H	1.440906290298	-2.068279574123	1.644009066673

SCF Done: E(RwB97X) = -669.363546143

Zero-point correction=	0.223981
Thermal correction to Energy=	0.237751
Thermal correction to Enthalpy=	0.238695
Thermal correction to Gibbs Free Energy=	0.182274
Sum of electronic and zero-point Energies=	-669.139565
Sum of electronic and thermal Energies=	-669.125795
Sum of electronic and thermal Enthalpies=	-669.124851
Sum of electronic and thermal Free Energies=	-669.181272

1 C	Isotropic =	54.5172	Anisotropy =	189.8804
2 C	Isotropic =	53.3535	Anisotropy =	172.7662
3 C	Isotropic =	71.7588	Anisotropy =	151.1251
4 C	Isotropic =	28.6922	Anisotropy =	146.6419
5 C	Isotropic =	71.7518	Anisotropy =	141.3162
6 C	Isotropic =	52.8927	Anisotropy =	177.1528
7 O	Isotropic =	229.4519	Anisotropy =	67.7099
8 C	Isotropic =	149.0673	Anisotropy =	33.6214
9 C	Isotropic =	127.9899	Anisotropy =	13.5460
10 N	Isotropic =	225.1976	Anisotropy =	49.4067
11 C	Isotropic =	6.9073	Anisotropy =	116.2269
12 O	Isotropic =	160.6569	Anisotropy =	156.7035
13 O	Isotropic =	-70.8229	Anisotropy =	569.3444
14 C	Isotropic =	138.1381	Anisotropy =	72.1740
15 H	Isotropic =	24.3516	Anisotropy =	7.2455
16 H	Isotropic =	24.6372	Anisotropy =	5.4054
17 H	Isotropic =	24.6533	Anisotropy =	5.0162
18 H	Isotropic =	24.1277	Anisotropy =	7.9769
19 H	Isotropic =	27.4085	Anisotropy =	14.3130
20 H	Isotropic =	28.8986	Anisotropy =	6.5257
21 H	Isotropic =	29.2338	Anisotropy =	4.0567
22 H	Isotropic =	28.5499	Anisotropy =	4.5479
23 H	Isotropic =	30.2773	Anisotropy =	15.4688

24	H	Isotropic =	30.4667	Anisotropy =	11.3514
25	H	Isotropic =	27.9882	Anisotropy =	8.3475
26	H	Isotropic =	28.1728	Anisotropy =	9.7823
27	H	Isotropic =	28.2824	Anisotropy =	7.9786

Conformer_6

C	-0.017428799168	1.283145306724	-0.607954599666
C	-0.649115071085	0.700137708229	0.489449329235
C	-1.028262085417	1.457096919196	1.594405811246
C	-0.774088084299	2.824687855726	1.611098783072
C	-0.146024384966	3.428860102975	0.524178303676
C	0.225518256894	2.658687719560	-0.568669910114
O	-1.123579894801	3.618527529582	2.663004314032
C	0.429342648962	0.456039849167	-1.788625942025
C	1.919005295614	0.083284695622	-1.748195935152
N	2.248248706144	-0.727608607528	-2.914133680383
C	2.260013432861	-0.593803688745	-0.423733264492
O	1.643153377557	-1.771715006695	-0.299052291389
O	2.997213743954	-0.136106024757	0.418372483605
C	1.861923362345	-2.486395815640	0.925782512654
H	-0.856550957704	-0.367330470454	0.486250392600
H	-1.523678474368	0.984975967463	2.439378187600
H	0.042410365853	4.497805580419	0.542630245863
H	0.712520936103	3.140021556237	-1.413441446890
H	-1.546682132565	3.082592091819	3.343223146991
H	0.261558625861	1.004226332751	-2.720378284825
H	-0.156962453110	-0.467399600513	-1.841738254823
H	2.519737228608	0.996241975863	-1.778322818279
H	3.237600081956	-0.954615803581	-2.925426291013
H	1.741127993545	-1.607169181177	-2.884364527495
H	2.921817283018	-2.713964876541	1.053227000381
H	1.504443886821	-1.902257889925	1.776353111156
H	1.288937111386	-3.407864225774	0.836883624434

SCF Done: E(RwB97X) = -669.363570247

Zero-point correction=	0.224079
Thermal correction to Energy=	0.237814
Thermal correction to Enthalpy=	0.238758
Thermal correction to Gibbs Free Energy=	0.182673
Sum of electronic and zero-point Energies=	-669.139491
Sum of electronic and thermal Energies=	-669.125756
Sum of electronic and thermal Enthalpies=	-669.124812
Sum of electronic and thermal Free Energies=	-669.180897

1	C	Isotropic =	54.4566	Anisotropy =	189.8638
2	C	Isotropic =	54.0968	Anisotropy =	171.5365
3	C	Isotropic =	72.6604	Anisotropy =	140.4628
4	C	Isotropic =	28.6748	Anisotropy =	146.6428
5	C	Isotropic =	70.8684	Anisotropy =	151.9605
6	C	Isotropic =	52.2679	Anisotropy =	178.2284
7	O	Isotropic =	229.2307	Anisotropy =	67.3173
8	C	Isotropic =	149.0399	Anisotropy =	33.5573
9	C	Isotropic =	127.9558	Anisotropy =	13.7392
10	N	Isotropic =	225.1686	Anisotropy =	49.4590
11	C	Isotropic =	6.8949	Anisotropy =	116.2197
12	O	Isotropic =	160.7336	Anisotropy =	156.4139
13	O	Isotropic =	-70.9454	Anisotropy =	569.7113
14	C	Isotropic =	138.1588	Anisotropy =	72.1546
15	H	Isotropic =	24.4233	Anisotropy =	7.3224
16	H	Isotropic =	24.8058	Anisotropy =	5.4982
17	H	Isotropic =	24.5229	Anisotropy =	4.8966
18	H	Isotropic =	24.0599	Anisotropy =	7.8977
19	H	Isotropic =	27.4186	Anisotropy =	13.9719
20	H	Isotropic =	28.9031	Anisotropy =	6.5647
21	H	Isotropic =	29.2222	Anisotropy =	4.0078
22	H	Isotropic =	28.5514	Anisotropy =	4.4824
23	H	Isotropic =	30.2744	Anisotropy =	15.4738
24	H	Isotropic =	30.4622	Anisotropy =	11.3205
25	H	Isotropic =	28.1746	Anisotropy =	9.7662
26	H	Isotropic =	28.2813	Anisotropy =	8.0304
27	H	Isotropic =	27.9915	Anisotropy =	8.3310

Conformer_7

C	0.323956430692	1.562502919272	-0.721040645626
C	-1.055700379473	1.584929607256	-0.517860613604
C	-1.611313325361	2.143413889494	0.629347838627
C	-0.779741850262	2.692615383383	1.600458861988
C	0.600631254629	2.689617192200	1.415720439267
C	1.137383761905	2.129798739159	0.264564860541
O	-1.265972587272	3.251675265333	2.744928732404
C	0.927272878209	0.915176024700	-1.945155282051
C	1.268624148695	-0.577079577670	-1.751639384800
N	0.068039931318	-1.360837557483	-1.520553811860
C	2.362040889334	-0.696253330081	-0.690540608845
O	1.931754650415	-1.221707524603	0.455328638848
O	3.502077983815	-0.330685121843	-0.869289849196
C	2.890317910798	-1.296065381662	1.521794827223

H	-1.716121071045	1.164307942356	-1.271889049752
H	-2.689976490209	2.154338267727	0.766952988126
H	1.242078421780	3.130891902992	2.172243833569
H	2.216348265913	2.142668793102	0.127891720439
H	-2.227953653871	3.192171356212	2.747422215357
H	1.840783644546	1.442915382487	-2.232546445654
H	0.229744286467	0.979001497613	-2.784605452795
H	1.732358940805	-0.925430366873	-2.679271957806
H	-0.359674905612	-1.104111405417	-0.636122788280
H	0.299622178462	-2.346214865493	-1.453199652450
H	3.735845902242	-1.922450468017	1.232483491079
H	3.243491494245	-0.297196381765	1.785769896250
H	2.362581288836	-1.742392182378	2.362907199003

SCF Done: E(RwB97X) = -669.363833579

Zero-point correction=	0.224313
Thermal correction to Energy=	0.237913
Thermal correction to Enthalpy=	0.238857
Thermal correction to Gibbs Free Energy=	0.183053
Sum of electronic and zero-point Energies=	-669.139521
Sum of electronic and thermal Energies=	-669.125921
Sum of electronic and thermal Enthalpies=	-669.124977
Sum of electronic and thermal Free Energies=	-669.180780

1 C	Isotropic = 56.2034	Anisotropy = 189.7084
2 C	Isotropic = 52.3420	Anisotropy = 173.7386
3 C	Isotropic = 72.6521	Anisotropy = 139.9986
4 C	Isotropic = 28.2823	Anisotropy = 147.2895
5 C	Isotropic = 71.3340	Anisotropy = 152.3927
6 C	Isotropic = 53.0387	Anisotropy = 175.6607
7 O	Isotropic = 229.3185	Anisotropy = 66.7406
8 C	Isotropic = 150.1272	Anisotropy = 11.9331
9 C	Isotropic = 132.7847	Anisotropy = 31.0331
10 N	Isotropic = 230.2128	Anisotropy = 25.0050
11 C	Isotropic = 6.4371	Anisotropy = 114.6016
12 O	Isotropic = 146.0420	Anisotropy = 177.7236
13 O	Isotropic = -53.3219	Anisotropy = 570.0401
14 C	Isotropic = 138.0566	Anisotropy = 72.4908
15 H	Isotropic = 24.2051	Anisotropy = 7.7052
16 H	Isotropic = 24.6694	Anisotropy = 5.0657
17 H	Isotropic = 24.5642	Anisotropy = 5.2380
18 H	Isotropic = 24.4435	Anisotropy = 7.4768
19 H	Isotropic = 27.3676	Anisotropy = 14.2458
20 H	Isotropic = 28.7235	Anisotropy = 7.0171
21 H	Isotropic = 29.0726	Anisotropy = 7.7303

22	H	Isotropic =	28.2702	Anisotropy =	6.9265
23	H	Isotropic =	30.8855	Anisotropy =	9.7544
24	H	Isotropic =	30.5682	Anisotropy =	15.8997
25	H	Isotropic =	28.1840	Anisotropy =	9.9660
26	H	Isotropic =	28.3199	Anisotropy =	7.6063
27	H	Isotropic =	28.3662	Anisotropy =	8.3599

Conformer_8

C	0.178236601898	1.355658495166	-0.669463150058
C	-0.652888006330	0.695077415936	0.233484318837
C	-1.024074872388	1.281716319958	1.439798189237
C	-0.562041763994	2.555296303806	1.755828913530
C	0.263645987450	3.237004398699	0.864750004587
C	0.625667614890	2.635402470409	-0.332439020107
O	-0.893923796421	3.182172403865	2.920417472590
C	0.621582971525	0.696283850715	-1.952270085228
C	2.010434636929	0.036856964743	-1.870765186771
N	2.330162400432	-0.564490468800	-3.157025512431
C	2.010699481986	-0.980179486918	-0.734018414309
O	2.599215166602	-0.513626840273	0.367187664464
O	1.519289781592	-2.082918104929	-0.812906483466
C	2.543064794343	-1.361353760804	1.525352923182
H	-1.025979634647	-0.298034926210	-0.005333468802
H	-1.674481100547	0.751702441338	2.131465515442
H	0.612430656127	4.233785292561	1.116513763637
H	1.269898610373	3.175881889320	-1.0219766666936
H	-1.464710077948	2.607228764993	3.442524843200
H	0.665740556482	1.430925674013	-2.761412440392
H	-0.102331946317	-0.072048172083	-2.246919056425
H	2.758275399968	0.801060693372	-1.643291142631
H	3.264769592386	-0.960470000380	-3.138247752696
H	1.691685033596	-1.333419105020	-3.341268114840
H	1.504758262363	-1.537722724355	1.814544657140
H	3.038450414756	-2.313930876417	1.329236741507
H	3.065623234890	-0.821158912707	2.312831487738

SCF Done: E(RwB97X) = -669.364624405

Zero-point correction=	0.224296
Thermal correction to Energy=	0.237960
Thermal correction to Enthalpy=	0.238905
Thermal correction to Gibbs Free Energy=	0.183151
Sum of electronic and zero-point Energies=	-669.140328
Sum of electronic and thermal Energies=	-669.126664

Sum of electronic and thermal Enthalpies= -669.125720
Sum of electronic and thermal Free Energies= -669.181473

1 C	Isotropic =	54.0400	Anisotropy =	191.2758
2 C	Isotropic =	54.1332	Anisotropy =	172.0820
3 C	Isotropic =	72.6345	Anisotropy =	140.4887
4 C	Isotropic =	28.5330	Anisotropy =	146.7298
5 C	Isotropic =	70.9244	Anisotropy =	152.2525
6 C	Isotropic =	52.2294	Anisotropy =	178.0797
7 O	Isotropic =	229.3838	Anisotropy =	67.3681
8 C	Isotropic =	147.7527	Anisotropy =	34.4782
9 C	Isotropic =	131.0612	Anisotropy =	24.0422
10 N	Isotropic =	226.1611	Anisotropy =	50.8273
11 C	Isotropic =	3.5043	Anisotropy =	114.6109
12 O	Isotropic =	145.6266	Anisotropy =	139.2976
13 O	Isotropic =	-43.6931	Anisotropy =	592.1423
14 C	Isotropic =	138.5238	Anisotropy =	72.0287
15 H	Isotropic =	24.5376	Anisotropy =	7.2351
16 H	Isotropic =	24.7705	Anisotropy =	5.2398
17 H	Isotropic =	24.5186	Anisotropy =	4.7521
18 H	Isotropic =	24.0239	Anisotropy =	7.6282
19 H	Isotropic =	27.3831	Anisotropy =	13.9375
20 H	Isotropic =	28.8593	Anisotropy =	6.4129
21 H	Isotropic =	29.3785	Anisotropy =	4.4231
22 H	Isotropic =	28.5175	Anisotropy =	3.8746
23 H	Isotropic =	30.4803	Anisotropy =	15.9494
24 H	Isotropic =	30.2662	Anisotropy =	11.8105
25 H	Isotropic =	28.6985	Anisotropy =	7.0399
26 H	Isotropic =	28.3068	Anisotropy =	9.7576
27 H	Isotropic =	28.6615	Anisotropy =	8.2264

Conformer_9

C	0.129954784696	1.297184102683	-0.638900652768
C	-0.711062139681	0.553401030785	0.190720177726
C	-1.154401805361	1.053050397163	1.409394165024
C	-0.756773516755	2.322697698959	1.816873430978
C	0.075552722520	3.086163699348	1.001967430489
C	0.510553624608	2.569552744241	-0.212908223380
O	-1.214297320308	2.777094839089	3.018340641962
C	0.651902399360	0.730130389030	-1.936253381225
C	2.066628726482	0.131415508950	-1.834027957242
N	2.463446429752	-0.383143775704	-3.136354886016
C	2.072841624258	-0.945477054777	-0.753828417684
O	2.597186949042	-0.514114340118	0.393218185875

O	1.637656948124	-2.063337964770	-0.910999088664
C	2.538007667041	-1.425711573651	1.501731651633
H	-1.032832580814	-0.437496694277	-0.121154280616
H	-1.809929757051	0.467858115255	2.047046822732
H	0.379405388562	4.081684335760	1.316981592676
H	1.159426183368	3.174587753302	-0.841656821239
H	-0.866248246136	3.660976221934	3.180908161170
H	0.691716797145	1.509412815932	-2.702733667012
H	-0.023115012682	-0.052924028075	-2.300078626633
H	2.767773459404	0.915530128710	-1.536465257619
H	1.870992206695	-1.170135146273	-3.386276665312
H	3.415087696205	-0.734967067531	-3.100970791043
H	3.084951905273	-2.342725397729	1.275441234860
H	3.004629640804	-0.906286913290	2.336875491748
H	1.499145225450	-1.664519824945	1.739509729580

SCF Done: E(RwB97X) = -669.364544392

Zero-point correction=	0.224178
Thermal correction to Energy=	0.237870
Thermal correction to Enthalpy=	0.238814
Thermal correction to Gibbs Free Energy=	0.182883
Sum of electronic and zero-point Energies=	-669.140366
Sum of electronic and thermal Energies=	-669.126674
Sum of electronic and thermal Enthalpies=	-669.125730
Sum of electronic and thermal Free Energies=	-669.181662

1 C	Isotropic =	53.9954	Anisotropy =	191.3011
2 C	Isotropic =	53.4561	Anisotropy =	173.3924
3 C	Isotropic =	71.7914	Anisotropy =	151.5132
4 C	Isotropic =	28.6544	Anisotropy =	146.7902
5 C	Isotropic =	71.7798	Anisotropy =	141.4900
6 C	Isotropic =	52.8322	Anisotropy =	176.9915
7 O	Isotropic =	229.4842	Anisotropy =	67.9293
8 C	Isotropic =	147.7651	Anisotropy =	34.4791
9 C	Isotropic =	131.0037	Anisotropy =	23.8361
10 N	Isotropic =	226.1720	Anisotropy =	50.7897
11 C	Isotropic =	3.4995	Anisotropy =	114.5737
12 O	Isotropic =	145.6768	Anisotropy =	139.1655
13 O	Isotropic =	-43.7070	Anisotropy =	592.1440
14 C	Isotropic =	138.4942	Anisotropy =	72.0664
15 H	Isotropic =	24.4653	Anisotropy =	7.1667
16 H	Isotropic =	24.6412	Anisotropy =	5.0789
17 H	Isotropic =	24.6749	Anisotropy =	4.8226
18 H	Isotropic =	24.0822	Anisotropy =	7.6891
19 H	Isotropic =	27.3600	Anisotropy =	14.3699

20	H	Isotropic =	28.8579	Anisotropy =	6.3671
21	H	Isotropic =	29.3789	Anisotropy =	4.4607
22	H	Isotropic =	28.5242	Anisotropy =	3.9203
23	H	Isotropic =	30.2642	Anisotropy =	11.8413
24	H	Isotropic =	30.4794	Anisotropy =	15.9355
25	H	Isotropic =	28.3056	Anisotropy =	9.7683
26	H	Isotropic =	28.6606	Anisotropy =	8.2288
27	H	Isotropic =	28.6904	Anisotropy =	6.9984

Methyl L-tyrosinate_protonated

Conformer_1

C	-0.378604285970	1.130287641926	0.023948761256
C	-1.521270942634	1.090235607167	0.826676016529
C	-2.368986269170	2.184445186971	0.933134579114
C	-2.080974934192	3.348215014515	0.225832022818
C	-0.950338174448	3.408749874095	-0.585733218375
C	-0.111366767132	2.305401510465	-0.680510946885
C	0.546749009099	-0.061144657364	-0.063709913034
C	1.708581302997	-0.025828835543	0.938036339296
N	1.202579304858	-0.053666596638	2.337732306764
C	2.593305320098	1.201164750988	0.791505890209
O	3.148496680544	1.239212407151	-0.405876928159
O	2.757133026278	2.018107981020	1.664665255889
C	3.990515723096	2.375260498418	-0.690964241534
O	-2.939867312534	4.395785280636	0.354472078199
H	-1.760600418783	0.180613981691	1.372717062342
H	-3.257197558721	2.141829944229	1.555456293735
H	-0.731318247634	4.313263187667	-1.147636593064
H	0.757739632562	2.363057309122	-1.331594414308
H	0.987587110402	-0.134166896579	-1.060059986633
H	-0.008749355215	-0.986870395738	0.111865259715
H	2.326769027217	-0.916448663537	0.810768561253
H	1.967906068645	-0.054761218897	3.016791557846
H	0.606273835341	0.751998395184	2.552573943558
H	0.649509345090	-0.900494494451	2.496226833918
H	3.413190127043	3.298228017477	-0.617406396796
H	4.832931550473	2.402898321744	0.001418767474
H	4.340661233105	2.226188991571	-1.709986774698
H	-2.632654030414	5.133937856707	-0.184242116432

SCF Done: E(RwB97X) = -669.826599547

Zero-point correction=	0.239688
Thermal correction to Energy=	0.253290

Thermal correction to Enthalpy=	0.254234
Thermal correction to Gibbs Free Energy=	0.198630
Sum of electronic and zero-point Energies=	-669.586911
Sum of electronic and thermal Energies=	-669.573309
Sum of electronic and thermal Enthalpies=	-669.572365
Sum of electronic and thermal Free Energies=	-669.627969

1 C	Isotropic =	60.7548	Anisotropy =	180.3326
2 C	Isotropic =	50.9244	Anisotropy =	175.5135
3 C	Isotropic =	70.8897	Anisotropy =	152.6283
4 C	Isotropic =	27.2265	Anisotropy =	149.2951
5 C	Isotropic =	70.8118	Anisotropy =	143.2244
6 C	Isotropic =	53.1915	Anisotropy =	176.8738
7 C	Isotropic =	154.8580	Anisotropy =	15.3023
8 C	Isotropic =	132.5289	Anisotropy =	34.0585
9 N	Isotropic =	217.6080	Anisotropy =	17.1591
10 C	Isotropic =	13.4327	Anisotropy =	103.1485
11 O	Isotropic =	152.9574	Anisotropy =	155.8673
12 O	Isotropic =	-65.9639	Anisotropy =	604.7731
13 C	Isotropic =	135.8196	Anisotropy =	76.5594
14 O	Isotropic =	227.1800	Anisotropy =	65.1059
15 H	Isotropic =	24.1661	Anisotropy =	7.7706
16 H	Isotropic =	24.4959	Anisotropy =	4.9104
17 H	Isotropic =	24.6338	Anisotropy =	5.7725
18 H	Isotropic =	24.3344	Anisotropy =	7.6253
19 H	Isotropic =	28.2679	Anisotropy =	7.1201
20 H	Isotropic =	28.6885	Anisotropy =	8.2329
21 H	Isotropic =	27.4278	Anisotropy =	7.2121
22 H	Isotropic =	26.8946	Anisotropy =	16.8728
23 H	Isotropic =	27.0415	Anisotropy =	11.5355
24 H	Isotropic =	26.9623	Anisotropy =	16.0057
25 H	Isotropic =	27.8509	Anisotropy =	8.1856
26 H	Isotropic =	27.8430	Anisotropy =	9.5930
27 H	Isotropic =	27.7251	Anisotropy =	8.3876
28 H	Isotropic =	27.2218	Anisotropy =	14.0495

Conformer_10

C	-0.462596971751	1.007003794586	0.107108165935
C	-0.254948499312	2.014611538127	-0.836678359417
C	-1.026920546039	3.169325268029	-0.840160797848
C	-2.032143951834	3.329581604951	0.111236248335
C	-2.262308124252	2.333366354708	1.055344786611
C	-1.480247319099	1.185839245396	1.046429983902
C	0.405726162870	-0.229469214995	0.127977585252

C	1.717341120398	-0.057442500611	0.908752200748
N	1.437142466351	0.199776258767	2.350933860895
C	2.571378428703	1.051557562256	0.314758496445
O	2.610985062884	2.130420472652	1.085073814334
O	3.115460154128	0.940089361174	-0.753168565985
C	3.345598388897	3.263924316237	0.577202762894
O	-2.821711420942	4.437029562543	0.154978512030
H	0.516148192409	1.896796928070	-1.594284093850
H	-0.854249702674	3.941817692145	-1.585365041247
H	-3.054436201989	2.461708723513	1.786116577069
H	-1.673773032973	0.409311522935	1.782820244242
H	0.680288587330	-0.525116768800	-0.887239088537
H	-0.135794436477	-1.068647133949	0.573943376201
H	2.293842470873	-0.982052487190	0.862619295318
H	0.937130449977	1.081327866270	2.499559124948
H	0.856705091675	-0.552024270757	2.734802803466
H	2.295629296393	0.233546767199	2.906890691938
H	3.273389082557	4.026638360868	1.349529682156
H	4.387101911077	2.989009805604	0.407702781846
H	2.889438550192	3.615640608996	-0.349390889561
H	-2.563675209373	5.046528761277	-0.545994158118

SCF Done: E(RwB97X) = -669.824578963

Zero-point correction=	0.239208
Thermal correction to Energy=	0.252915
Thermal correction to Enthalpy=	0.253860
Thermal correction to Gibbs Free Energy=	0.197976
Sum of electronic and zero-point Energies=	-669.585371
Sum of electronic and thermal Energies=	-669.571663
Sum of electronic and thermal Enthalpies=	-669.570719
Sum of electronic and thermal Free Energies=	-669.626603

1 C	Isotropic =	60.8251	Anisotropy =	181.2928
2 C	Isotropic =	52.8878	Anisotropy =	177.7992
3 C	Isotropic =	71.0530	Anisotropy =	143.9470
4 C	Isotropic =	27.1026	Anisotropy =	149.3828
5 C	Isotropic =	70.9435	Anisotropy =	152.3598
6 C	Isotropic =	51.2806	Anisotropy =	175.2680
7 C	Isotropic =	153.9222	Anisotropy =	13.3712
8 C	Isotropic =	131.8458	Anisotropy =	26.8005
9 N	Isotropic =	216.9968	Anisotropy =	18.9024
10 C	Isotropic =	16.3091	Anisotropy =	100.9084
11 O	Isotropic =	145.8123	Anisotropy =	168.0641
12 O	Isotropic =	-61.9208	Anisotropy =	584.8430
13 C	Isotropic =	135.9518	Anisotropy =	77.3199

14	O	Isotropic =	226.9042	Anisotropy =	64.8903
15	H	Isotropic =	24.3737	Anisotropy =	7.5370
16	H	Isotropic =	24.6225	Anisotropy =	5.3662
17	H	Isotropic =	24.4642	Anisotropy =	4.9499
18	H	Isotropic =	24.1358	Anisotropy =	7.6186
19	H	Isotropic =	28.4020	Anisotropy =	7.8187
20	H	Isotropic =	28.7642	Anisotropy =	8.2269
21	H	Isotropic =	27.4915	Anisotropy =	7.4507
22	H	Isotropic =	26.9844	Anisotropy =	10.3592
23	H	Isotropic =	26.9942	Anisotropy =	15.7563
24	H	Isotropic =	26.8606	Anisotropy =	16.6657
25	H	Isotropic =	28.1498	Anisotropy =	8.5562
26	H	Isotropic =	27.9473	Anisotropy =	9.9955
27	H	Isotropic =	28.1344	Anisotropy =	7.7209
28	H	Isotropic =	27.2294	Anisotropy =	13.9995

Conformer_11

C	-0.375217335585	1.158360418105	0.023665146603
C	-0.037561736525	2.205379664898	-0.839398362260
C	-0.671137985718	3.436714512504	-0.760426325869
C	-1.666016617293	3.641225485159	0.193624799326
C	-2.024535352347	2.610582704390	1.057074521209
C	-1.379006872795	1.382201923150	0.965474126502
C	0.340203052328	-0.170877894777	-0.043411568507
C	1.647795638791	-0.215346237231	0.759259207417
N	1.379992568975	0.025775553889	2.206802422294
C	2.674746365326	0.767260575899	0.217239995259
O	2.977479564530	1.725362538631	1.082444414941
O	3.137867990025	0.659845969314	-0.888594973431
C	3.921643074088	2.721917321849	0.634979467150
O	-2.260531254821	4.864568431381	0.234851346100
H	0.726119684487	2.055074517759	-1.598541635934
H	-0.407600024643	4.242443456824	-1.438129236747
H	-2.808001159071	2.764355422978	1.794930036609
H	-1.673999330068	0.580836481938	1.638883059763
H	0.595318451416	-0.421836857383	-1.075437321552
H	-0.305776422928	-0.968426421302	0.334050790327
H	2.084898605720	-1.212591662192	0.687339016242
H	2.223837778574	-0.078511991770	2.775679706747
H	0.999655712462	0.960178875932	2.385664277352
H	0.696243102993	-0.654557774264	2.551929875514
H	3.520241184897	3.246415117269	-0.233217656975
H	4.040980550162	3.405894459258	1.472173331321
H	4.873286932028	2.249914153796	0.388054586311

H -2.930226165007 4.874641253998 0.928336954287

SCF Done: E(RwB97X) = -669.824605103

Zero-point correction= 0.239450
Thermal correction to Energy= 0.253144
Thermal correction to Enthalpy= 0.254088
Thermal correction to Gibbs Free Energy= 0.198107
Sum of electronic and zero-point Energies= -669.585155
Sum of electronic and thermal Energies= -669.571461
Sum of electronic and thermal Enthalpies= -669.570517
Sum of electronic and thermal Free Energies= -669.626498

1	C	Isotropic =	60.9579	Anisotropy =	180.8255
2	C	Isotropic =	52.4330	Anisotropy =	178.5916
3	C	Isotropic =	70.1151	Anisotropy =	154.5121
4	C	Isotropic =	27.0812	Anisotropy =	149.4797
5	C	Isotropic =	71.8055	Anisotropy =	141.8468
6	C	Isotropic =	51.6152	Anisotropy =	174.1438
7	C	Isotropic =	154.1433	Anisotropy =	14.1516
8	C	Isotropic =	131.9554	Anisotropy =	27.1078
9	N	Isotropic =	217.3304	Anisotropy =	18.1007
10	C	Isotropic =	16.1668	Anisotropy =	100.2665
11	O	Isotropic =	145.3256	Anisotropy =	166.6143
12	O	Isotropic =	-60.4329	Anisotropy =	586.6711
13	C	Isotropic =	135.4943	Anisotropy =	77.6720
14	O	Isotropic =	226.7871	Anisotropy =	64.5731
15	H	Isotropic =	24.2914	Anisotropy =	7.6395
16	H	Isotropic =	24.4693	Anisotropy =	5.2910
17	H	Isotropic =	24.6155	Anisotropy =	5.0657
18	H	Isotropic =	24.2104	Anisotropy =	7.7196
19	H	Isotropic =	28.3341	Anisotropy =	7.7399
20	H	Isotropic =	28.7582	Anisotropy =	8.2282
21	H	Isotropic =	27.4712	Anisotropy =	7.3890
22	H	Isotropic =	26.8335	Anisotropy =	16.5124
23	H	Isotropic =	27.0865	Anisotropy =	10.4844
24	H	Isotropic =	27.0037	Anisotropy =	15.7243
25	H	Isotropic =	28.0532	Anisotropy =	7.8819
26	H	Isotropic =	28.0652	Anisotropy =	8.5551
27	H	Isotropic =	27.9127	Anisotropy =	9.8834
28	H	Isotropic =	27.2256	Anisotropy =	14.1711

Conformer_12

C -0.433144954657 1.045686821821 0.097271620187

C	-1.443863506280	1.369414102652	1.001334793927
C	-2.167026658754	2.551982213838	0.884155168167
C	-1.880452057652	3.433071267290	-0.153909351187
C	-0.880543931245	3.124467862095	-1.074336572210
C	-0.170026377270	1.940792006962	-0.944379402023
C	0.374634216845	-0.221730311261	0.252731053982
C	1.682544263871	-0.034185590178	1.036338655836
N	1.394488300601	0.365627884768	2.444102431628
C	2.591075287806	0.979817713863	0.359092559411
O	2.662864745864	2.122915535674	1.027758984260
O	3.146654834410	0.748508173454	-0.683345507532
C	3.449418335052	3.175840544217	0.431909554913
O	-2.551523084878	4.605219550214	-0.319592289290
H	-1.682166114092	0.684155344113	1.811432307772
H	-2.955230414280	2.785726166739	1.595582428605
H	-0.673523167126	3.811342573913	-1.888773128019
H	0.597824383124	1.705380404889	-1.677467436638
H	0.648184608819	-0.626304035510	-0.724492600653
H	-0.211193150984	-0.988387378417	0.767943905103
H	2.219093462506	-0.982420852059	1.084298034453
H	0.775219842483	-0.321744762595	2.883931280971
H	2.245823121160	0.412202552789	3.010035358271
H	0.933215010840	1.278326447209	2.502910825504
H	3.397548106469	4.008068135662	1.130615120351
H	4.481145329657	2.846284947303	0.305778279080
H	3.020103095534	3.459039318510	-0.530315762821
H	-3.217643527822	4.696403362046	0.371389687952

SCF Done: E(RwB97X) = -669.824588273

Zero-point correction=	0.239258
Thermal correction to Energy=	0.252958
Thermal correction to Enthalpy=	0.253902
Thermal correction to Gibbs Free Energy=	0.198101
Sum of electronic and zero-point Energies=	-669.585330
Sum of electronic and thermal Energies=	-669.571631
Sum of electronic and thermal Enthalpies=	-669.570686
Sum of electronic and thermal Free Energies=	-669.626487

1 C	Isotropic =	60.8211	Anisotropy =	181.4424
2 C	Isotropic =	51.9573	Anisotropy =	174.1662
3 C	Isotropic =	71.8829	Anisotropy =	141.7365
4 C	Isotropic =	27.0847	Anisotropy =	149.5371
5 C	Isotropic =	70.1254	Anisotropy =	154.5845
6 C	Isotropic =	52.2788	Anisotropy =	178.7334
7 C	Isotropic =	153.8783	Anisotropy =	13.2414

8	C	Isotropic =	131.8856	Anisotropy =	26.8853
9	N	Isotropic =	216.9280	Anisotropy =	19.0178
10	C	Isotropic =	16.3828	Anisotropy =	100.8731
11	O	Isotropic =	145.9571	Anisotropy =	167.9420
12	O	Isotropic =	-61.9817	Anisotropy =	584.9882
13	C	Isotropic =	135.9542	Anisotropy =	77.3278
14	O	Isotropic =	226.8266	Anisotropy =	64.5827
15	H	Isotropic =	24.2086	Anisotropy =	7.6700
16	H	Isotropic =	24.6063	Anisotropy =	5.0549
17	H	Isotropic =	24.4623	Anisotropy =	5.2529
18	H	Isotropic =	24.3093	Anisotropy =	7.4537
19	H	Isotropic =	28.4033	Anisotropy =	7.8755
20	H	Isotropic =	28.7686	Anisotropy =	8.1745
21	H	Isotropic =	27.4965	Anisotropy =	7.4659
22	H	Isotropic =	27.0066	Anisotropy =	15.7171
23	H	Isotropic =	26.8639	Anisotropy =	16.6713
24	H	Isotropic =	26.9710	Anisotropy =	10.4229
25	H	Isotropic =	28.1551	Anisotropy =	8.5574
26	H	Isotropic =	27.9491	Anisotropy =	10.0181
27	H	Isotropic =	28.1389	Anisotropy =	7.6624
28	H	Isotropic =	27.2179	Anisotropy =	14.1881

Conformer_13

C	-0.430109418853	1.422287667424	1.150406036580
C	-1.441451460368	1.037414656286	0.268700678882
C	-2.209808834717	1.980429934926	-0.399049224231
C	-1.971432425579	3.337027518466	-0.189347523941
C	-0.972748598346	3.740972106636	0.691940709435
C	-0.212175704538	2.783272030821	1.353385710406
C	0.435761720029	0.393314380502	1.834017555454
C	1.593764131977	-0.092232747818	0.947417917189
N	2.434023336489	-1.038454852193	1.733583830118
C	2.484181915370	1.063376176987	0.518014911731
O	2.127328150370	1.541437723667	-0.658010234302
O	3.382525159978	1.489271061795	1.204501463625
C	2.815048882339	2.728482464663	-1.101852613743
O	-2.747579552381	4.228156731623	-0.865940545751
H	-1.633528495880	-0.019215650886	0.099440074630
H	-2.997286098808	1.676327525423	-1.081391224631
H	-0.793101512879	4.799243079542	0.863660937456
H	0.563590213493	3.109609584520	2.042277464947
H	-0.155701748828	-0.485492540220	2.107746411566
H	0.856833192622	0.809769302147	2.755381598297
H	1.222034414007	-0.628748557148	0.074382051868

H	3.158498555037	-1.476258311194	1.158236885940
H	2.898475627633	-0.560634012399	2.512218524457
H	1.859503303721	-1.789734227620	2.125798845832
H	2.360541883735	2.987827886033	-2.055656948356
H	2.673977309680	3.535726724404	-0.381214774758
H	3.877806679121	2.520186145775	-1.231902599699
H	-2.482770624422	5.125938197837	-0.635345919002

SCF Done: E(RwB97X) = -669.825074683

Zero-point correction=	0.239432
Thermal correction to Energy=	0.253156
Thermal correction to Enthalpy=	0.254101
Thermal correction to Gibbs Free Energy=	0.198392
Sum of electronic and zero-point Energies=	-669.585643
Sum of electronic and thermal Energies=	-669.571918
Sum of electronic and thermal Enthalpies=	-669.570974
Sum of electronic and thermal Free Energies=	-669.626683

1 C	Isotropic = 58.6632	Anisotropy = 182.2607
2 C	Isotropic = 51.8844	Anisotropy = 179.4651
3 C	Isotropic = 70.5668	Anisotropy = 153.1255
4 C	Isotropic = 27.4455	Anisotropy = 148.6416
5 C	Isotropic = 72.0868	Anisotropy = 141.9409
6 C	Isotropic = 52.9464	Anisotropy = 174.3888
7 C	Isotropic = 151.9498	Anisotropy = 30.2768
8 C	Isotropic = 132.0682	Anisotropy = 25.8986
9 N	Isotropic = 213.5900	Anisotropy = 31.1674
10 C	Isotropic = 12.5593	Anisotropy = 104.0270
11 O	Isotropic = 140.2237	Anisotropy = 155.6753
12 O	Isotropic = -52.6396	Anisotropy = 593.5788
13 C	Isotropic = 136.3883	Anisotropy = 76.2021
14 O	Isotropic = 227.4769	Anisotropy = 65.7574
15 H	Isotropic = 23.9897	Anisotropy = 7.5292
16 H	Isotropic = 24.4664	Anisotropy = 4.7423
17 H	Isotropic = 24.6864	Anisotropy = 5.2325
18 H	Isotropic = 24.4288	Anisotropy = 7.1397
19 H	Isotropic = 28.5256	Anisotropy = 7.1141
20 H	Isotropic = 28.9455	Anisotropy = 5.4162
21 H	Isotropic = 27.7466	Anisotropy = 4.5847
22 H	Isotropic = 26.8147	Anisotropy = 16.8479
23 H	Isotropic = 26.5135	Anisotropy = 12.9032
24 H	Isotropic = 26.8284	Anisotropy = 15.3132
25 H	Isotropic = 28.4926	Anisotropy = 8.0178
26 H	Isotropic = 28.3543	Anisotropy = 7.1500
27 H	Isotropic = 28.1536	Anisotropy = 9.9381

28 H Isotropic = 27.2482 Anisotropy = 13.8882

Conformer_14

C	-0.383704797425	1.500829012373	1.176917401123
C	-1.433544864682	1.204381277748	0.309726000468
C	-2.177780171735	2.214100234907	-0.288132863823
C	-1.873852254593	3.546544203777	-0.018692206500
C	-0.831967380386	3.862226190838	0.849108840848
C	-0.097772706559	2.841287751947	1.437697224274
C	0.445857355913	0.400511065073	1.790329909870
C	1.543388622565	-0.115270396369	0.846318388811
N	2.312901318209	-1.182324046050	1.544853278535
C	2.514911316430	0.994362171834	0.476431464952
O	2.167226834638	1.585715124780	-0.650185980701
O	3.460000725096	1.298041300337	1.164981174198
C	2.927336614084	2.752740416179	-1.023419878595
O	-2.570316412237	4.576254208914	-0.574522299088
H	-1.678976104490	0.167424867654	0.094387035822
H	-2.996484699220	1.968595818218	-0.959965915178
H	-0.607805531034	4.903151738755	1.060031436790
H	0.712952408060	3.096018317923	2.116545716319
H	-0.187613695926	-0.452884496108	2.050843372584
H	0.919537188900	0.754853495266	2.712153293747
H	1.113108329193	-0.557372268605	-0.052319926561
H	3.007312300543	-1.617909608820	0.932020908464
H	2.805662918709	-0.812081056504	2.363430145736
H	1.683518286821	-1.922420056189	1.868174760881
H	3.972251465737	2.485532209729	-1.186097789327
H	2.478616310474	3.107535877430	-1.948829463117
H	2.848923288668	3.514929678941	-0.246397949111
H	-3.260586665756	4.225726966021	-1.148886081418

SCF Done: E(RwB97X) = -669.825015973

Zero-point correction=	0.239500
Thermal correction to Energy=	0.253211
Thermal correction to Enthalpy=	0.254155
Thermal correction to Gibbs Free Energy=	0.198465
Sum of electronic and zero-point Energies=	-669.585516
Sum of electronic and thermal Energies=	-669.571805
Sum of electronic and thermal Enthalpies=	-669.570861
Sum of electronic and thermal Free Energies=	-669.626551

1 C Isotropic = 58.6127 Anisotropy = 182.1255

2 C	Isotropic =	52.4312	Anisotropy =	178.2222
3 C	Isotropic =	71.4518	Anisotropy =	142.2915
4 C	Isotropic =	27.5638	Anisotropy =	148.6512
5 C	Isotropic =	71.3309	Anisotropy =	152.7018
6 C	Isotropic =	52.2286	Anisotropy =	175.6409
7 C	Isotropic =	151.8814	Anisotropy =	30.0729
8 C	Isotropic =	131.9357	Anisotropy =	25.4836
9 N	Isotropic =	213.6529	Anisotropy =	31.1070
10 C	Isotropic =	12.5397	Anisotropy =	103.7265
11 O	Isotropic =	140.5334	Anisotropy =	154.9834
12 O	Isotropic =	-52.2079	Anisotropy =	591.9177
13 C	Isotropic =	136.3931	Anisotropy =	76.2099
14 O	Isotropic =	227.5529	Anisotropy =	66.4090
15 H	Isotropic =	24.0441	Anisotropy =	7.6831
16 H	Isotropic =	24.6157	Anisotropy =	4.8754
17 H	Isotropic =	24.5554	Anisotropy =	5.0646
18 H	Isotropic =	24.3618	Anisotropy =	7.0692
19 H	Isotropic =	28.5512	Anisotropy =	6.9887
20 H	Isotropic =	28.9496	Anisotropy =	5.3949
21 H	Isotropic =	27.7741	Anisotropy =	4.5064
22 H	Isotropic =	26.8157	Anisotropy =	16.7890
23 H	Isotropic =	26.5316	Anisotropy =	12.9460
24 H	Isotropic =	26.8173	Anisotropy =	15.3397
25 H	Isotropic =	28.1110	Anisotropy =	9.8683
26 H	Isotropic =	28.4664	Anisotropy =	8.0135
27 H	Isotropic =	28.3236	Anisotropy =	7.2176
28 H	Isotropic =	27.2292	Anisotropy =	14.3151

Conformer_15

C	-0.379668415191	1.642497290274	1.219333974825
C	-0.169631572393	3.012001274513	1.076258499212
C	-1.117144628487	3.825758097270	0.463740234988
C	-2.297303845507	3.265899671631	-0.015946304863
C	-2.526648687640	1.898159860809	0.120599287516
C	-1.571776086460	1.100832276903	0.733589079192
C	0.657284983842	0.757538826442	1.865676607222
C	1.528806278941	0.018843008183	0.840804100883
N	2.470572109723	-0.880708788030	1.569961913886
C	2.311354436015	0.982687914080	-0.040059911901
O	3.370375257259	1.468162627884	0.599372091888
O	1.981554854454	1.279942966983	-1.158019707481
C	4.179998491122	2.421539383441	-0.119988915186
O	-3.262945671881	4.010893905524	-0.621310504558
H	0.746357986233	3.460863412516	1.453099250835

H	-0.940450623407	4.893712378443	0.363137269154
H	-3.453644270177	1.472098896431	-0.249843823112
H	-1.760227055726	0.035438909444	0.840810783362
H	0.168613880539	-0.003010218956	2.482699122775
H	1.304894247308	1.348418454453	2.521510087857
H	0.918800334242	-0.611717435307	0.194350147271
H	3.054195412158	-1.425928361288	0.929247296550
H	3.092871134797	-0.357038922465	2.192495090967
H	1.947948225396	-1.546712581008	2.146756836933
H	4.980950460949	2.697503371871	0.562301315982
H	4.588296775786	1.960344943111	-1.020236689241
H	3.581251971013	3.295389909815	-0.380140133749
H	-2.986185982909	4.933788927032	-0.652597001206

SCF Done: E(RwB97X) = -669.822956919

Zero-point correction=	0.239644
Thermal correction to Energy=	0.253358
Thermal correction to Enthalpy=	0.254302
Thermal correction to Gibbs Free Energy=	0.198215
Sum of electronic and zero-point Energies=	-669.583313
Sum of electronic and thermal Energies=	-669.569599
Sum of electronic and thermal Enthalpies=	-669.568655
Sum of electronic and thermal Free Energies=	-669.624742

1 C	Isotropic = 59.0353	Anisotropy = 180.3668
2 C	Isotropic = 52.8437	Anisotropy = 173.6946
3 C	Isotropic = 72.3717	Anisotropy = 141.4216
4 C	Isotropic = 27.6554	Anisotropy = 148.3600
5 C	Isotropic = 70.5953	Anisotropy = 152.6025
6 C	Isotropic = 51.8298	Anisotropy = 179.3519
7 C	Isotropic = 152.4027	Anisotropy = 29.7166
8 C	Isotropic = 129.7010	Anisotropy = 12.5799
9 N	Isotropic = 213.2133	Anisotropy = 31.0208
10 C	Isotropic = 17.0637	Anisotropy = 100.4117
11 O	Isotropic = 155.0104	Anisotropy = 156.5913
12 O	Isotropic = -86.2698	Anisotropy = 599.4269
13 C	Isotropic = 135.6339	Anisotropy = 76.9993
14 O	Isotropic = 227.4031	Anisotropy = 65.8923
15 H	Isotropic = 24.3845	Anisotropy = 7.4945
16 H	Isotropic = 24.7503	Anisotropy = 5.3557
17 H	Isotropic = 24.4620	Anisotropy = 4.9453
18 H	Isotropic = 23.9961	Anisotropy = 7.9781
19 H	Isotropic = 28.5801	Anisotropy = 6.8460
20 H	Isotropic = 28.8515	Anisotropy = 5.0445
21 H	Isotropic = 27.8510	Anisotropy = 4.9285

22	H	Isotropic =	26.6932	Anisotropy =	16.2619
23	H	Isotropic =	26.6211	Anisotropy =	12.3138
24	H	Isotropic =	26.7265	Anisotropy =	15.4879
25	H	Isotropic =	27.7687	Anisotropy =	8.4296
26	H	Isotropic =	27.9590	Anisotropy =	9.6010
27	H	Isotropic =	27.9140	Anisotropy =	8.2595
28	H	Isotropic =	27.2946	Anisotropy =	13.9610

Conformer_16

C	-0.339850491694	1.709893527582	1.224726736973
C	-0.047068913242	3.071797734634	1.147073232160
C	-0.937992497764	3.968335482099	0.571841729055
C	-2.147039077880	3.504462251852	0.061572071428
C	-2.458919692481	2.148332056158	0.130933334923
C	-1.556691590437	1.264726613714	0.709880001351
C	0.639714071121	0.737161692778	1.833494844228
C	1.477857540780	0.000503519595	0.779789475832
N	2.372983002098	-0.972613105486	1.472398525182
C	2.308768454718	0.960493910026	-0.060108348943
O	3.385979315688	1.370971432236	0.600993962458
O	1.998844238963	1.315547469290	-1.166844158618
C	4.242669027537	2.312292507045	-0.078812714245
O	-2.993410016879	4.417662324995	-0.489684978334
H	0.891818574816	3.444970652840	1.549466087686
H	-0.706653105729	5.027453370495	0.518816846900
H	-3.405950728608	1.786093415895	-0.261497730182
H	-1.810927490294	0.209138388242	0.764529491912
H	0.104506947610	-0.023054751566	2.410985308540
H	1.313799207762	1.259446980294	2.520202500504
H	0.840465980167	-0.572789971987	0.106977591804
H	2.932118549375	-1.518308593068	0.810591916438
H	3.017423132193	-0.505444139818	2.116998871618
H	1.817207589231	-1.635899856991	2.020634441310
H	5.053888538831	2.521922198084	0.614857634971
H	4.630983204529	1.868256884839	-0.996363954725
H	3.687317929865	3.223611603093	-0.304414308705
H	-3.789841700275	3.972836403129	-0.801238411523

SCF Done: E(RwB97X) = -669.822907935

Zero-point correction=	0.239547
Thermal correction to Energy=	0.253294
Thermal correction to Enthalpy=	0.254238
Thermal correction to Gibbs Free Energy=	0.197757

Sum of electronic and zero-point Energies=	-669.583361
Sum of electronic and thermal Energies=	-669.569614
Sum of electronic and thermal Enthalpies=	-669.568670
Sum of electronic and thermal Free Energies=	-669.625151

1 C	Isotropic =	59.0993	Anisotropy =	180.3918
2 C	Isotropic =	52.2342	Anisotropy =	174.8822
3 C	Isotropic =	71.4204	Anisotropy =	152.0482
4 C	Isotropic =	27.6668	Anisotropy =	148.4362
5 C	Isotropic =	71.5095	Anisotropy =	142.0070
6 C	Isotropic =	52.4044	Anisotropy =	178.1165
7 C	Isotropic =	152.4589	Anisotropy =	29.7577
8 C	Isotropic =	129.7006	Anisotropy =	12.5382
9 N	Isotropic =	213.2344	Anisotropy =	31.0468
10 C	Isotropic =	17.0625	Anisotropy =	100.4736
11 O	Isotropic =	154.8515	Anisotropy =	156.8949
12 O	Isotropic =	-86.4248	Anisotropy =	599.3887
13 C	Isotropic =	135.6138	Anisotropy =	77.0012
14 O	Isotropic =	227.6318	Anisotropy =	66.2482
15 H	Isotropic =	24.3200	Anisotropy =	7.4342
16 H	Isotropic =	24.5808	Anisotropy =	5.2907
17 H	Isotropic =	24.5958	Anisotropy =	5.0520
18 H	Isotropic =	24.0634	Anisotropy =	8.0343
19 H	Isotropic =	28.5820	Anisotropy =	6.8358
20 H	Isotropic =	28.8567	Anisotropy =	5.0832
21 H	Isotropic =	27.8567	Anisotropy =	4.9709
22 H	Isotropic =	26.6961	Anisotropy =	16.2581
23 H	Isotropic =	26.6280	Anisotropy =	12.3291
24 H	Isotropic =	26.7297	Anisotropy =	15.4731
25 H	Isotropic =	27.7623	Anisotropy =	8.4477
26 H	Isotropic =	27.9544	Anisotropy =	9.6113
27 H	Isotropic =	27.9068	Anisotropy =	8.2317
28 H	Isotropic =	27.2851	Anisotropy =	14.2063

Conformer_2

C	-0.138250892927	2.383276089433	-0.075257115436
C	-0.404346291074	3.701405176780	0.297281722350
C	-1.706599855392	4.154880291349	0.466665859758
C	-2.769574386225	3.281413665365	0.261043953477
C	-2.525679463023	1.961162633376	-0.114797384696
C	-1.218435874150	1.523052918344	-0.278360856183
C	1.281084867473	1.895312962301	-0.243038465463
C	1.769982640024	1.050094040942	0.940988184270
N	1.728566886049	1.841565671585	2.200000965313

C	3.205566302175	0.602546039785	0.725228012936
O	3.268963892275	-0.369137049202	-0.165569570339
O	4.151033189971	1.104654255616	1.283722149714
C	4.587174414199	-0.854254900830	-0.496346501640
O	-4.029741685379	3.764974762837	0.435871450164
H	0.421862207741	4.390605233884	0.453915993900
H	-1.905883685235	5.182541406976	0.753400347431
H	-3.357656522505	1.282494009254	-0.284930463215
H	-1.038549825761	0.493277043893	-0.577243507568
H	1.957738380766	2.746568296870	-0.373028210271
H	1.363818179184	1.271078384921	-1.136125103101
H	1.127672684884	0.180114765331	1.087667899911
H	2.002750524240	1.280110577789	3.010434155739
H	2.353744270738	2.652158453164	2.157108233317
H	0.780519154916	2.187030573393	2.378006447595
H	5.186758531394	-0.049610241139	-0.923756857464
H	5.072198121858	-1.256024872987	0.394190191188
H	4.429461946144	-1.641335700491	-1.230417602383
H	-4.671377712360	3.068245511460	0.256446070693

SCF Done: E(RwB97X) = -669.825904217

Zero-point correction=	0.239155
Thermal correction to Energy=	0.253001
Thermal correction to Enthalpy=	0.253945
Thermal correction to Gibbs Free Energy=	0.197381
Sum of electronic and zero-point Energies=	-669.586749
Sum of electronic and thermal Energies=	-669.572904
Sum of electronic and thermal Enthalpies=	-669.571959
Sum of electronic and thermal Free Energies=	-669.628523

1 C	Isotropic =	59.1184	Anisotropy =	179.3860
2 C	Isotropic =	50.7758	Anisotropy =	173.1752
3 C	Isotropic =	71.3902	Anisotropy =	151.3237
4 C	Isotropic =	27.3241	Anisotropy =	148.6058
5 C	Isotropic =	70.7499	Anisotropy =	143.1638
6 C	Isotropic =	52.3278	Anisotropy =	181.0700
7 C	Isotropic =	153.1265	Anisotropy =	21.6778
8 C	Isotropic =	131.1829	Anisotropy =	25.1642
9 N	Isotropic =	217.7723	Anisotropy =	13.1393
10 C	Isotropic =	12.8042	Anisotropy =	100.3816
11 O	Isotropic =	152.0506	Anisotropy =	145.1154
12 O	Isotropic =	-51.0325	Anisotropy =	583.0090
13 C	Isotropic =	135.3103	Anisotropy =	77.6882
14 O	Isotropic =	227.1425	Anisotropy =	65.8055
15 H	Isotropic =	24.1543	Anisotropy =	7.7270

16	H	Isotropic =	24.5332	Anisotropy =	5.0253
17	H	Isotropic =	24.5622	Anisotropy =	5.2365
18	H	Isotropic =	23.9871	Anisotropy =	8.2334
19	H	Isotropic =	29.0762	Anisotropy =	5.7581
20	H	Isotropic =	28.4343	Anisotropy =	6.8180
21	H	Isotropic =	27.7268	Anisotropy =	5.9507
22	H	Isotropic =	27.0507	Anisotropy =	16.9882
23	H	Isotropic =	26.8960	Anisotropy =	13.4311
24	H	Isotropic =	27.2604	Anisotropy =	14.1005
25	H	Isotropic =	27.8664	Anisotropy =	8.7182
26	H	Isotropic =	27.8286	Anisotropy =	9.0558
27	H	Isotropic =	27.7696	Anisotropy =	8.2163
28	H	Isotropic =	27.2279	Anisotropy =	14.1675

Conformer_3

C	-0.190228431544	2.235189591156	-0.114385660376
C	-1.220686263276	1.291541239456	-0.168190739320
C	-2.545282132312	1.663526264900	-0.001801898882
C	-2.862163882252	3.002441065235	0.225504531075
C	-1.852672317597	3.957405425914	0.280175525113
C	-0.527073249704	3.567431471057	0.111271342092
C	1.250063163427	1.809398062940	-0.273087096936
C	1.781572696873	1.061970452543	0.955916498384
N	1.700712451075	1.927240072432	2.163549757490
C	3.231769501745	0.644837813463	0.780785070978
O	3.352723790719	-0.250917051873	-0.181171100082
O	4.140220075035	1.091841448920	1.438404420879
C	4.690599736312	-0.710968208863	-0.465106682431
O	-4.175655836078	3.321034725214	0.385766895779
H	-0.982356602218	0.246037173798	-0.348527922546
H	-3.341593555971	0.927414373125	-0.049163738633
H	-2.100075140323	5.001904272697	0.452635066488
H	0.254983742034	4.321279436115	0.152363097378
H	1.885625339180	2.681598958914	-0.459453516572
H	1.356160072483	1.136603152594	-1.127146998589
H	1.175899424257	0.176167186332	1.159346094961
H	2.044923621954	1.448899531510	2.999736273492
H	2.245879698639	2.787453308992	2.052225384709
H	0.729255107773	2.198097657537	2.344522415487
H	4.586192376929	-1.418634229090	-1.284550561289
H	5.320743079523	0.127236286256	-0.764787873212
H	5.109979692662	-1.204288043361	0.412698612836
H	-4.262316159343	4.270258562087	0.530372801726

SCF Done: E(RwB97X) = -669.826005731

Zero-point correction=	0.239089
Thermal correction to Energy=	0.252907
Thermal correction to Enthalpy=	0.253851
Thermal correction to Gibbs Free Energy=	0.197673
Sum of electronic and zero-point Energies=	-669.586917
Sum of electronic and thermal Energies=	-669.573099
Sum of electronic and thermal Enthalpies=	-669.572155
Sum of electronic and thermal Free Energies=	-669.628333

1 C	Isotropic =	58.7920	Anisotropy =	179.8119
2 C	Isotropic =	51.9586	Anisotropy =	182.8994
3 C	Isotropic =	69.9260	Anisotropy =	153.9399
4 C	Isotropic =	27.3465	Anisotropy =	148.4139
5 C	Isotropic =	72.3255	Anisotropy =	140.5215
6 C	Isotropic =	51.5777	Anisotropy =	171.6626
7 C	Isotropic =	153.3818	Anisotropy =	21.5226
8 C	Isotropic =	130.9257	Anisotropy =	27.0042
9 N	Isotropic =	217.4455	Anisotropy =	11.8492
10 C	Isotropic =	13.1927	Anisotropy =	100.1311
11 O	Isotropic =	153.6818	Anisotropy =	149.9234
12 O	Isotropic =	-52.6302	Anisotropy =	582.7120
13 C	Isotropic =	135.3647	Anisotropy =	77.6140
14 O	Isotropic =	226.9477	Anisotropy =	65.1236
15 H	Isotropic =	23.9018	Anisotropy =	8.3084
16 H	Isotropic =	24.4234	Anisotropy =	5.1239
17 H	Isotropic =	24.6936	Anisotropy =	5.0659
18 H	Isotropic =	24.2377	Anisotropy =	7.6213
19 H	Isotropic =	29.0698	Anisotropy =	5.9106
20 H	Isotropic =	28.3328	Anisotropy =	7.1096
21 H	Isotropic =	27.6400	Anisotropy =	5.7567
22 H	Isotropic =	26.9817	Anisotropy =	16.7617
23 H	Isotropic =	27.1030	Anisotropy =	13.4291
24 H	Isotropic =	27.3284	Anisotropy =	13.8270
25 H	Isotropic =	27.7846	Anisotropy =	8.1805
26 H	Isotropic =	27.8545	Anisotropy =	8.7651
27 H	Isotropic =	27.8561	Anisotropy =	9.1373
28 H	Isotropic =	27.2236	Anisotropy =	14.0815

Conformer_4

C	-0.340227756847	1.191363366337	-0.014881991745
C	-1.505772578233	1.244740980574	0.749143338412
C	-2.299934443084	2.386054034262	0.777945342586

C	-1.929524692044	3.499744435132	0.030173719165
C	-0.772518996545	3.465497805849	-0.745469963165
C	0.009117743864	2.320032223298	-0.762776941546
C	0.526693430283	-0.046271090013	-0.019254361333
C	1.666773351914	-0.013834447265	1.007307150366
N	1.128319843742	0.055855138521	2.393271397305
C	2.613608857356	1.160224929849	0.820111898054
O	3.198494600792	1.107326914766	-0.362484475917
O	2.796071992344	2.014352960661	1.653078226842
C	4.104312192026	2.183281984391	-0.683202228677
O	-2.664890491394	4.644573158320	0.014458996491
H	-1.809618081765	0.375247102569	1.327231692772
H	-3.207913589725	2.406579134904	1.375481317289
H	-0.499826721485	4.335504022176	-1.334381100029
H	0.900200661644	2.302194532361	-1.385924423381
H	0.984582934859	-0.192624841549	-0.999737706044
H	-0.077278047783	-0.933749561183	0.190334552418
H	2.243524512884	-0.938251439686	0.941115188937
H	0.532094399492	-0.754882387769	2.581283122386
H	1.876959044023	0.055340789396	3.090688111852
H	0.566066261247	0.898502526545	2.550395233618
H	3.574728189939	3.137131556253	-0.667528903194
H	4.932744304630	2.201828962742	0.026188266228
H	4.466859986924	1.966135423001	-1.685493764307
H	-3.438546909058	4.540201785558	0.580128304618

SCF Done: E(RwB97X) = -669.826578447

Zero-point correction=	0.239756
Thermal correction to Energy=	0.253316
Thermal correction to Enthalpy=	0.254260
Thermal correction to Gibbs Free Energy=	0.199023
Sum of electronic and zero-point Energies=	-669.586823
Sum of electronic and thermal Energies=	-669.573262
Sum of electronic and thermal Enthalpies=	-669.572318
Sum of electronic and thermal Free Energies=	-669.627556

1 C	Isotropic =	60.7846	Anisotropy =	180.2273
2 C	Isotropic =	51.4638	Anisotropy =	174.1387
3 C	Isotropic =	71.9080	Anisotropy =	141.9851
4 C	Isotropic =	27.2177	Anisotropy =	149.3473
5 C	Isotropic =	69.8562	Anisotropy =	154.0075
6 C	Isotropic =	52.6919	Anisotropy =	178.2423
7 C	Isotropic =	154.8481	Anisotropy =	15.3373
8 C	Isotropic =	132.5834	Anisotropy =	34.0946
9 N	Isotropic =	217.6338	Anisotropy =	17.1841

10	C	Isotropic =	13.4311	Anisotropy =	103.1419
11	O	Isotropic =	152.8810	Anisotropy =	155.8242
12	O	Isotropic =	-66.1556	Anisotropy =	605.0097
13	C	Isotropic =	135.8095	Anisotropy =	76.5452
14	O	Isotropic =	226.9897	Anisotropy =	65.0203
15	H	Isotropic =	24.2332	Anisotropy =	7.8050
16	H	Isotropic =	24.6446	Anisotropy =	5.0115
17	H	Isotropic =	24.4824	Anisotropy =	5.6821
18	H	Isotropic =	24.2783	Anisotropy =	7.5953
19	H	Isotropic =	28.2614	Anisotropy =	7.1677
20	H	Isotropic =	28.7009	Anisotropy =	8.2051
21	H	Isotropic =	27.4300	Anisotropy =	7.2214
22	H	Isotropic =	26.9850	Anisotropy =	16.0018
23	H	Isotropic =	26.9035	Anisotropy =	16.8679
24	H	Isotropic =	27.0572	Anisotropy =	11.5607
25	H	Isotropic =	27.8209	Anisotropy =	8.1558
26	H	Isotropic =	27.8394	Anisotropy =	9.6206
27	H	Isotropic =	27.7123	Anisotropy =	8.4049
28	H	Isotropic =	27.2027	Anisotropy =	14.3430

Conformer_5

C	-0.283093656155	2.251072163133	0.972689167591
C	-1.380220461777	1.428029070930	1.226509317855
C	-2.675780653565	1.846545835093	0.947214228867
C	-2.887526985446	3.108421702416	0.401452321817
C	-1.804353435708	3.946104392308	0.139358312628
C	-0.516804909629	3.513731514010	0.425567480558
C	1.124835730395	1.792796854591	1.271609535605
C	1.936791885490	1.496090609526	0.006475212580
N	1.301186813344	0.391705586139	-0.768508407119
C	3.382303159155	1.172163642364	0.351097322032
O	3.757572137218	-0.024359923773	-0.082237630525
O	4.084606170798	1.941719878760	0.953468890283
C	5.116492594423	-0.418627663929	0.204598002460
O	-4.171116530530	3.480597077335	0.142435698781
H	-1.222164363202	0.441980678798	1.656003167408
H	-3.525195896138	1.202572970685	1.151546489016
H	-1.970738634199	4.934737282289	-0.281134213698
H	0.320639283915	4.177342830741	0.223776035320
H	1.107563215799	0.895468500101	1.899275339039
H	1.667888246062	2.566380806512	1.819254763970
H	1.948467762309	2.367627414804	-0.652451964902
H	1.825949545654	0.161181886453	-1.615562612830
H	1.207244296930	-0.464053880960	-0.212990727959

H	0.359016386763	0.669003103381	-1.061307214907
H	5.278797833702	-0.439237951819	1.282863547474
H	5.224099514734	-1.415454482419	-0.217223186589
H	5.812749860807	0.273918718537	-0.269608328134
H	-4.181308911149	4.372541383993	-0.223170546619

SCF Done: E(RwB97X) = -669.824207546

Zero-point correction=	0.239557
Thermal correction to Energy=	0.253178
Thermal correction to Enthalpy=	0.254123
Thermal correction to Gibbs Free Energy=	0.198751
Sum of electronic and zero-point Energies=	-669.584650
Sum of electronic and thermal Energies=	-669.571029
Sum of electronic and thermal Enthalpies=	-669.570085
Sum of electronic and thermal Free Energies=	-669.625456

1 C	Isotropic = 58.5700	Anisotropy = 180.1259
2 C	Isotropic = 51.0686	Anisotropy = 172.3672
3 C	Isotropic = 71.5256	Anisotropy = 151.0664
4 C	Isotropic = 27.4434	Anisotropy = 148.3166
5 C	Isotropic = 70.8743	Anisotropy = 143.2217
6 C	Isotropic = 52.6563	Anisotropy = 182.4777
7 C	Isotropic = 152.9517	Anisotropy = 22.3908
8 C	Isotropic = 130.0897	Anisotropy = 22.0302
9 N	Isotropic = 217.5917	Anisotropy = 12.5379
10 C	Isotropic = 16.1895	Anisotropy = 95.9679
11 O	Isotropic = 151.2334	Anisotropy = 152.6766
12 O	Isotropic = -55.2425	Anisotropy = 581.0182
13 C	Isotropic = 135.1431	Anisotropy = 78.2508
14 O	Isotropic = 227.3174	Anisotropy = 66.2440
15 H	Isotropic = 24.1311	Anisotropy = 7.5883
16 H	Isotropic = 24.5453	Anisotropy = 4.9994
17 H	Isotropic = 24.5526	Anisotropy = 5.2110
18 H	Isotropic = 23.9925	Anisotropy = 8.4173
19 H	Isotropic = 29.0366	Anisotropy = 5.9654
20 H	Isotropic = 28.3035	Anisotropy = 6.9317
21 H	Isotropic = 27.6205	Anisotropy = 5.5664
22 H	Isotropic = 26.7745	Anisotropy = 16.0651
23 H	Isotropic = 27.0676	Anisotropy = 13.0278
24 H	Isotropic = 27.2634	Anisotropy = 13.7297
25 H	Isotropic = 27.8426	Anisotropy = 8.7792
26 H	Isotropic = 27.7611	Anisotropy = 8.3670
27 H	Isotropic = 27.8525	Anisotropy = 9.1699
28 H	Isotropic = 27.2195	Anisotropy = 14.1791

Conformer_6

C	-0.435690471326	1.891756136394	-0.121725323508
C	-1.461411988068	1.379998133400	0.674722323960
C	-2.632150220182	2.095029550816	0.885797034003
C	-2.790325931273	3.348798881638	0.296795392494
C	-1.780630631195	3.875638593107	-0.501993443488
C	-0.615137495099	3.146440589352	-0.705025573028
C	0.840830242423	1.110634544951	-0.323164954911
C	1.777083498294	1.188310596483	0.890904414201
N	2.190566212252	2.600241081061	1.133443827430
C	2.986014748592	0.291204136410	0.683671340029
O	4.082531614749	0.977978427953	0.389423484205
O	2.917028467956	-0.908120531346	0.753624653512
C	5.280343177555	0.210844907194	0.143186262690
O	-3.915138356032	4.095048302908	0.471049589342
H	-1.348706513286	0.401103509094	1.134233608833
H	-3.424548179069	1.680252333309	1.503915628741
H	-1.915323597609	4.849786908082	-0.961168037790
H	0.166486603086	3.561972477553	-1.336229978782
H	1.373394983898	1.472595319431	-1.209001970889
H	0.615995525217	0.053503872209	-0.483648528275
H	1.260754835022	0.852414135285	1.791625481812
H	1.361434323836	3.193343993437	1.243566400529
H	2.744658374432	2.696647253734	1.988528502625
H	2.739639784451	2.979315545401	0.356993973228
H	5.137181405790	-0.436858283864	-0.722386742484
H	6.059488017069	0.943932248223	-0.053175366044
H	5.528528446031	-0.382863595550	1.023518404414
H	-4.536496877517	3.616850933336	1.032019597153

SCF Done: E(RwB97X) = -669.824120573

Zero-point correction=	0.239597
Thermal correction to Energy=	0.253277
Thermal correction to Enthalpy=	0.254221
Thermal correction to Gibbs Free Energy=	0.198537
Sum of electronic and zero-point Energies=	-669.584523
Sum of electronic and thermal Energies=	-669.570844
Sum of electronic and thermal Enthalpies=	-669.569900
Sum of electronic and thermal Free Energies=	-669.625583

1 C	Isotropic =	58.9162	Anisotropy =	180.0469
2 C	Isotropic =	51.9820	Anisotropy =	180.5701
3 C	Isotropic =	70.6224	Anisotropy =	143.3676

4	C	Isotropic =	27.3307	Anisotropy =	148.5137
5	C	Isotropic =	71.4592	Anisotropy =	151.3592
6	C	Isotropic =	51.1772	Anisotropy =	173.6976
7	C	Isotropic =	152.7823	Anisotropy =	22.1402
8	C	Isotropic =	129.9387	Anisotropy =	20.3918
9	N	Isotropic =	217.9786	Anisotropy =	12.8568
10	C	Isotropic =	16.3007	Anisotropy =	96.8839
11	O	Isotropic =	152.9774	Anisotropy =	155.5370
12	O	Isotropic =	-59.7331	Anisotropy =	578.6004
13	C	Isotropic =	135.1478	Anisotropy =	78.3381
14	O	Isotropic =	226.9845	Anisotropy =	65.8474
15	H	Isotropic =	23.9847	Anisotropy =	8.2578
16	H	Isotropic =	24.5406	Anisotropy =	5.2242
17	H	Isotropic =	24.5102	Anisotropy =	5.0897
18	H	Isotropic =	24.1406	Anisotropy =	7.6987
19	H	Isotropic =	29.0065	Anisotropy =	5.7659
20	H	Isotropic =	28.4965	Anisotropy =	6.6098
21	H	Isotropic =	27.8165	Anisotropy =	5.8665
22	H	Isotropic =	27.2132	Anisotropy =	14.5553
23	H	Isotropic =	26.9328	Anisotropy =	16.5585
24	H	Isotropic =	26.8835	Anisotropy =	13.0151
25	H	Isotropic =	27.8867	Anisotropy =	8.7884
26	H	Isotropic =	27.7431	Anisotropy =	8.3825
27	H	Isotropic =	27.8558	Anisotropy =	9.1484
28	H	Isotropic =	27.1969	Anisotropy =	14.1952

Conformer_7

C	-0.380022367794	1.941063176485	-0.153460673813
C	-0.568930719326	3.284693441332	-0.466511070652
C	-1.793850846444	3.910260813492	-0.250903662089
C	-2.850371238729	3.184518219735	0.289046384575
C	-2.680735593045	1.837768191532	0.609074226243
C	-1.455352752268	1.229812098583	0.387394852596
C	0.950299949486	1.263287535862	-0.381616836587
C	1.688441568193	0.944514238250	0.922732837185
N	1.992850372372	2.201764887032	1.665026004243
C	2.950435795500	0.139921878240	0.651973468479
O	4.045777899176	0.733970682382	1.107713756783
O	2.923841973511	-0.920279597616	0.083199930601
C	5.294001921874	0.041477537922	0.891382573920
O	-4.071459739023	3.738650438206	0.523886747274
H	0.250914562698	3.857801954195	-0.891928391049
H	-1.925412837982	4.959192497289	-0.504714634115
H	-3.513679879485	1.278603955527	1.023573235367

H	-1.334280702024	0.177585193598	0.633795607219
H	1.594010854248	1.889499348903	-1.008454917637
H	0.808197018890	0.313506863011	-0.902254394948
H	1.056803940821	0.343598247306	1.581469915483
H	2.492391928789	2.023962188903	2.539590622965
H	2.554821679758	2.852024254347	1.107293180172
H	1.120810783969	2.683284705222	1.906012645743
H	5.463957319403	-0.095180835639	-0.177200606774
H	6.059769865889	0.683456255382	1.321077212380
H	5.276474121539	-0.924020187652	1.398116358997
H	-4.063304879995	4.664162018170	0.254185627439

SCF Done: E(RwB97X) = -669.824242872

Zero-point correction=	0.239596
Thermal correction to Energy=	0.253215
Thermal correction to Enthalpy=	0.254159
Thermal correction to Gibbs Free Energy=	0.198717
Sum of electronic and zero-point Energies=	-669.584647
Sum of electronic and thermal Energies=	-669.571028
Sum of electronic and thermal Enthalpies=	-669.570084
Sum of electronic and thermal Free Energies=	-669.625526

1 C	Isotropic =	58.5876	Anisotropy =	180.1054
2 C	Isotropic =	51.6382	Anisotropy =	171.0381
3 C	Isotropic =	72.4412	Anisotropy =	140.3442
4 C	Isotropic =	27.3567	Anisotropy =	148.2754
5 C	Isotropic =	69.9668	Anisotropy =	153.9647
6 C	Isotropic =	52.1612	Anisotropy =	183.7011
7 C	Isotropic =	152.9244	Anisotropy =	22.3904
8 C	Isotropic =	130.1568	Anisotropy =	22.0896
9 N	Isotropic =	217.6229	Anisotropy =	12.5666
10 C	Isotropic =	16.1806	Anisotropy =	95.9496
11 O	Isotropic =	151.2177	Anisotropy =	152.6442
12 O	Isotropic =	-55.2777	Anisotropy =	581.0725
13 C	Isotropic =	135.1402	Anisotropy =	78.2496
14 O	Isotropic =	227.0914	Anisotropy =	65.1970
15 H	Isotropic =	24.1988	Anisotropy =	7.6292
16 H	Isotropic =	24.6852	Anisotropy =	5.0929
17 H	Isotropic =	24.4001	Anisotropy =	5.1228
18 H	Isotropic =	23.9301	Anisotropy =	8.3576
19 H	Isotropic =	29.0359	Anisotropy =	5.9394
20 H	Isotropic =	28.2978	Anisotropy =	6.9735
21 H	Isotropic =	27.6057	Anisotropy =	5.5618
22 H	Isotropic =	26.7755	Anisotropy =	16.0694
23 H	Isotropic =	27.0780	Anisotropy =	13.0365

24	H	Isotropic =	27.2643	Anisotropy =	13.7628
25	H	Isotropic =	27.8427	Anisotropy =	8.7724
26	H	Isotropic =	27.7626	Anisotropy =	8.3591
27	H	Isotropic =	27.8519	Anisotropy =	9.1779
28	H	Isotropic =	27.2212	Anisotropy =	14.0804

Conformer_8

C	-0.465410564707	1.819350573640	-0.068892909539
C	-0.715566214565	3.099312630180	-0.558101909577
C	-1.923782381649	3.743588135177	-0.306877631828
C	-2.900948235033	3.101433433834	0.446113433477
C	-2.670057402109	1.818981537376	0.942900855552
C	-1.461787225008	1.191635991421	0.684866079372
C	0.853206495688	1.128403251571	-0.321898542652
C	1.774013693377	1.149657061304	0.906133857926
N	2.103708861075	2.555554782410	1.277309498521
C	3.033727757555	0.343586587583	0.636641217156
O	4.093794623191	1.113842117589	0.427499249993
O	3.030949037762	-0.858940268546	0.592660478538
C	5.335730185634	0.439877639462	0.132038426584
O	-4.101453938658	3.677913184256	0.726107848823
H	0.040369027371	3.606093717218	-1.152711968390
H	-2.105075129540	4.741322406138	-0.698791395565
H	-3.442353754836	1.324631826397	1.523679353852
H	-1.291338388897	0.189518414800	1.070850610258
H	1.372109824937	1.595102579132	-1.165859984414
H	0.687739802591	0.078913589358	-0.576993317678
H	1.270542227354	0.706795342434	1.767072869855
H	2.635142211528	3.032910125057	0.543991610874
H	1.240677079512	3.087986697097	1.429109191844
H	2.645229199693	2.607303970152	2.144219662684
H	6.074614807581	1.229766043927	0.017089752757
H	5.606621455415	-0.218342833417	0.958132537642
H	5.239429863474	-0.131666079460	-0.791683404002
H	-4.142132918737	4.552167543912	0.321794527936

SCF Done: E(RwB97X) = -669.824154919

Zero-point correction=	0.239508
Thermal correction to Energy=	0.253255
Thermal correction to Enthalpy=	0.254199
Thermal correction to Gibbs Free Energy=	0.198202
Sum of electronic and zero-point Energies=	-669.584647
Sum of electronic and thermal Energies=	-669.570900

Sum of electronic and thermal Enthalpies= -669.569956
Sum of electronic and thermal Free Energies= -669.625953

1 C	Isotropic =	58.9682	Anisotropy =	179.8658
2 C	Isotropic =	51.7127	Anisotropy =	172.2897
3 C	Isotropic =	72.4470	Anisotropy =	140.6747
4 C	Isotropic =	27.2660	Anisotropy =	148.5393
5 C	Isotropic =	69.7962	Anisotropy =	154.1769
6 C	Isotropic =	51.5328	Anisotropy =	182.0989
7 C	Isotropic =	152.7478	Anisotropy =	22.2177
8 C	Isotropic =	130.0457	Anisotropy =	20.6192
9 N	Isotropic =	217.9698	Anisotropy =	12.8315
10 C	Isotropic =	16.3054	Anisotropy =	96.8749
11 O	Isotropic =	152.9326	Anisotropy =	155.3756
12 O	Isotropic =	-59.6263	Anisotropy =	578.6642
13 C	Isotropic =	135.1505	Anisotropy =	78.3415
14 O	Isotropic =	226.7896	Anisotropy =	65.1218
15 H	Isotropic =	24.2024	Anisotropy =	7.7444
16 H	Isotropic =	24.6613	Anisotropy =	5.1716
17 H	Isotropic =	24.4153	Anisotropy =	5.1042
18 H	Isotropic =	23.9217	Anisotropy =	8.2119
19 H	Isotropic =	29.0112	Anisotropy =	5.7535
20 H	Isotropic =	28.4881	Anisotropy =	6.6577
21 H	Isotropic =	27.7902	Anisotropy =	5.8732
22 H	Isotropic =	26.9045	Anisotropy =	13.0083
23 H	Isotropic =	27.2322	Anisotropy =	14.5481
24 H	Isotropic =	26.9354	Anisotropy =	16.5440
25 H	Isotropic =	27.7447	Anisotropy =	8.3735
26 H	Isotropic =	27.8570	Anisotropy =	9.1579
27 H	Isotropic =	27.8854	Anisotropy =	8.7865
28 H	Isotropic =	27.1707	Anisotropy =	14.0957

Conformer_9

C	-0.429063934804	1.113347463281	0.078218886235
C	-0.179656854250	2.238776947209	-0.709169656044
C	-0.861075619543	3.431026550743	-0.498167703458
C	-1.814301817627	3.511417817946	0.514543626839
C	-2.083472597635	2.399291823726	1.306887444331
C	-1.393145895401	1.215562155789	1.083868807937
C	0.331748127405	-0.174735806162	-0.135152955328
C	1.680053857683	-0.232613460324	0.595258505537
N	1.481756109271	-0.128257438818	2.070027227611
C	2.640856480781	0.834128923330	0.092259030082
O	2.972686563209	1.710752798258	1.030164915865

O	3.035190272524	0.852006985971	-1.044862856353
C	3.863317706878	2.775227536019	0.631972666719
O	-2.515417615601	4.650490150397	0.764820293923
H	0.549402623103	2.186734916419	-1.513893601880
H	-0.658853139009	4.295771299179	-1.125163515890
H	-2.834725087319	2.467323989414	2.087280404279
H	-1.618627538631	0.348948134521	1.701080701390
H	0.541680772193	-0.328990793373	-1.195884155804
H	-0.264023826891	-1.026635567867	0.204268335913
H	2.149611686407	-1.200999512500	0.414438732401
H	2.358386757727	-0.246219849291	2.583957506310
H	1.078472818233	0.771176798039	2.349526861045
H	0.842590925896	-0.862856377003	2.388271284475
H	3.390813066127	3.380384753549	-0.142930843883
H	4.028881319636	3.366773477584	1.529589804682
H	4.803319792229	2.358740904707	0.268406660763
H	-2.241704952590	5.340925379255	0.150183592304

SCF Done: E(RwB97X) = -669.824575947

Zero-point correction=	0.239409
Thermal correction to Energy=	0.253110
Thermal correction to Enthalpy=	0.254054
Thermal correction to Gibbs Free Energy=	0.197882
Sum of electronic and zero-point Energies=	-669.585167
Sum of electronic and thermal Energies=	-669.571466
Sum of electronic and thermal Enthalpies=	-669.570522
Sum of electronic and thermal Free Energies=	-669.626694

1 C	Isotropic =	60.8726	Anisotropy =	180.8610
2 C	Isotropic =	52.9378	Anisotropy =	177.4721
3 C	Isotropic =	71.0449	Anisotropy =	143.8379
4 C	Isotropic =	27.1366	Anisotropy =	149.2892
5 C	Isotropic =	70.8634	Anisotropy =	152.4529
6 C	Isotropic =	51.0156	Anisotropy =	175.3389
7 C	Isotropic =	154.2890	Anisotropy =	14.2692
8 C	Isotropic =	131.8568	Anisotropy =	27.0314
9 N	Isotropic =	217.3010	Anisotropy =	18.0694
10 C	Isotropic =	16.2049	Anisotropy =	100.1247
11 O	Isotropic =	145.4039	Anisotropy =	166.3526
12 O	Isotropic =	-59.9917	Anisotropy =	586.9923
13 C	Isotropic =	135.4744	Anisotropy =	77.7079
14 O	Isotropic =	226.9708	Anisotropy =	64.8036
15 H	Isotropic =	24.3492	Anisotropy =	7.7474
16 H	Isotropic =	24.6303	Anisotropy =	5.3898
17 H	Isotropic =	24.4699	Anisotropy =	4.9730

18 H	Isotropic =	24.1391	Anisotropy =	7.6867
19 H	Isotropic =	28.3273	Anisotropy =	7.7051
20 H	Isotropic =	28.7593	Anisotropy =	8.2592
21 H	Isotropic =	27.4607	Anisotropy =	7.3547
22 H	Isotropic =	26.8146	Anisotropy =	16.4728
23 H	Isotropic =	27.0718	Anisotropy =	10.4338
24 H	Isotropic =	26.9834	Anisotropy =	15.7401
25 H	Isotropic =	28.0865	Anisotropy =	7.9560
26 H	Isotropic =	28.0568	Anisotropy =	8.5857
27 H	Isotropic =	27.9065	Anisotropy =	9.8056
28 H	Isotropic =	27.2357	Anisotropy =	14.0339

2-(pyrrolidin-1-yl)ethan-1-ol_neutral

Conformer_1

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N      -0.396108483440    1.289608498059    0.151309831797
C      -1.844075652730    1.385235923035   -0.023606854041
C      -2.167635393025    2.834504650118    0.349843846213
C      -1.023559342921    3.246891872393    1.306640201733
C      -0.140778601132    1.999025142525    1.405139894663
C       0.104192273215   -0.075402362609    0.116822675142
C       1.613932617680   -0.081604791696   -0.057566719160
O       1.987312645252    0.687990881344   -1.193418959977
H      -2.128444138207    1.121469768246   -1.046053102669
H      -2.358681602823    0.688465876870    0.662637002110
H      -2.171968232190    3.467409858569   -0.541268544354
H      -3.152900582100    2.914833307287    0.814516235095
H      -0.456805004327    4.084664662314    0.892402410733
H      -1.388334811978    3.552078259332    2.290008286669
H      -0.448638462428    1.373898223730    2.263071035810
H       0.920461613830    2.232966142207    1.523499956499
H      -0.171540617667   -0.635368792223    1.027885066303
H      -0.353728624898   -0.580736406662   -0.740313413461
H       2.106483740652    0.309732938517    0.843314329589
H       1.970121136433   -1.103130163599   -0.214204765211
H       1.368195522803    1.430566512242   -1.202358413483

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SCF Done: E(RwB97X) = -366.449365990

Zero-point correction=	0.193039
Thermal correction to Energy=	0.201353
Thermal correction to Enthalpy=	0.202297
Thermal correction to Gibbs Free Energy=	0.159494
Sum of electronic and zero-point Energies=	-366.256327
Sum of electronic and thermal Energies=	-366.248013

Sum of electronic and thermal Enthalpies= -366.247069
Sum of electronic and thermal Free Energies= -366.289872

1 N	Isotropic =	205.7368	Anisotropy =	57.2572
2 C	Isotropic =	134.7237	Anisotropy =	63.1333
3 C	Isotropic =	167.7937	Anisotropy =	23.0489
4 C	Isotropic =	166.7910	Anisotropy =	24.7277
5 C	Isotropic =	139.0209	Anisotropy =	57.1979
6 C	Isotropic =	133.8944	Anisotropy =	39.9940
7 C	Isotropic =	131.0646	Anisotropy =	57.6298
8 O	Isotropic =	314.4877	Anisotropy =	41.8701
9 H	Isotropic =	28.9680	Anisotropy =	9.1513
10 H	Isotropic =	29.6891	Anisotropy =	8.2156
11 H	Isotropic =	30.0770	Anisotropy =	10.7093
12 H	Isotropic =	30.1578	Anisotropy =	10.9625
13 H	Isotropic =	30.0889	Anisotropy =	10.5698
14 H	Isotropic =	30.0965	Anisotropy =	10.8999
15 H	Isotropic =	30.2054	Anisotropy =	8.2980
16 H	Isotropic =	28.7388	Anisotropy =	8.0791
17 H	Isotropic =	29.8200	Anisotropy =	7.2889
18 H	Isotropic =	28.9339	Anisotropy =	9.2897
19 H	Isotropic =	28.1306	Anisotropy =	6.3745
20 H	Isotropic =	28.4207	Anisotropy =	7.8606
21 H	Isotropic =	29.6209	Anisotropy =	17.2857

Conformer_10

N	-0.646453483355	1.809240406355	-0.022084842864
C	-2.045328414017	1.429015399569	0.162777430966
C	-2.668100551369	2.642148018719	0.854885908740
C	-1.488330256084	3.285177636352	1.621401237267
C	-0.276638826890	2.419595640026	1.255525258717
C	0.188325417973	0.688287769774	-0.413162330048
C	1.601987788702	1.115125756115	-0.780786626081
O	2.373066356028	0.014330413208	-1.253041330359
H	-2.510912040054	1.181346178588	-0.795289834829
H	-2.116182751910	0.538685546372	0.815315359892
H	-3.069844876655	3.338075842772	0.113823440863
H	-3.489547996622	2.350157935043	1.513022975899
H	-1.335199464186	4.317987977347	1.298451364374
H	-1.649498115298	3.300509164803	2.701668526289
H	-0.118115909241	1.634560930880	2.018542633259
H	0.647499775278	2.996248241906	1.170516952687
H	-0.264192753939	0.205640657900	-1.286064912052
H	0.234934916689	-0.068262196650	0.395674567455

H	2.102503391067	1.588801965106	0.072425057044
H	1.569705821910	1.841376644478	-1.597285794730
H	2.488421971974	-0.602149928664	-0.523815042489

SCF Done: E(RwB97X) = -366.445467640

Zero-point correction=	0.192502
Thermal correction to Energy=	0.201190
Thermal correction to Enthalpy=	0.202134
Thermal correction to Gibbs Free Energy=	0.158381
Sum of electronic and zero-point Energies=	-366.252966
Sum of electronic and thermal Energies=	-366.244278
Sum of electronic and thermal Enthalpies=	-366.243334
Sum of electronic and thermal Free Energies=	-366.287087

1 N	Isotropic = 199.5093	Anisotropy = 61.9607
2 C	Isotropic = 133.9445	Anisotropy = 64.3018
3 C	Isotropic = 167.8221	Anisotropy = 22.5816
4 C	Isotropic = 166.8854	Anisotropy = 25.1157
5 C	Isotropic = 137.0214	Anisotropy = 58.8182
6 C	Isotropic = 131.4349	Anisotropy = 63.1464
7 C	Isotropic = 126.6882	Anisotropy = 65.0478
8 O	Isotropic = 309.7014	Anisotropy = 54.0386
9 H	Isotropic = 28.9559	Anisotropy = 9.0161
10 H	Isotropic = 29.9105	Anisotropy = 7.5780
11 H	Isotropic = 30.1700	Anisotropy = 10.8739
12 H	Isotropic = 30.2153	Anisotropy = 10.8726
13 H	Isotropic = 30.1349	Anisotropy = 10.7340
14 H	Isotropic = 30.1435	Anisotropy = 10.6988
15 H	Isotropic = 30.2251	Anisotropy = 7.4517
16 H	Isotropic = 28.9369	Anisotropy = 8.0274
17 H	Isotropic = 28.9478	Anisotropy = 7.0174
18 H	Isotropic = 29.9990	Anisotropy = 5.5236
19 H	Isotropic = 27.9343	Anisotropy = 6.2485
20 H	Isotropic = 28.3339	Anisotropy = 4.0551
21 H	Isotropic = 31.5000	Anisotropy = 17.2036

Conformer_11

N	-0.609310845760	1.110367896639	0.425876251123
C	-0.091312685129	2.452951728354	0.158662417327
C	-1.042614907408	3.390989300665	0.916075686919
C	-2.331267611059	2.560922945768	1.115126568300
C	-2.060302254848	1.269186102911	0.346803049677
C	-0.124131281699	0.071166801262	-0.468895347643

C	1.353107062008	-0.259352993417	-0.326269194501
O	2.231539899954	0.627105115812	-1.017977044671
H	0.941900230843	2.558997924145	0.504047431751
H	-0.116692804301	2.668228041918	-0.924875545690
H	-0.615160412313	3.681973067152	1.878612343834
H	-1.221069941985	4.306439824869	0.347574995433
H	-2.488880446132	2.344582176749	2.174993176387
H	-3.223317139844	3.071220637486	0.744942527023
H	-2.378901013874	1.375900024050	-0.707115973303
H	-2.568063523928	0.395144239349	0.764467381388
H	-0.328276753956	0.329083029426	-1.525615071867
H	-0.686164047534	-0.842255669617	-0.243718957550
H	1.531281441351	-1.242922607715	-0.767869197472
H	1.620797797510	-0.315867325052	0.736796929305
H	2.257339238103	1.464739739247	-0.548742425770

SCF Done: E(RwB97X) = -366.444698321

Zero-point correction=	0.192303
Thermal correction to Energy=	0.200984
Thermal correction to Enthalpy=	0.201928
Thermal correction to Gibbs Free Energy=	0.157886
Sum of electronic and zero-point Energies=	-366.252395
Sum of electronic and thermal Energies=	-366.243714
Sum of electronic and thermal Enthalpies=	-366.242770
Sum of electronic and thermal Free Energies=	-366.286813

1 N	Isotropic = 192.2012	Anisotropy = 76.8731
2 C	Isotropic = 136.2796	Anisotropy = 55.7619
3 C	Isotropic = 166.1729	Anisotropy = 26.9767
4 C	Isotropic = 167.8547	Anisotropy = 22.2201
5 C	Isotropic = 133.5892	Anisotropy = 64.0541
6 C	Isotropic = 130.6770	Anisotropy = 37.6062
7 C	Isotropic = 124.0230	Anisotropy = 48.9839
8 O	Isotropic = 296.3179	Anisotropy = 22.5375
9 H	Isotropic = 28.8931	Anisotropy = 7.6284
10 H	Isotropic = 29.9081	Anisotropy = 6.8142
11 H	Isotropic = 30.0110	Anisotropy = 10.6099
12 H	Isotropic = 30.0478	Anisotropy = 10.5776
13 H	Isotropic = 30.1851	Anisotropy = 10.8692
14 H	Isotropic = 30.2127	Anisotropy = 10.9604
15 H	Isotropic = 29.8815	Anisotropy = 7.7053
16 H	Isotropic = 28.9785	Anisotropy = 9.0589
17 H	Isotropic = 29.7696	Anisotropy = 6.9167
18 H	Isotropic = 28.9820	Anisotropy = 7.9706
19 H	Isotropic = 28.1743	Anisotropy = 7.4871

20 H Isotropic = 27.9280 Anisotropy = 6.0851
 21 H Isotropic = 30.8955 Anisotropy = 15.0874

Conformer_12

N	-0.714534380701	1.241107858449	-0.057276520514
C	0.004647184565	2.333774708344	0.599304142711
C	-1.061870352724	3.414997182195	0.827402768480
C	-2.406083180547	2.653912068038	0.771642267677
C	-1.995253068295	1.188423255996	0.645461467694
C	-0.031913446412	-0.043355528684	-0.045468540712
C	1.230191754048	-0.106427733824	-0.891011126851
O	2.396277050838	0.422464310490	-0.261383803406
H	0.425088652399	1.995155086972	1.563468868113
H	0.827379199336	2.701298647309	-0.022069446695
H	-0.907899972638	3.917929976297	1.784711795520
H	-1.014205787912	4.177406915636	0.046168603818
H	-3.024844688472	2.824989279166	1.655417935489
H	-2.985305180209	2.960993369074	-0.103093468043
H	-2.714302601087	0.576853588750	0.093044433210
H	-1.865994228435	0.738777752453	1.647831802129
H	0.218965086910	-0.350873599737	0.987655464691
H	-0.729899553192	-0.787818875753	-0.444860842759
H	1.461481905613	-1.155980732110	-1.088767742389
H	1.056231905897	0.386025549198	-1.856511562326
H	2.325543701018	1.379946921741	-0.234866495835

SCF Done: E(RwB97X) = -366.444698297

Zero-point correction=	0.192301
Thermal correction to Energy=	0.200984
Thermal correction to Enthalpy=	0.201928
Thermal correction to Gibbs Free Energy=	0.157870
Sum of electronic and zero-point Energies=	-366.252397
Sum of electronic and thermal Energies=	-366.243714
Sum of electronic and thermal Enthalpies=	-366.242770
Sum of electronic and thermal Free Energies=	-366.286828

1 N	Isotropic = 192.2007	Anisotropy = 76.8653
2 C	Isotropic = 136.2796	Anisotropy = 55.7580
3 C	Isotropic = 166.1717	Anisotropy = 26.9774
4 C	Isotropic = 167.8572	Anisotropy = 22.2200
5 C	Isotropic = 133.5903	Anisotropy = 64.0589
6 C	Isotropic = 130.6772	Anisotropy = 37.6045
7 C	Isotropic = 124.0245	Anisotropy = 48.9855

8	O	Isotropic =	296.3152	Anisotropy =	22.5262
9	H	Isotropic =	29.9082	Anisotropy =	6.8145
10	H	Isotropic =	28.8932	Anisotropy =	7.6283
11	H	Isotropic =	30.0478	Anisotropy =	10.5778
12	H	Isotropic =	30.0110	Anisotropy =	10.6098
13	H	Isotropic =	30.2127	Anisotropy =	10.9603
14	H	Isotropic =	30.1851	Anisotropy =	10.8695
15	H	Isotropic =	28.9784	Anisotropy =	9.0589
16	H	Isotropic =	29.8816	Anisotropy =	7.7052
17	H	Isotropic =	29.7697	Anisotropy =	6.9166
18	H	Isotropic =	28.9818	Anisotropy =	7.9709
19	H	Isotropic =	28.1742	Anisotropy =	7.4871
20	H	Isotropic =	27.9281	Anisotropy =	6.0849
21	H	Isotropic =	30.8954	Anisotropy =	15.0874

Conformer_13

N	-0.465553478074	1.310128080959	0.720937245902
C	-0.641402591711	2.390448813411	-0.251020399765
C	-1.995582836615	3.003749162865	0.119046363792
C	-2.170977489416	2.669489272279	1.619611870428
C	-0.893029848969	1.910633441816	1.983737119196
C	0.880155401480	0.765305192515	0.796018549391
C	1.261052977473	-0.139908450564	-0.355814571143
O	1.479921484989	0.628685913151	-1.538960208391
H	0.164433683205	3.139029800964	-0.131593033250
H	-0.591803178896	2.013379922917	-1.273007250937
H	-2.010974336524	4.078698097008	-0.075827965412
H	-2.796690897849	2.552698817463	-0.472510344808
H	-2.295993164732	3.561393231327	2.237953451460
H	-3.048461660672	2.036127580310	1.773858287274
H	-1.041558572917	1.142759571302	2.748274806543
H	-0.124045103760	2.614428327141	2.353982639351
H	1.631238618189	1.573049572967	0.884516888563
H	0.944981661811	0.163079707264	1.708793189899
H	2.178303674041	-0.678311610002	-0.085155315380
H	0.465090009578	-0.877834375050	-0.520318361227
H	1.739895649368	0.025269929956	-2.240122961488

SCF Done: E(RwB97X) = -366.444700200

Zero-point correction=	0.192349
Thermal correction to Energy=	0.200930
Thermal correction to Enthalpy=	0.201874
Thermal correction to Gibbs Free Energy=	0.158659

Sum of electronic and zero-point Energies=	-366.252351
Sum of electronic and thermal Energies=	-366.243770
Sum of electronic and thermal Enthalpies=	-366.242826
Sum of electronic and thermal Free Energies=	-366.286041

1	N	Isotropic =	190.7894	Anisotropy =	72.7798
2	C	Isotropic =	134.6136	Anisotropy =	57.6472
3	C	Isotropic =	166.2229	Anisotropy =	25.8805
4	C	Isotropic =	168.1081	Anisotropy =	22.3235
5	C	Isotropic =	133.7269	Anisotropy =	64.1926
6	C	Isotropic =	134.0149	Anisotropy =	42.9039
7	C	Isotropic =	123.8741	Anisotropy =	45.7707
8	O	Isotropic =	306.8592	Anisotropy =	101.6161
9	H	Isotropic =	30.0956	Anisotropy =	6.8513
10	H	Isotropic =	28.3604	Anisotropy =	7.4604
11	H	Isotropic =	30.1294	Anisotropy =	10.6577
12	H	Isotropic =	30.0978	Anisotropy =	10.5335
13	H	Isotropic =	30.2310	Anisotropy =	10.8971
14	H	Isotropic =	30.1876	Anisotropy =	10.8664
15	H	Isotropic =	28.9647	Anisotropy =	8.9838
16	H	Isotropic =	29.8488	Anisotropy =	7.6623
17	H	Isotropic =	29.7226	Anisotropy =	7.1023
18	H	Isotropic =	29.0975	Anisotropy =	8.2405
19	H	Isotropic =	27.9692	Anisotropy =	7.7507
20	H	Isotropic =	27.9424	Anisotropy =	6.3122
21	H	Isotropic =	31.2864	Anisotropy =	21.0047

Conformer_14

N	-0.184926394631	1.633917626754	0.820727183769
C	-0.970329631292	1.999760756407	-0.358583147441
C	-1.901771449209	3.105389960186	0.147558340500
C	-2.040918474162	2.826635442126	1.662665549749
C	-1.173766123881	1.586830189127	1.896768470053
C	0.561514877696	0.392377213394	0.702212277989
C	1.778385365380	0.470392203581	-0.195243771158
O	1.380904015733	0.495979634597	-1.566481056269
H	-0.324699726398	2.309657543023	-1.181216529362
H	-1.559585988273	1.130043228608	-0.705231911939
H	-1.457133641235	4.089314792062	-0.024113677699
H	-2.862690507161	3.084529233382	-0.371999357935
H	-1.667115890489	3.671358193467	2.247124221151
H	-3.076596309602	2.651155223738	1.962807214859
H	-1.788154488376	0.670813350463	1.813604604952
H	-0.682542980464	1.573527740525	2.873946364666

H	0.916949423467	0.121854657733	1.702441666483
H	-0.089601315331	-0.431764671929	0.353802057043
H	2.359516177756	1.368215118990	0.052335615765
H	2.407182786947	-0.408809517551	-0.006063597304
H	2.176180273528	0.534322081316	-2.104460517875

SCF Done: E(RwB97X) = -366.444679906

Zero-point correction=	0.192202
Thermal correction to Energy=	0.200869
Thermal correction to Enthalpy=	0.201813
Thermal correction to Gibbs Free Energy=	0.158082
Sum of electronic and zero-point Energies=	-366.252478
Sum of electronic and thermal Energies=	-366.243811
Sum of electronic and thermal Enthalpies=	-366.242867
Sum of electronic and thermal Free Energies=	-366.286598

1 N	Isotropic = 190.9627	Anisotropy = 73.4669
2 C	Isotropic = 134.8045	Anisotropy = 56.4738
3 C	Isotropic = 166.1294	Anisotropy = 25.9935
4 C	Isotropic = 168.2232	Anisotropy = 22.3830
5 C	Isotropic = 133.9339	Anisotropy = 64.4244
6 C	Isotropic = 133.9824	Anisotropy = 42.3952
7 C	Isotropic = 124.0609	Anisotropy = 45.9723
8 O	Isotropic = 306.8060	Anisotropy = 103.0611
9 H	Isotropic = 28.3868	Anisotropy = 7.5135
10 H	Isotropic = 30.0835	Anisotropy = 6.8546
11 H	Isotropic = 30.0957	Anisotropy = 10.5295
12 H	Isotropic = 30.1219	Anisotropy = 10.6492
13 H	Isotropic = 30.1769	Anisotropy = 10.8821
14 H	Isotropic = 30.2263	Anisotropy = 10.8914
15 H	Isotropic = 29.8510	Anisotropy = 7.6683
16 H	Isotropic = 28.9559	Anisotropy = 8.9930
17 H	Isotropic = 29.0755	Anisotropy = 8.3007
18 H	Isotropic = 29.7338	Anisotropy = 7.0641
19 H	Isotropic = 27.9467	Anisotropy = 6.2141
20 H	Isotropic = 27.9583	Anisotropy = 7.7577
21 H	Isotropic = 31.3058	Anisotropy = 20.9894

Conformer_15

N	-0.432596767195	2.274882308203	-0.168748373903
C	-0.289856770464	2.921142131547	1.144639028957
C	-1.439634710843	2.385878521424	2.032496687285
C	-2.475117837078	1.838780169482	1.026310351414

C	-1.888434153741	2.223273971214	-0.344458562690
C	0.185782190818	0.948571676913	-0.195881311338
C	1.674247276624	1.051462407669	-0.499496450384
O	2.309994996979	-0.222476769033	-0.483884949324
H	0.701477959747	2.735382757174	1.564102792696
H	-0.394233273879	4.002715564212	1.008515849503
H	-1.087444927507	1.597252710719	2.702544582112
H	-1.850187830247	3.182864905920	2.657489077891
H	-2.564123024659	0.751831115618	1.111593376786
H	-3.472186352633	2.261560687218	1.172618614602
H	-2.231569214205	3.224982476009	-0.628367304607
H	-2.156593892835	1.535193110136	-1.149475660615
H	0.050564619347	0.393262317794	0.746874406998
H	-0.289937564906	0.361804939804	-0.989928912963
H	2.183648571388	1.651644527750	0.259073976052
H	1.815230992985	1.545625379181	-1.469190804403
H	1.937169712305	-0.747934908951	-1.198126414069

SCF Done: E(RwB97X) = -366.441750187

Zero-point correction=	0.192675
Thermal correction to Energy=	0.201259
Thermal correction to Enthalpy=	0.202203
Thermal correction to Gibbs Free Energy=	0.158816
Sum of electronic and zero-point Energies=	-366.249076
Sum of electronic and thermal Energies=	-366.240491
Sum of electronic and thermal Enthalpies=	-366.239547
Sum of electronic and thermal Free Energies=	-366.282935

1 N	Isotropic =	202.2691	Anisotropy =	35.5224
2 C	Isotropic =	139.1960	Anisotropy =	59.2856
3 C	Isotropic =	169.6184	Anisotropy =	30.7380
4 C	Isotropic =	167.9182	Anisotropy =	26.8659
5 C	Isotropic =	133.2899	Anisotropy =	64.9293
6 C	Isotropic =	133.0010	Anisotropy =	63.6872
7 C	Isotropic =	125.4888	Anisotropy =	70.1547
8 O	Isotropic =	307.7377	Anisotropy =	46.8622
9 H	Isotropic =	28.9826	Anisotropy =	7.7191
10 H	Isotropic =	29.4104	Anisotropy =	11.2142
11 H	Isotropic =	29.9985	Anisotropy =	10.1283
12 H	Isotropic =	30.3401	Anisotropy =	11.4056
13 H	Isotropic =	30.1773	Anisotropy =	9.9180
14 H	Isotropic =	30.2801	Anisotropy =	11.3180
15 H	Isotropic =	29.2259	Anisotropy =	11.0383
16 H	Isotropic =	29.0563	Anisotropy =	8.6150
17 H	Isotropic =	29.3389	Anisotropy =	7.1950

18 H	Isotropic =	29.6662	Anisotropy =	6.9935
19 H	Isotropic =	28.3243	Anisotropy =	4.6381
20 H	Isotropic =	28.1362	Anisotropy =	4.1612
21 H	Isotropic =	31.4635	Anisotropy =	17.1650

Conformer_16

N	-0.753932078038	1.018759233171	0.678956721169
C	-0.542728855988	1.932696378425	1.811707932573
C	-1.211928997322	3.276059329126	1.431793083039
C	-2.202661338185	2.903833566927	0.307582253764
C	-2.107006919491	1.368841318215	0.232155673142
C	0.251265741749	1.204517101626	-0.368564055781
C	1.508088393024	0.401914961250	-0.061116294066
O	2.521244163275	0.603261875851	-1.041072613489
H	-1.032882953738	1.506247152554	2.693249201889
H	0.521009986260	2.029983007330	2.040172066815
H	-1.713391237881	3.717720406811	2.296563451767
H	-0.472629915285	4.000680598916	1.080661556160
H	-1.898971620949	3.351911371866	-0.643023982751
H	-3.222939119074	3.235898464512	0.515094269832
H	-2.303357877867	0.961424896094	-0.762266581383
H	-2.822057261834	0.916724608561	0.929335192413
H	-0.166377725645	0.844749402483	-1.315800624758
H	0.528528584045	2.261608129953	-0.513906793288
H	1.943949148379	0.714640600796	0.891441029083
H	1.250549199059	-0.661757170062	0.020466341439
H	2.195130685507	0.260384765595	-1.878527827570

SCF Done: E(RwB97X) = -366.441750185

Zero-point correction=	0.192675
Thermal correction to Energy=	0.201259
Thermal correction to Enthalpy=	0.202203
Thermal correction to Gibbs Free Energy=	0.158816
Sum of electronic and zero-point Energies=	-366.249076
Sum of electronic and thermal Energies=	-366.240491
Sum of electronic and thermal Enthalpies=	-366.239547
Sum of electronic and thermal Free Energies=	-366.282934

1 N	Isotropic =	202.2692	Anisotropy =	35.5222
2 C	Isotropic =	139.1960	Anisotropy =	59.2857
3 C	Isotropic =	169.6183	Anisotropy =	30.7380
4 C	Isotropic =	167.9181	Anisotropy =	26.8658
5 C	Isotropic =	133.2899	Anisotropy =	64.9292

6 C	Isotropic =	133.0009	Anisotropy =	63.6874
7 C	Isotropic =	125.4887	Anisotropy =	70.1548
8 O	Isotropic =	307.7376	Anisotropy =	46.8623
9 H	Isotropic =	29.4104	Anisotropy =	11.2142
10 H	Isotropic =	28.9826	Anisotropy =	7.7191
11 H	Isotropic =	30.3401	Anisotropy =	11.4056
12 H	Isotropic =	29.9985	Anisotropy =	10.1283
13 H	Isotropic =	30.1773	Anisotropy =	9.9179
14 H	Isotropic =	30.2801	Anisotropy =	11.3180
15 H	Isotropic =	29.0563	Anisotropy =	8.6150
16 H	Isotropic =	29.2259	Anisotropy =	11.0383
17 H	Isotropic =	29.6662	Anisotropy =	6.9935
18 H	Isotropic =	29.3389	Anisotropy =	7.1950
19 H	Isotropic =	28.3244	Anisotropy =	4.6381
20 H	Isotropic =	28.1362	Anisotropy =	4.1612
21 H	Isotropic =	31.4634	Anisotropy =	17.1650

Conformer_17

N	-0.747827446951	1.381387080499	-0.087727837965
C	-0.052080168608	2.463262201456	0.610786924071
C	-1.159014848638	3.474609561959	0.929042676624
C	-2.456660595639	2.632546558285	0.947406780919
C	-1.976789492293	1.204258367686	0.684125102459
C	0.008632766111	0.147835691507	-0.215230866981
C	1.121750979424	0.188329654827	-1.247606434391
O	2.240554882998	0.992927702770	-0.881099099326
H	0.397684501120	2.079168107152	1.546204620674
H	0.753739811504	2.873031753606	0.000702015399
H	-0.973068965901	3.977778805885	1.880825720432
H	-1.210091553599	4.245903162743	0.156130510257
H	-2.994064094831	2.706324516859	1.895632388315
H	-3.137622941067	2.957077366490	0.156242948849
H	-2.697301018384	0.594488481135	0.131706312624
H	-1.759829390187	0.691740091543	1.640173429101
H	0.427725241981	-0.162497500710	0.763113249207
H	-0.685853649521	-0.641020120987	-0.526047614680
H	0.742299279113	0.608462671702	-2.183032194967
H	1.450065398783	-0.840118321270	-1.447211539015
H	2.620351304586	0.621304166864	-0.079137091605

SCF Done: E(RwB97X) = -366.445078376

Zero-point correction=	0.192495
Thermal correction to Energy=	0.201005

Thermal correction to Enthalpy=	0.201950
Thermal correction to Gibbs Free Energy=	0.158995
Sum of electronic and zero-point Energies=	-366.252584
Sum of electronic and thermal Energies=	-366.244073
Sum of electronic and thermal Enthalpies=	-366.243129
Sum of electronic and thermal Free Energies=	-366.286083

1 N	Isotropic =	191.1891	Anisotropy =	72.7722
2 C	Isotropic =	134.7789	Anisotropy =	57.3801
3 C	Isotropic =	166.2715	Anisotropy =	25.9859
4 C	Isotropic =	168.1328	Anisotropy =	22.1399
5 C	Isotropic =	133.6697	Anisotropy =	64.0794
6 C	Isotropic =	131.1307	Anisotropy =	40.5594
7 C	Isotropic =	123.0922	Anisotropy =	47.1051
8 O	Isotropic =	297.7966	Anisotropy =	71.3172
9 H	Isotropic =	30.1431	Anisotropy =	6.9217
10 H	Isotropic =	28.3415	Anisotropy =	7.5181
11 H	Isotropic =	30.1189	Anisotropy =	10.6276
12 H	Isotropic =	30.0743	Anisotropy =	10.5551
13 H	Isotropic =	30.2361	Anisotropy =	10.9033
14 H	Isotropic =	30.1891	Anisotropy =	10.9005
15 H	Isotropic =	28.9745	Anisotropy =	9.0188
16 H	Isotropic =	29.8867	Anisotropy =	7.6758
17 H	Isotropic =	29.8985	Anisotropy =	6.9319
18 H	Isotropic =	29.0673	Anisotropy =	7.8349
19 H	Isotropic =	28.1854	Anisotropy =	6.1370
20 H	Isotropic =	27.9247	Anisotropy =	7.8394
21 H	Isotropic =	31.7458	Anisotropy =	15.9995

Conformer_18

N	-0.648427078401	1.174888841237	0.453337833774
C	-0.081555326325	2.524360565487	0.450433503657
C	-1.103942207394	3.360293727368	1.228457663825
C	-2.433197844109	2.583866740881	1.075030504174
C	-2.068605528808	1.394808112906	0.184615895672
C	-0.042256964975	0.253276167415	-0.491824349845
C	1.333727606336	-0.251741636296	-0.094222078319
O	2.369839907770	0.724438293836	-0.177673562610
H	0.917015390569	2.534017312659	0.888868589510
H	0.005156803362	2.893857708601	-0.589169407066
H	-1.165299458581	4.377293460624	0.834005731827
H	-0.819529390384	3.434723137029	2.281295551457
H	-2.790234009354	2.235484372502	2.047718851371
H	-3.226398870180	3.189164087448	0.630255850978

H	-2.648233254446	0.492500334884	0.399080255644
H	-2.222947037194	1.653136093821	-0.879909996930
H	-0.693870337006	-0.624556907340	-0.569416367963
H	0.010933315690	0.702340436994	-1.504052102242
H	1.317657021523	-0.585506613485	0.946861633836
H	1.583106214387	-1.116511031064	-0.722967529833
H	2.433661047522	1.008366794491	-1.094626470916

SCF Done: E(RwB97X) = -366.445078370

Zero-point correction=	0.192494
Thermal correction to Energy=	0.201005
Thermal correction to Enthalpy=	0.201949
Thermal correction to Gibbs Free Energy=	0.158991
Sum of electronic and zero-point Energies=	-366.252585
Sum of electronic and thermal Energies=	-366.244073
Sum of electronic and thermal Enthalpies=	-366.243129
Sum of electronic and thermal Free Energies=	-366.286087

1 N	Isotropic = 191.1885	Anisotropy = 72.7665
2 C	Isotropic = 134.7792	Anisotropy = 57.3729
3 C	Isotropic = 166.2702	Anisotropy = 25.9859
4 C	Isotropic = 168.1348	Anisotropy = 22.1391
5 C	Isotropic = 133.6710	Anisotropy = 64.0827
6 C	Isotropic = 131.1306	Anisotropy = 40.5562
7 C	Isotropic = 123.0938	Anisotropy = 47.1057
8 O	Isotropic = 297.7939	Anisotropy = 71.3137
9 H	Isotropic = 28.3415	Anisotropy = 7.5184
10 H	Isotropic = 30.1432	Anisotropy = 6.9220
11 H	Isotropic = 30.1189	Anisotropy = 10.6278
12 H	Isotropic = 30.0744	Anisotropy = 10.5550
13 H	Isotropic = 30.1891	Anisotropy = 10.9007
14 H	Isotropic = 30.2361	Anisotropy = 10.9033
15 H	Isotropic = 28.9745	Anisotropy = 9.0187
16 H	Isotropic = 29.8868	Anisotropy = 7.6758
17 H	Isotropic = 29.0673	Anisotropy = 7.8351
18 H	Isotropic = 29.8987	Anisotropy = 6.9319
19 H	Isotropic = 28.1855	Anisotropy = 6.1367
20 H	Isotropic = 27.9247	Anisotropy = 7.8395
21 H	Isotropic = 31.7456	Anisotropy = 16.0001

Conformer_19

N	-0.227766124431	2.422788714904	0.190077517103
C	-1.556319575264	2.210478339616	-0.404041791785

C	-2.499102086132	1.786486688148	0.748713366398
C	-1.772896565356	2.257334137767	2.027315696423
C	-0.550805695782	3.023965715677	1.488945673905
C	0.520034675350	1.171350585416	0.322524282796
C	1.243970533631	0.838682941383	-0.968714966105
O	1.907345937509	-0.409710132230	-0.785655683434
H	-1.507915062022	1.478287573614	-1.213299622875
H	-1.894962250775	3.158369026937	-0.835386119780
H	-3.482183954870	2.250424315678	0.635887834047
H	-2.650621540652	0.703973522254	0.758228538323
H	-2.399275830512	2.888688984116	2.662420756496
H	-1.451425776737	1.402571591403	2.629610105771
H	0.315790554481	2.998450693820	2.153559179367
H	-0.815600106454	4.074228387826	1.319843182319
H	1.265252054526	1.291485429015	1.115053095009
H	-0.120901146886	0.318834069987	0.601320355627
H	1.965840526278	1.632739635964	-1.197972110303
H	0.531610510834	0.773803083814	-1.801254895384
H	2.366130923264	-0.627533305110	-1.601074393917

SCF Done: E(RwB97X) = -366.441411558

Zero-point correction=	0.192820
Thermal correction to Energy=	0.201335
Thermal correction to Enthalpy=	0.202279
Thermal correction to Gibbs Free Energy=	0.159302
Sum of electronic and zero-point Energies=	-366.248591
Sum of electronic and thermal Energies=	-366.240077
Sum of electronic and thermal Enthalpies=	-366.239132
Sum of electronic and thermal Free Energies=	-366.282110

1 N	Isotropic =	202.6988	Anisotropy =	36.2616
2 C	Isotropic =	138.9746	Anisotropy =	59.5883
3 C	Isotropic =	169.6463	Anisotropy =	30.6953
4 C	Isotropic =	167.9110	Anisotropy =	27.0344
5 C	Isotropic =	133.2683	Anisotropy =	64.8523
6 C	Isotropic =	135.2419	Anisotropy =	61.9997
7 C	Isotropic =	126.1767	Anisotropy =	69.5556
8 O	Isotropic =	315.5280	Anisotropy =	99.5637
9 H	Isotropic =	28.9871	Anisotropy =	7.7733
10 H	Isotropic =	29.4068	Anisotropy =	11.1842
11 H	Isotropic =	30.3391	Anisotropy =	11.3956
12 H	Isotropic =	29.9928	Anisotropy =	10.1433
13 H	Isotropic =	30.2678	Anisotropy =	11.3336
14 H	Isotropic =	30.1544	Anisotropy =	9.9085
15 H	Isotropic =	29.0103	Anisotropy =	8.6626

16	H	Isotropic =	29.2102	Anisotropy =	11.0696
17	H	Isotropic =	29.4826	Anisotropy =	6.9314
18	H	Isotropic =	29.3583	Anisotropy =	7.3116
19	H	Isotropic =	28.1396	Anisotropy =	4.1962
20	H	Isotropic =	28.1410	Anisotropy =	5.1241
21	H	Isotropic =	31.3058	Anisotropy =	20.5800

Conformer_2

N	-0.404800385004	1.314504399186	0.087859650974
C	-0.384213194152	2.700728092855	-0.379598269395
C	-1.101973709305	3.473006225314	0.731522950143
C	-2.024958275111	2.423388781520	1.395475242538
C	-1.757417654730	1.135348420881	0.611955603588
C	-0.037213738686	0.331866495149	-0.919139393310
C	1.464618249705	0.348392556918	-1.151505551421
O	2.160671663507	0.187923743824	0.077970000276
H	0.637246383376	3.049341319114	-0.552969583210
H	-0.938952368948	2.787294059241	-1.331636653611
H	-0.380261659269	3.864171909211	1.453178911832
H	-1.655958829752	4.323530324573	0.327887267812
H	-1.763993708295	2.291766384368	2.448681108119
H	-3.079675334259	2.703956735747	1.351043233838
H	-2.479008800405	1.035199853153	-0.219016759870
H	-1.819158173543	0.229754664569	1.221810074839
H	-0.327525536854	-0.656673818021	-0.547328354569
H	-0.567269793945	0.504969735525	-1.872397688404
H	1.752487315145	-0.476341622473	-1.808669723498
H	1.767860827241	1.285466666024	-1.638613725991
H	1.631196723285	0.672205073323	0.725991659318

SCF Done: E(RwB97X) = -366.449365987

Zero-point correction=	0.193039
Thermal correction to Energy=	0.201353
Thermal correction to Enthalpy=	0.202297
Thermal correction to Gibbs Free Energy=	0.159494
Sum of electronic and zero-point Energies=	-366.256327
Sum of electronic and thermal Energies=	-366.248013
Sum of electronic and thermal Enthalpies=	-366.247069
Sum of electronic and thermal Free Energies=	-366.289872

1	N	Isotropic =	205.7370	Anisotropy =	57.2560
2	C	Isotropic =	139.0211	Anisotropy =	57.1986
3	C	Isotropic =	166.7915	Anisotropy =	24.7276

4	C	Isotropic =	167.7933	Anisotropy =	23.0491
5	C	Isotropic =	134.7236	Anisotropy =	63.1328
6	C	Isotropic =	133.8944	Anisotropy =	39.9942
7	C	Isotropic =	131.0647	Anisotropy =	57.6300
8	O	Isotropic =	314.4883	Anisotropy =	41.8701
9	H	Isotropic =	28.7388	Anisotropy =	8.0791
10	H	Isotropic =	30.2054	Anisotropy =	8.2979
11	H	Isotropic =	30.0889	Anisotropy =	10.5699
12	H	Isotropic =	30.0965	Anisotropy =	10.8999
13	H	Isotropic =	30.0770	Anisotropy =	10.7092
14	H	Isotropic =	30.1577	Anisotropy =	10.9625
15	H	Isotropic =	29.6891	Anisotropy =	8.2157
16	H	Isotropic =	28.9680	Anisotropy =	9.1513
17	H	Isotropic =	28.9338	Anisotropy =	9.2897
18	H	Isotropic =	29.8200	Anisotropy =	7.2889
19	H	Isotropic =	28.4207	Anisotropy =	7.8606
20	H	Isotropic =	28.1306	Anisotropy =	6.3745
21	H	Isotropic =	29.6209	Anisotropy =	17.2857

Conformer_20

N	-0.788725317682	1.951547099506	-0.355494895588
C	-2.201473942405	1.688339091485	-0.059372361965
C	-2.359239065177	1.843901369103	1.464432423939
C	-1.259469160577	2.859638406480	1.842161646312
C	-0.484485940930	3.091977131613	0.521981992235
C	0.067225836183	0.798253755226	-0.072460873268
C	1.384390969129	0.911006390002	-0.817049491004
O	2.183654972313	-0.213655618854	-0.458752935309
H	-2.802735765627	2.446364987529	-0.574779453331
H	-2.500121412337	0.707968169980	-0.437570278570
H	-3.361797362866	2.184495580524	1.734970487825
H	-2.192315979718	0.885404257758	1.964573597810
H	-1.673929435626	3.798228482910	2.218577704300
H	-0.604502190457	2.459246797539	2.620357159279
H	0.593414133518	3.194543544375	0.666746641575
H	-0.841111366781	4.005239431516	0.034125787483
H	0.275495728269	0.675284871810	1.003091437898
H	-0.444206186107	-0.108250521604	-0.410943365122
H	1.193409190990	0.923986267699	-1.897576353086
H	1.896795734802	1.844080664943	-0.549461560543
H	3.020726561088	-0.147100159541	-0.925357310870

SCF Done: E(RwB97X) = -366.441411555

Zero-point correction=	0.192820
Thermal correction to Energy=	0.201335
Thermal correction to Enthalpy=	0.202279
Thermal correction to Gibbs Free Energy=	0.159302
Sum of electronic and zero-point Energies=	-366.248591
Sum of electronic and thermal Energies=	-366.240077
Sum of electronic and thermal Enthalpies=	-366.239132
Sum of electronic and thermal Free Energies=	-366.282110

1 N	Isotropic = 202.6988	Anisotropy = 36.2603
2 C	Isotropic = 133.2683	Anisotropy = 64.8519
3 C	Isotropic = 167.9110	Anisotropy = 27.0342
4 C	Isotropic = 169.6462	Anisotropy = 30.6952
5 C	Isotropic = 138.9744	Anisotropy = 59.5887
6 C	Isotropic = 135.2418	Anisotropy = 62.0000
7 C	Isotropic = 126.1766	Anisotropy = 69.5559
8 O	Isotropic = 315.5279	Anisotropy = 99.5636
9 H	Isotropic = 29.2102	Anisotropy = 11.0696
10 H	Isotropic = 29.0103	Anisotropy = 8.6627
11 H	Isotropic = 30.2678	Anisotropy = 11.3336
12 H	Isotropic = 30.1544	Anisotropy = 9.9085
13 H	Isotropic = 30.3391	Anisotropy = 11.3956
14 H	Isotropic = 29.9928	Anisotropy = 10.1433
15 H	Isotropic = 28.9871	Anisotropy = 7.7733
16 H	Isotropic = 29.4068	Anisotropy = 11.1842
17 H	Isotropic = 29.3584	Anisotropy = 7.3116
18 H	Isotropic = 29.4826	Anisotropy = 6.9314
19 H	Isotropic = 28.1396	Anisotropy = 4.1962
20 H	Isotropic = 28.1410	Anisotropy = 5.1240
21 H	Isotropic = 31.3058	Anisotropy = 20.5800

Conformer_21

N	0.031838105797	1.502395262563	0.464654022948
C	-0.018812909086	2.945201532005	0.724005215404
C	-1.452769435934	3.393763269108	0.383292923199
C	-2.300307299060	2.122985802037	0.612048965779
C	-1.264818447298	1.033744698054	0.975563804231
C	0.220527721129	1.185241475862	-0.955231820813
C	0.722192244526	-0.243339361749	-1.096998818615
O	1.862448028435	-0.452682069558	-0.275329985903
H	0.179365289927	3.106393202047	1.789786814181
H	0.753861856874	3.466861523998	0.154822022677
H	-1.770339890895	4.232973738600	1.007062734736
H	-1.514491643663	3.718504640344	-0.659383952538

H	-3.031859671978	2.248619004467	1.414021136773
H	-2.852745605185	1.854092591896	-0.292009819125
H	-1.511105063326	0.049575911250	0.570168138726
H	-1.188559378194	0.934747480784	2.063439711490
H	0.980934750208	1.865475135815	-1.351430173677
H	-0.693871800053	1.316181272696	-1.555285374773
H	-0.070299135048	-0.956901134270	-0.831169577532
H	1.013314054942	-0.438956280141	-2.132456782900
H	1.675098227882	0.059822304193	0.524030815733

SCF Done: E(RwB97X) = -366.446124962

Zero-point correction=	0.193361
Thermal correction to Energy=	0.201526
Thermal correction to Enthalpy=	0.202471
Thermal correction to Gibbs Free Energy=	0.160229
Sum of electronic and zero-point Energies=	-366.252764
Sum of electronic and thermal Energies=	-366.244599
Sum of electronic and thermal Enthalpies=	-366.243654
Sum of electronic and thermal Free Energies=	-366.285896

1 N	Isotropic = 206.3942	Anisotropy = 55.4679
2 C	Isotropic = 133.7322	Anisotropy = 65.2099
3 C	Isotropic = 167.7095	Anisotropy = 26.6675
4 C	Isotropic = 169.7976	Anisotropy = 30.2869
5 C	Isotropic = 141.8737	Anisotropy = 56.6716
6 C	Isotropic = 135.2282	Anisotropy = 40.5339
7 C	Isotropic = 130.8978	Anisotropy = 55.0517
8 O	Isotropic = 315.1977	Anisotropy = 38.8842
9 H	Isotropic = 29.0715	Anisotropy = 10.9002
10 H	Isotropic = 29.0692	Anisotropy = 8.6916
11 H	Isotropic = 30.2256	Anisotropy = 11.3461
12 H	Isotropic = 30.1540	Anisotropy = 10.1789
13 H	Isotropic = 30.3138	Anisotropy = 11.4128
14 H	Isotropic = 30.0936	Anisotropy = 10.3859
15 H	Isotropic = 28.8856	Anisotropy = 7.8420
16 H	Isotropic = 29.4442	Anisotropy = 11.2481
17 H	Isotropic = 29.5458	Anisotropy = 9.0407
18 H	Isotropic = 29.3226	Anisotropy = 6.9455
19 H	Isotropic = 28.2512	Anisotropy = 6.8817
20 H	Isotropic = 28.4370	Anisotropy = 7.7247
21 H	Isotropic = 29.1838	Anisotropy = 17.0095

Conformer_22

N	-0.057393922310	1.716997609940	-0.094352763121
C	-1.485821282093	1.565509177958	-0.408504641922
C	-2.263264071049	2.033559136028	0.843415356591
C	-1.257521347064	2.923711173156	1.606126866437
C	-0.025526358263	2.961197314288	0.681826380965
C	0.476619360648	0.569320168397	0.647178568810
C	0.845825074708	-0.539523633793	-0.325756063385
O	1.690284266597	-0.037709676542	-1.352540292588
H	-1.719363600142	2.212509343689	-1.260531667012
H	-1.714016055504	0.537887591983	-0.700927901234
H	-3.168656458011	2.575862409397	0.560062924395
H	-2.572907780852	1.182048339411	1.454863751889
H	-1.643461137859	3.927095244343	1.802300353611
H	-0.998760629098	2.477627476813	2.570743573193
H	0.923087103038	3.059518016327	1.214360161663
H	-0.109230221878	3.800687765060	-0.017746328542
H	1.382941719744	0.898591275262	1.164940616427
H	-0.220838490764	0.178190180899	1.404729248795
H	-0.059227624932	-0.982295131594	-0.764744562169
H	1.386292718379	-1.333707956532	0.196114781132
H	1.346438736706	0.849724175511	-1.528658363937

SCF Done: E(RwB97X) = -366.446125002

Zero-point correction=	0.193365
Thermal correction to Energy=	0.201528
Thermal correction to Enthalpy=	0.202472
Thermal correction to Gibbs Free Energy=	0.160239
Sum of electronic and zero-point Energies=	-366.252760
Sum of electronic and thermal Energies=	-366.244597
Sum of electronic and thermal Enthalpies=	-366.243653
Sum of electronic and thermal Free Energies=	-366.285886

1 N	Isotropic = 206.3820	Anisotropy = 55.4546
2 C	Isotropic = 141.8736	Anisotropy = 56.6586
3 C	Isotropic = 169.7963	Anisotropy = 30.2877
4 C	Isotropic = 167.7093	Anisotropy = 26.6654
5 C	Isotropic = 133.7297	Anisotropy = 65.2218
6 C	Isotropic = 135.2362	Anisotropy = 40.5321
7 C	Isotropic = 130.9026	Anisotropy = 55.0445
8 O	Isotropic = 315.1714	Anisotropy = 38.8933
9 H	Isotropic = 29.4445	Anisotropy = 11.2482
10 H	Isotropic = 28.8853	Anisotropy = 7.8432
11 H	Isotropic = 30.3136	Anisotropy = 11.4124
12 H	Isotropic = 30.0937	Anisotropy = 10.3851
13 H	Isotropic = 30.2257	Anisotropy = 11.3462

14	H	Isotropic =	30.1540	Anisotropy =	10.1798
15	H	Isotropic =	29.0693	Anisotropy =	8.6908
16	H	Isotropic =	29.0712	Anisotropy =	10.8992
17	H	Isotropic =	29.5460	Anisotropy =	9.0415
18	H	Isotropic =	29.3220	Anisotropy =	6.9451
19	H	Isotropic =	28.2519	Anisotropy =	6.8846
20	H	Isotropic =	28.4371	Anisotropy =	7.7262
21	H	Isotropic =	29.1779	Anisotropy =	17.0198

Conformer_23

N	-0.856111187009	1.774652362351	-0.480566095594
C	-2.181908158198	1.478050664622	0.073846907659
C	-2.139480782107	1.914366840598	1.550233169096
C	-1.099974654355	3.056202636114	1.561934998527
C	-0.544922081370	3.082130891051	0.117007052927
C	0.138307261111	0.760045685920	-0.129520109055
C	1.331233153431	0.820643463994	-1.073245131184
O	2.331816393514	-0.131693445825	-0.726567436932
H	-2.919062088327	2.079558933526	-0.470563475312
H	-2.435006465966	0.425047959551	-0.069457068201
H	-3.122340001721	2.232156222600	1.906911854431
H	-1.812901452422	1.084480191650	2.183797000695
H	-1.545170425617	4.019399764386	1.823462842364
H	-0.306550348551	2.858341584102	2.287331166946
H	0.527139776596	3.286626906403	0.070186669754
H	-1.054945795151	3.855479814125	-0.466947402431
H	0.495535227351	0.860996106247	0.910700181091
H	-0.322589319242	-0.228485415184	-0.218583873978
H	1.011351277267	0.574671103840	-2.088988952188
H	1.756595897616	1.832272831919	-1.092983418820
H	2.685683773151	0.110654898011	0.134411120203

SCF Done: E(RwB97X) = -366.441776584

Zero-point correction=	0.193013
Thermal correction to Energy=	0.201456
Thermal correction to Enthalpy=	0.202401
Thermal correction to Gibbs Free Energy=	0.159648
Sum of electronic and zero-point Energies=	-366.248764
Sum of electronic and thermal Energies=	-366.240320
Sum of electronic and thermal Enthalpies=	-366.239376
Sum of electronic and thermal Free Energies=	-366.282128

1	N	Isotropic =	201.9449	Anisotropy =	34.6677

2 C	Isotropic =	133.4407	Anisotropy =	64.6959
3 C	Isotropic =	167.9601	Anisotropy =	27.0866
4 C	Isotropic =	169.7676	Anisotropy =	30.8599
5 C	Isotropic =	139.2190	Anisotropy =	59.1749
6 C	Isotropic =	133.1123	Anisotropy =	63.7182
7 C	Isotropic =	125.8179	Anisotropy =	70.9108
8 O	Isotropic =	308.6355	Anisotropy =	60.9708
9 H	Isotropic =	29.2309	Anisotropy =	11.0973
10 H	Isotropic =	29.0299	Anisotropy =	8.6509
11 H	Isotropic =	30.2777	Anisotropy =	11.3312
12 H	Isotropic =	30.1740	Anisotropy =	9.9070
13 H	Isotropic =	30.3492	Anisotropy =	11.3810
14 H	Isotropic =	30.0290	Anisotropy =	10.1500
15 H	Isotropic =	29.0057	Anisotropy =	7.6879
16 H	Isotropic =	29.4158	Anisotropy =	11.2140
17 H	Isotropic =	29.5362	Anisotropy =	7.7057
18 H	Isotropic =	29.4676	Anisotropy =	6.7321
19 H	Isotropic =	28.3122	Anisotropy =	4.1420
20 H	Isotropic =	28.1336	Anisotropy =	5.1640
21 H	Isotropic =	31.6283	Anisotropy =	16.7723

Conformer_24

N	-0.757204358795	0.953973172368	0.766224572572
C	-0.419686107214	2.043517872593	1.694882898726
C	-1.131043041152	3.314275287253	1.169793348880
C	-2.243064771774	2.773603987459	0.244816959952
C	-2.154050403998	1.246718923573	0.425335928767
C	0.116153422591	0.943211600568	-0.407938398581
C	1.407072265890	0.190860396943	-0.116635331629
O	2.291552822315	0.201358303760	-1.232825928526
H	-0.804731233601	1.780386507407	2.685689490832
H	0.663003626756	2.159875921195	1.781895258317
H	-1.531241303033	3.904594417750	1.997869102969
H	-0.438888369260	3.956408849268	0.618923891813
H	-3.233569981613	3.154994493187	0.504937568949
H	-2.049435881158	3.046287369084	-0.796778289933
H	-2.465587750818	0.678109777496	-0.453889634419
H	-2.781070757143	0.934863745295	1.268652349933
H	-0.402662214118	0.434799482630	-1.226412093662
H	0.362917278310	1.960562357616	-0.760026600046
H	1.904326295172	0.606384791517	0.769251247044
H	1.184103568133	-0.859135055155	0.089172613997
H	2.565006894511	1.110847798194	-1.385438955955

SCF Done: E(RwB97X) = -366.441776589

Zero-point correction=	0.193013
Thermal correction to Energy=	0.201456
Thermal correction to Enthalpy=	0.202401
Thermal correction to Gibbs Free Energy=	0.159648
Sum of electronic and zero-point Energies=	-366.248764
Sum of electronic and thermal Energies=	-366.240320
Sum of electronic and thermal Enthalpies=	-366.239376
Sum of electronic and thermal Free Energies=	-366.282128

1	N	Isotropic =	201.9449	Anisotropy =	34.6679
2	C	Isotropic =	139.2190	Anisotropy =	59.1749
3	C	Isotropic =	169.7677	Anisotropy =	30.8599
4	C	Isotropic =	167.9602	Anisotropy =	27.0867
5	C	Isotropic =	133.4407	Anisotropy =	64.6959
6	C	Isotropic =	133.1123	Anisotropy =	63.7181
7	C	Isotropic =	125.8180	Anisotropy =	70.9110
8	O	Isotropic =	308.6352	Anisotropy =	60.9713
9	H	Isotropic =	29.4158	Anisotropy =	11.2140
10	H	Isotropic =	29.0057	Anisotropy =	7.6879
11	H	Isotropic =	30.3492	Anisotropy =	11.3810
12	H	Isotropic =	30.0290	Anisotropy =	10.1500
13	H	Isotropic =	30.2777	Anisotropy =	11.3312
14	H	Isotropic =	30.1740	Anisotropy =	9.9070
15	H	Isotropic =	29.0299	Anisotropy =	8.6509
16	H	Isotropic =	29.2309	Anisotropy =	11.0973
17	H	Isotropic =	29.4676	Anisotropy =	6.7321
18	H	Isotropic =	29.5362	Anisotropy =	7.7057
19	H	Isotropic =	28.1336	Anisotropy =	5.1640
20	H	Isotropic =	28.3122	Anisotropy =	4.1420
21	H	Isotropic =	31.6283	Anisotropy =	16.7722

Conformer_25

N	-0.432545116784	2.204963733619	0.073307808770
C	-1.696237128799	1.487713212673	-0.062799444025
C	-2.643136452837	2.270914960975	0.854910037742
C	-1.709061339112	2.931995876323	1.899287182920
C	-0.304824375873	2.461617367781	1.503677983774
C	0.722266106675	1.627305259392	-0.591005349230
C	1.222392063821	0.278551147643	-0.067726192138
O	2.316788117068	-0.190883953714	-0.852639234349
H	-1.615592456035	0.443926933460	0.285791249570
H	-2.018458333549	1.468238427222	-1.108355686755

H	-3.182959262302	3.032078426056	0.285867482421
H	-3.386566958642	1.615557843327	1.314663777553
H	-1.776258553302	4.021280430640	1.838953202028
H	-1.954939472534	2.642901541668	2.923756881622
H	-0.046941005052	1.544002118268	2.060435416227
H	0.476822982865	3.202900220980	1.696657489618
H	0.472073586789	1.512549515968	-1.654126382349
H	1.550455349040	2.343877937720	-0.533679614043
H	1.606974446668	0.369388382394	0.950862274429
H	0.415459725621	-0.464356773060	-0.057685736656
H	2.000188076274	-0.323722609334	-1.751353147130

SCF Done: E(RwB97X) = -366.441982997

Zero-point correction=	0.192643
Thermal correction to Energy=	0.201299
Thermal correction to Enthalpy=	0.202243
Thermal correction to Gibbs Free Energy=	0.158864
Sum of electronic and zero-point Energies=	-366.249340
Sum of electronic and thermal Energies=	-366.240684
Sum of electronic and thermal Enthalpies=	-366.239740
Sum of electronic and thermal Free Energies=	-366.283119

1 N	Isotropic = 204.8102	Anisotropy = 59.7493
2 C	Isotropic = 140.1088	Anisotropy = 55.4542
3 C	Isotropic = 167.0940	Anisotropy = 24.1943
4 C	Isotropic = 166.7435	Anisotropy = 24.5989
5 C	Isotropic = 140.4067	Anisotropy = 53.4020
6 C	Isotropic = 137.7047	Anisotropy = 53.8002
7 C	Isotropic = 134.4890	Anisotropy = 66.7154
8 O	Isotropic = 315.9847	Anisotropy = 72.5255
9 H	Isotropic = 29.3239	Anisotropy = 7.4788
10 H	Isotropic = 29.0799	Anisotropy = 8.7591
11 H	Isotropic = 30.1587	Anisotropy = 10.8455
12 H	Isotropic = 30.2491	Anisotropy = 10.6118
13 H	Isotropic = 30.1656	Anisotropy = 10.8569
14 H	Isotropic = 30.2342	Anisotropy = 10.6378
15 H	Isotropic = 29.4772	Anisotropy = 7.5378
16 H	Isotropic = 29.0547	Anisotropy = 8.7701
17 H	Isotropic = 29.0927	Anisotropy = 6.6688
18 H	Isotropic = 28.7503	Anisotropy = 6.6441
19 H	Isotropic = 28.1833	Anisotropy = 5.8249
20 H	Isotropic = 27.8990	Anisotropy = 6.7568
21 H	Isotropic = 31.9743	Anisotropy = 17.6580

Conformer_26

N	-0.742870511771	1.255939044527	0.634951489856
C	-0.369140897090	2.264926432456	1.620047046677
C	-1.673348467539	3.041225213922	1.834633211199
C	-2.451123651185	2.858292988057	0.507286521857
C	-1.535452623114	1.979649828119	-0.353960673729
C	0.325277747609	0.413264387371	0.127458572128
C	1.496243853487	1.116322798317	-0.563650697517
O	2.432246791564	0.162480555205	-1.061891658092
H	0.016441005234	1.794780806300	2.529994107897
H	0.410551972513	2.943282544787	1.232216723322
H	-2.235511278655	2.616602563483	2.670315595567
H	-1.481317015900	4.091446584180	2.066427960174
H	-3.404446281543	2.354757868429	0.686775311144
H	-2.669285288444	3.809503374996	0.016206371989
H	-0.905669293568	2.615447134328	-0.999440024773
H	-2.079366793038	1.282182898393	-0.998236142697
H	-0.119085312630	-0.295301864526	-0.584206267423
H	0.725633649032	-0.178753451196	0.959257900606
H	2.054183206030	1.737318072693	0.141151431615
H	1.143736557419	1.763332574424	-1.376220535781
H	1.983002631590	-0.376000354265	-1.720516244020

SCF Done: E(RwB97X) = -366.441982998

Zero-point correction=	0.192643
Thermal correction to Energy=	0.201299
Thermal correction to Enthalpy=	0.202243
Thermal correction to Gibbs Free Energy=	0.158864
Sum of electronic and zero-point Energies=	-366.249340
Sum of electronic and thermal Energies=	-366.240684
Sum of electronic and thermal Enthalpies=	-366.239740
Sum of electronic and thermal Free Energies=	-366.283119

1	N	Isotropic =	204.8102	Anisotropy =	59.7494
2	C	Isotropic =	140.4067	Anisotropy =	53.4021
3	C	Isotropic =	166.7435	Anisotropy =	24.5989
4	C	Isotropic =	167.0940	Anisotropy =	24.1943
5	C	Isotropic =	140.1088	Anisotropy =	55.4541
6	C	Isotropic =	137.7047	Anisotropy =	53.8002
7	C	Isotropic =	134.4890	Anisotropy =	66.7154
8	O	Isotropic =	315.9847	Anisotropy =	72.5253
9	H	Isotropic =	29.0547	Anisotropy =	8.7701
10	H	Isotropic =	29.4772	Anisotropy =	7.5378
11	H	Isotropic =	30.1656	Anisotropy =	10.8569

12	H	Isotropic =	30.2342	Anisotropy =	10.6378
13	H	Isotropic =	30.1587	Anisotropy =	10.8455
14	H	Isotropic =	30.2491	Anisotropy =	10.6118
15	H	Isotropic =	29.3239	Anisotropy =	7.4788
16	H	Isotropic =	29.0799	Anisotropy =	8.7591
17	H	Isotropic =	29.0927	Anisotropy =	6.6688
18	H	Isotropic =	28.7503	Anisotropy =	6.6441
19	H	Isotropic =	28.1833	Anisotropy =	5.8249
20	H	Isotropic =	27.8990	Anisotropy =	6.7568
21	H	Isotropic =	31.9743	Anisotropy =	17.6580

Conformer_27

N	-0.786347163503	1.221286644610	0.736918827189
C	-0.343024380543	2.380818579912	1.502861205219
C	-1.643650557745	3.153975405840	1.747554568590
C	-2.558029815398	2.749297633335	0.564158351368
C	-1.712460120621	1.763491835608	-0.251658056225
C	0.246624496414	0.328083172425	0.244503477408
C	1.289291746320	0.932170393248	-0.692181649743
O	2.132903909989	-0.140975052595	-1.108816259542
H	0.360342182881	3.005656231579	0.925358408219
H	0.161683303758	2.068766703543	2.422436380630
H	-2.091342899252	2.853768851631	2.698424871761
H	-1.467623189063	4.231313155060	1.791757025943
H	-3.466185949118	2.262763924457	0.928981050172
H	-2.864549146900	3.606938239822	-0.039245346136
H	-1.183213637526	2.301911770844	-1.056602752075
H	-2.298214596432	0.962549369537	-0.712869393469
H	0.770053428923	-0.103167170138	1.106197087117
H	-0.242647625272	-0.500083981166	-0.281561807718
H	0.810112604101	1.397508529756	-1.562379905364
H	1.880687238546	1.698312974404	-0.176227344683
H	2.822790170440	0.221712788288	-1.670408738660

SCF Done: E(RwB97X) = -366.441726870

Zero-point correction=	0.192456
Thermal correction to Energy=	0.201230
Thermal correction to Enthalpy=	0.202174
Thermal correction to Gibbs Free Energy=	0.158491
Sum of electronic and zero-point Energies=	-366.249271
Sum of electronic and thermal Energies=	-366.240497
Sum of electronic and thermal Enthalpies=	-366.239553
Sum of electronic and thermal Free Energies=	-366.283236

1	N	Isotropic = 206.1466	Anisotropy = 56.3441
2	C	Isotropic = 140.1200	Anisotropy = 53.9848
3	C	Isotropic = 166.7328	Anisotropy = 24.5592
4	C	Isotropic = 167.0601	Anisotropy = 24.2030
5	C	Isotropic = 140.0309	Anisotropy = 55.7099
6	C	Isotropic = 140.0093	Anisotropy = 51.8221
7	C	Isotropic = 135.4589	Anisotropy = 65.4917
8	O	Isotropic = 321.7721	Anisotropy = 94.3348
9	H	Isotropic = 29.5259	Anisotropy = 7.5634
10	H	Isotropic = 29.0688	Anisotropy = 8.8182
11	H	Isotropic = 30.1624	Anisotropy = 10.8632
12	H	Isotropic = 30.2414	Anisotropy = 10.6069
13	H	Isotropic = 30.1445	Anisotropy = 10.8635
14	H	Isotropic = 30.2443	Anisotropy = 10.6072
15	H	Isotropic = 29.3930	Anisotropy = 7.4941
16	H	Isotropic = 29.0656	Anisotropy = 8.8508
17	H	Isotropic = 28.7703	Anisotropy = 6.8907
18	H	Isotropic = 28.9040	Anisotropy = 6.7157
19	H	Isotropic = 27.9484	Anisotropy = 6.7154
20	H	Isotropic = 27.9834	Anisotropy = 6.5201
21	H	Isotropic = 31.3306	Anisotropy = 20.4608

Conformer_28

N	0.087749572413	1.875979647794	0.970854576294
C	-0.458796409653	2.744608040711	-0.084204053491
C	-1.993283533160	2.550975635283	-0.064228895176
C	-2.289683901727	2.015019558618	1.353541035867
C	-0.908963824188	2.019161131477	2.039392562936
C	0.232465843963	0.483079927868	0.538812888242
C	1.531923559823	0.198110111306	-0.184232002223
O	1.525360389372	0.797750339546	-1.480504711346
H	-0.212872253158	3.781257049824	0.172083080591
H	0.001633564301	2.513356959911	-1.044348765023
H	-2.509295702429	3.491991481561	-0.270997057234
H	-2.308432698176	1.834144302463	-0.827511765827
H	-3.010764930436	2.630803416605	1.897088611149
H	-2.694232438478	0.999574150947	1.310291495558
H	-0.786867242665	1.236683499123	2.792066363437
H	-0.742770072628	2.985717370443	2.528889183514
H	0.231687047543	-0.145850882969	1.434932384953
H	-0.607287148916	0.146113264418	-0.092043815469
H	2.371039322499	0.583881002395	0.408674215185
H	1.645901715083	-0.889902741732	-0.277348894272

H 2.370089140615 0.610246734409 -1.898306437666

SCF Done: E(RwB97X) = -366.440796960

Zero-point correction= 0.192677
Thermal correction to Energy= 0.201202
Thermal correction to Enthalpy= 0.202146
Thermal correction to Gibbs Free Energy= 0.158697
Sum of electronic and zero-point Energies= -366.248120
Sum of electronic and thermal Energies= -366.239595
Sum of electronic and thermal Enthalpies= -366.238651
Sum of electronic and thermal Free Energies= -366.282100

1 N	Isotropic =	191.4590	Anisotropy =	29.8125
2 C	Isotropic =	137.7067	Anisotropy =	60.1899
3 C	Isotropic =	169.8438	Anisotropy =	31.1643
4 C	Isotropic =	167.8866	Anisotropy =	26.8798
5 C	Isotropic =	132.5204	Anisotropy =	66.7561
6 C	Isotropic =	136.6634	Anisotropy =	42.7754
7 C	Isotropic =	122.2648	Anisotropy =	43.4425
8 O	Isotropic =	308.3347	Anisotropy =	98.8156
9 H	Isotropic =	29.3304	Anisotropy =	10.8742
10 H	Isotropic =	28.1932	Anisotropy =	7.6453
11 H	Isotropic =	30.3601	Anisotropy =	11.3376
12 H	Isotropic =	29.9914	Anisotropy =	9.9412
13 H	Isotropic =	30.2949	Anisotropy =	11.3411
14 H	Isotropic =	30.1561	Anisotropy =	10.0021
15 H	Isotropic =	29.0511	Anisotropy =	8.5225
16 H	Isotropic =	29.2035	Anisotropy =	10.9817
17 H	Isotropic =	29.7874	Anisotropy =	7.7729
18 H	Isotropic =	29.0573	Anisotropy =	8.1103
19 H	Isotropic =	27.9395	Anisotropy =	6.6510
20 H	Isotropic =	28.0221	Anisotropy =	7.6269
21 H	Isotropic =	31.2261	Anisotropy =	21.0773

Conformer_29

N	-0.707002881668	0.945564510525	0.677526480546
C	-1.356963687117	1.494670635752	1.874082201072
C	-1.430407918754	3.021135387446	1.670836209081
C	-1.453583006033	3.183001686483	0.135116280159
C	-1.318195198444	1.738559118177	-0.401352604341
C	0.750476152369	1.089680694736	0.730042719164
C	1.492371838301	0.151945330987	-0.198846358530
O	1.312654965532	0.548917995164	-1.559011391817

H	-2.370263616981	1.080239668966	1.928197811834
H	-0.823046491684	1.194315990900	2.778745761863
H	-2.311455847260	3.449600807979	2.155360204005
H	-0.551053182875	3.508898478791	2.101512168330
H	-2.375991979869	3.648215598238	-0.221633157465
H	-0.623039589729	3.807594193132	-0.205249374474
H	-0.726359179037	1.661208865093	-1.312998211681
H	-2.312168087967	1.323513858917	-0.602743576313
H	1.081118876236	2.123055479790	0.531237062864
H	1.073886654052	0.840271830304	1.745811205988
H	1.127194269010	-0.872315745292	-0.050499652782
H	2.559067480574	0.179391551090	0.059689765633
H	1.781660431346	-0.078465937178	-2.115523543137

SCF Done: E(RwB97X) = -366.440796959

Zero-point correction=	0.192677
Thermal correction to Energy=	0.201202
Thermal correction to Enthalpy=	0.202146
Thermal correction to Gibbs Free Energy=	0.158697
Sum of electronic and zero-point Energies=	-366.248120
Sum of electronic and thermal Energies=	-366.239595
Sum of electronic and thermal Enthalpies=	-366.238651
Sum of electronic and thermal Free Energies=	-366.282100

1 N	Isotropic = 191.4591	Anisotropy = 29.8124
2 C	Isotropic = 132.5204	Anisotropy = 66.7562
3 C	Isotropic = 167.8866	Anisotropy = 26.8797
4 C	Isotropic = 169.8438	Anisotropy = 31.1644
5 C	Isotropic = 137.7066	Anisotropy = 60.1899
6 C	Isotropic = 136.6634	Anisotropy = 42.7756
7 C	Isotropic = 122.2648	Anisotropy = 43.4424
8 O	Isotropic = 308.3348	Anisotropy = 98.8153
9 H	Isotropic = 29.2035	Anisotropy = 10.9817
10 H	Isotropic = 29.0511	Anisotropy = 8.5225
11 H	Isotropic = 30.2949	Anisotropy = 11.3411
12 H	Isotropic = 30.1561	Anisotropy = 10.0021
13 H	Isotropic = 30.3601	Anisotropy = 11.3376
14 H	Isotropic = 29.9914	Anisotropy = 9.9412
15 H	Isotropic = 28.1932	Anisotropy = 7.6453
16 H	Isotropic = 29.3304	Anisotropy = 10.8742
17 H	Isotropic = 29.0573	Anisotropy = 8.1103
18 H	Isotropic = 29.7874	Anisotropy = 7.7729
19 H	Isotropic = 27.9395	Anisotropy = 6.6511
20 H	Isotropic = 28.0221	Anisotropy = 7.6269
21 H	Isotropic = 31.2261	Anisotropy = 21.0773

Conformer_3

N	-0.313367935677	1.197384107950	0.331032131946
C	-0.016075233193	2.297340901007	1.260420166841
C	-1.129128938272	3.352359229529	1.063288469506
C	-2.290632068065	2.565198219813	0.417628455880
C	-1.776769399208	1.113172187702	0.384669780009
C	0.193042725068	1.456048028767	-1.021313179139
C	1.662944974292	1.073842150205	-1.097242456818
O	1.855842420757	-0.251847760680	-0.623385467958
H	-0.048853874113	1.901523007695	2.280887138488
H	0.988764209328	2.690942200712	1.090227791108
H	-1.411371073390	3.804367232998	2.017303949365
H	-0.793259447428	4.160269708253	0.408086480459
H	-3.223658684440	2.648692641204	0.980393458196
H	-2.486241955933	2.924972375577	-0.596638614388
H	-2.160547109307	0.527935473097	-0.453984396172
H	-2.054022646720	0.598054444834	1.311459901682
H	0.067137923592	2.502857288375	-1.340147132303
H	-0.370393049883	0.824707012247	-1.715471008791
H	2.272980165732	1.775985129951	-0.511808370012
H	2.009476342074	1.114468934544	-2.133308969271
H	1.233732654787	-0.332172513781	0.113701871371

SCF Done: E(RwB97X) = -366.446124882

Zero-point correction=	0.193362
Thermal correction to Energy=	0.201526
Thermal correction to Enthalpy=	0.202470
Thermal correction to Gibbs Free Energy=	0.160231
Sum of electronic and zero-point Energies=	-366.252763
Sum of electronic and thermal Energies=	-366.244599
Sum of electronic and thermal Enthalpies=	-366.243655
Sum of electronic and thermal Free Energies=	-366.285894

1 N	Isotropic =	206.3798	Anisotropy =	55.4462
2 C	Isotropic =	141.8716	Anisotropy =	56.6660
3 C	Isotropic =	169.7969	Anisotropy =	30.2843
4 C	Isotropic =	167.7091	Anisotropy =	26.6624
5 C	Isotropic =	133.7293	Anisotropy =	65.2159
6 C	Isotropic =	135.2336	Anisotropy =	40.5256
7 C	Isotropic =	130.9012	Anisotropy =	55.0347
8 O	Isotropic =	315.1681	Anisotropy =	38.9021
9 H	Isotropic =	29.4444	Anisotropy =	11.2480

10	H	Isotropic =	28.8854	Anisotropy =	7.8430
11	H	Isotropic =	30.3136	Anisotropy =	11.4126
12	H	Isotropic =	30.0936	Anisotropy =	10.3854
13	H	Isotropic =	30.2256	Anisotropy =	11.3462
14	H	Isotropic =	30.1541	Anisotropy =	10.1794
15	H	Isotropic =	29.0693	Anisotropy =	8.6912
16	H	Isotropic =	29.0714	Anisotropy =	10.8993
17	H	Isotropic =	29.3220	Anisotropy =	6.9456
18	H	Isotropic =	29.5464	Anisotropy =	9.0410
19	H	Isotropic =	28.2520	Anisotropy =	6.8843
20	H	Isotropic =	28.4372	Anisotropy =	7.7263
21	H	Isotropic =	29.1783	Anisotropy =	17.0196

Conformer_30

N	-0.985734287858	1.202054863596	-0.402358618929
C	-0.542176943042	2.603308179162	-0.465965669301
C	-0.760964172849	3.197579402948	0.943129115602
C	-1.860785842842	2.305020191729	1.559871297419
C	-2.184511202325	1.292490179599	0.440404975699
C	0.013535407850	0.302377107970	0.178868483656
C	1.158443243427	-0.048136395075	-0.758097740533
O	2.142915158556	0.975101677926	-0.905206958971
H	0.487955259593	2.666138537801	-0.816222688403
H	-1.180507665070	3.123164440952	-1.189256684988
H	0.157577496595	3.150838078021	1.534959756509
H	-1.056854910080	4.248119667325	0.886409427229
H	-1.491645999858	1.792301443897	2.452594520255
H	-2.747950284152	2.872083695896	1.852660610727
H	-3.005624462769	1.672905972169	-0.177767470728
H	-2.472583767673	0.305740110020	0.811016098919
H	0.434526970838	0.685017116342	1.126614996805
H	-0.497834674145	-0.635772339500	0.419155518580
H	0.767587996087	-0.238906078419	-1.761284073100
H	1.633880510016	-0.970031934413	-0.399581721814
H	2.580852169702	1.084906082055	-0.055743174632

SCF Done: E(RwB97X) = -366.440709059

Zero-point correction=	0.192958
Thermal correction to Energy=	0.201368
Thermal correction to Enthalpy=	0.202312
Thermal correction to Gibbs Free Energy=	0.159406
Sum of electronic and zero-point Energies=	-366.247751
Sum of electronic and thermal Energies=	-366.239341

Sum of electronic and thermal Enthalpies= -366.238397
Sum of electronic and thermal Free Energies= -366.281303

1 N	Isotropic =	190.4133	Anisotropy =	38.2381
2 C	Isotropic =	138.9736	Anisotropy =	57.8376
3 C	Isotropic =	169.9823	Anisotropy =	32.3228
4 C	Isotropic =	168.3025	Anisotropy =	28.2489
5 C	Isotropic =	133.5670	Anisotropy =	66.2191
6 C	Isotropic =	134.2360	Anisotropy =	37.1441
7 C	Isotropic =	122.0465	Anisotropy =	46.3037
8 O	Isotropic =	296.6175	Anisotropy =	69.8164
9 H	Isotropic =	28.0170	Anisotropy =	7.6250
10 H	Isotropic =	29.3751	Anisotropy =	11.0264
11 H	Isotropic =	30.0153	Anisotropy =	9.7897
12 H	Isotropic =	30.3537	Anisotropy =	11.2733
13 H	Isotropic =	30.1171	Anisotropy =	10.0690
14 H	Isotropic =	30.3165	Anisotropy =	11.3334
15 H	Isotropic =	29.1917	Anisotropy =	10.9994
16 H	Isotropic =	29.0757	Anisotropy =	8.4940
17 H	Isotropic =	29.2261	Anisotropy =	7.9634
18 H	Isotropic =	29.6993	Anisotropy =	7.7727
19 H	Isotropic =	28.1639	Anisotropy =	5.8943
20 H	Isotropic =	27.9040	Anisotropy =	7.6741
21 H	Isotropic =	31.6490	Anisotropy =	16.1047

Conformer_4

N	-0.243880947450	1.632785191875	-0.161410886609
C	-1.654830000798	1.877203675409	-0.479208191838
C	-2.353317838744	2.172357082829	0.861881018614
C	-1.225361972302	2.748903799762	1.745565533583
C	0.040124525137	2.648893328818	0.862754753967
C	0.003516771039	0.269352885875	0.320297749879
C	1.481945800214	-0.059379317241	0.183763116119
O	1.928514509177	0.204088341574	-1.139250368262
H	-1.709316852651	2.757342224103	-1.130009944210
H	-2.080492882306	1.030046863002	-1.021669826955
H	-3.189057611789	2.865088059651	0.735875852876
H	-2.753422770906	1.251420461755	1.295735976347
H	-1.414442841874	3.784048016393	2.040255660407
H	-1.111549987169	2.165835237505	2.663114020424
H	0.941525557571	2.394463981343	1.425188472869
H	0.222860496656	3.602823328421	0.357062975024
H	-0.314604162430	0.111969066225	1.363056663750
H	-0.568790927880	-0.417151948046	-0.311431291464

H	2.072969680810	0.523288726749	0.904227975528
H	1.652783386624	-1.118979198481	0.391684061614
H	1.446828069072	1.003200192481	-1.396483321662

SCF Done: E(RwB97X) = -366.446124884

Zero-point correction=	0.193362
Thermal correction to Energy=	0.201526
Thermal correction to Enthalpy=	0.202470
Thermal correction to Gibbs Free Energy=	0.160231
Sum of electronic and zero-point Energies=	-366.252763
Sum of electronic and thermal Energies=	-366.244599
Sum of electronic and thermal Enthalpies=	-366.243655
Sum of electronic and thermal Free Energies=	-366.285893

1 N	Isotropic = 206.3798	Anisotropy = 55.4464
2 C	Isotropic = 133.7293	Anisotropy = 65.2159
3 C	Isotropic = 167.7090	Anisotropy = 26.6624
4 C	Isotropic = 169.7969	Anisotropy = 30.2843
5 C	Isotropic = 141.8717	Anisotropy = 56.6659
6 C	Isotropic = 135.2336	Anisotropy = 40.5257
7 C	Isotropic = 130.9013	Anisotropy = 55.0348
8 O	Isotropic = 315.1682	Anisotropy = 38.9024
9 H	Isotropic = 29.0714	Anisotropy = 10.8993
10 H	Isotropic = 29.0693	Anisotropy = 8.6912
11 H	Isotropic = 30.2256	Anisotropy = 11.3462
12 H	Isotropic = 30.1541	Anisotropy = 10.1794
13 H	Isotropic = 30.3136	Anisotropy = 11.4126
14 H	Isotropic = 30.0936	Anisotropy = 10.3854
15 H	Isotropic = 28.8854	Anisotropy = 7.8430
16 H	Isotropic = 29.4444	Anisotropy = 11.2480
17 H	Isotropic = 29.3220	Anisotropy = 6.9456
18 H	Isotropic = 29.5464	Anisotropy = 9.0410
19 H	Isotropic = 28.2520	Anisotropy = 6.8843
20 H	Isotropic = 28.4372	Anisotropy = 7.7263
21 H	Isotropic = 29.1782	Anisotropy = 17.0197

Conformer_5

N	-0.648412578113	1.481476440341	0.370954164143
C	-1.914408022564	1.905193997597	-0.222844213102
C	-2.686965204819	2.510197509488	0.950740724304
C	-1.582443799661	3.004395306806	1.914873833574
C	-0.270677498402	2.603465115719	1.230455099593
C	0.347846766763	1.131039715138	-0.624268327004

C	1.604919814650	0.540615808893	-0.001327660626
O	2.534929297355	0.123010847369	-0.995042355981
H	-1.734952810870	2.672948322489	-0.998543404468
H	-2.423332941543	1.061162651593	-0.696940942944
H	-3.349565151728	3.313907376959	0.621801806735
H	-3.305594152344	1.748747429356	1.432763471352
H	-1.626056374387	4.082458849087	2.085262094114
H	-1.672649436242	2.514693128412	2.887799387991
H	0.510180523426	2.318032167664	1.939769655257
H	0.116505316931	3.438366304399	0.616782716846
H	-0.091342328373	0.384600725144	-1.297739090323
H	0.625000608210	2.008223952878	-1.239087754639
H	2.129745092764	1.285530145901	0.601694976016
H	1.333136147580	-0.296365887770	0.655218726574
H	2.125536731367	-0.581899907464	-1.505922907415

SCF Done: E(RwB97X) = -366.445624755

Zero-point correction= 0.192500
Thermal correction to Energy= 0.201158
Thermal correction to Enthalpy= 0.202102
Thermal correction to Gibbs Free Energy= 0.158393
Sum of electronic and zero-point Energies= -366.253124
Sum of electronic and thermal Energies= -366.244466
Sum of electronic and thermal Enthalpies= -366.243522
Sum of electronic and thermal Free Energies= -366.287231

1 N	Isotropic =	199.6670	Anisotropy =	61.5843
2 C	Isotropic =	134.1546	Anisotropy =	64.3601
3 C	Isotropic =	167.8001	Anisotropy =	22.6868
4 C	Isotropic =	166.8298	Anisotropy =	25.0699
5 C	Isotropic =	137.1985	Anisotropy =	58.2632
6 C	Isotropic =	131.5920	Anisotropy =	63.0639
7 C	Isotropic =	126.0796	Anisotropy =	64.4249
8 O	Isotropic =	307.0039	Anisotropy =	56.5216
9 H	Isotropic =	29.8927	Anisotropy =	7.6027
10 H	Isotropic =	28.9705	Anisotropy =	9.0167
11 H	Isotropic =	30.2087	Anisotropy =	10.8782
12 H	Isotropic =	30.1663	Anisotropy =	10.8426
13 H	Isotropic =	30.1372	Anisotropy =	10.7543
14 H	Isotropic =	30.1408	Anisotropy =	10.7090
15 H	Isotropic =	28.9798	Anisotropy =	8.0182
16 H	Isotropic =	30.2022	Anisotropy =	7.5037
17 H	Isotropic =	29.1432	Anisotropy =	7.3096
18 H	Isotropic =	29.7949	Anisotropy =	5.3146
19 H	Isotropic =	28.1463	Anisotropy =	5.4030

20 H Isotropic = 28.1246 Anisotropy = 4.2360
 21 H Isotropic = 31.5127 Anisotropy = 17.0931

Conformer_6

N	-0.553945974625	1.830415917782	0.127488287508
C	-0.392904696725	2.151853579440	1.545595370945
C	-1.554891418562	3.106175520802	1.843858513000
C	-2.617627492483	2.766320470109	0.772017889840
C	-1.991827881221	1.619065694831	-0.023190926725
C	0.229399390034	0.693318139332	-0.318813379745
C	1.724095978982	0.980829554217	-0.308456666224
O	2.471083907161	-0.112995928181	-0.830314277858
H	0.585386434176	2.595871375034	1.745927588392
H	-0.480350415812	1.233200598111	2.155508704905
H	-1.927220419533	2.969786114920	2.861662163865
H	-1.231160590406	4.145815657113	1.749645115204
H	-3.576505613769	2.475394976155	1.206878963977
H	-2.797256401568	3.626809060435	0.122289652472
H	-2.274877490204	1.609525026282	-1.079577736057
H	-2.283417862252	0.646485357664	0.415469347434
H	0.027310021485	-0.200105758704	0.301849924671
H	-0.072593182874	0.453728801526	-1.345954329355
H	1.927204030251	1.898380875563	-0.876175392447
H	2.087155848232	1.128118937687	0.711576959005
H	2.221043829714	-0.229193970118	-1.751985772808

SCF Done: E(RwB97X) = -366.445624756

Zero-point correction=	0.192500
Thermal correction to Energy=	0.201158
Thermal correction to Enthalpy=	0.202102
Thermal correction to Gibbs Free Energy=	0.158393
Sum of electronic and zero-point Energies=	-366.253124
Sum of electronic and thermal Energies=	-366.244466
Sum of electronic and thermal Enthalpies=	-366.243522
Sum of electronic and thermal Free Energies=	-366.287231

1 N	Isotropic = 199.6669	Anisotropy = 61.5841
2 C	Isotropic = 137.1985	Anisotropy = 58.2631
3 C	Isotropic = 166.8298	Anisotropy = 25.0699
4 C	Isotropic = 167.8001	Anisotropy = 22.6867
5 C	Isotropic = 134.1546	Anisotropy = 64.3602
6 C	Isotropic = 131.5920	Anisotropy = 63.0639
7 C	Isotropic = 126.0796	Anisotropy = 64.4249

8	O	Isotropic =	307.0039	Anisotropy =	56.5217
9	H	Isotropic =	28.9798	Anisotropy =	8.0182
10	H	Isotropic =	30.2022	Anisotropy =	7.5037
11	H	Isotropic =	30.1372	Anisotropy =	10.7543
12	H	Isotropic =	30.1408	Anisotropy =	10.7090
13	H	Isotropic =	30.2087	Anisotropy =	10.8782
14	H	Isotropic =	30.1663	Anisotropy =	10.8426
15	H	Isotropic =	28.9705	Anisotropy =	9.0167
16	H	Isotropic =	29.8927	Anisotropy =	7.6027
17	H	Isotropic =	29.7949	Anisotropy =	5.3146
18	H	Isotropic =	29.1432	Anisotropy =	7.3096
19	H	Isotropic =	28.1246	Anisotropy =	4.2360
20	H	Isotropic =	28.1463	Anisotropy =	5.4030
21	H	Isotropic =	31.5127	Anisotropy =	17.0931

Conformer_7

N	-0.719232718285	1.739888051513	0.063520424693
C	-0.343209800605	2.381721692282	1.323563555855
C	-1.537800693850	3.284150579658	1.655676472207
C	-2.726108363486	2.646464864414	0.897858390599
C	-2.127109968915	1.397066784277	0.251059474277
C	0.091785676739	0.587620800798	-0.284235469028
C	1.516420339649	0.970216122448	-0.638456338263
O	2.183393693396	-0.218663460595	-1.055888608087
H	-0.205288625625	1.617817424586	2.111585333700
H	0.593914757087	2.935227606358	1.225627505020
H	-1.706644304694	3.332680660255	2.733794405890
H	-1.359439610375	4.304138274274	1.306041077015
H	-3.561069967665	2.396397313033	1.556273950516
H	-3.102787881308	3.327933654809	0.130623526568
H	-2.592303428296	1.128100305266	-0.701490717722
H	-2.222474082856	0.530866329369	0.932402334805
H	0.109911759397	-0.148979641182	0.541120266546
H	-0.359423065699	0.096319824006	-1.153197155277
H	2.028492669217	1.406076412586	0.227964978184
H	1.508609024032	1.715208184150	-1.444785330708
H	3.105764592143	-0.003751782305	-1.216658076789

SCF Done: E(RwB97X) = -366.445204181

Zero-point correction=	0.192334
Thermal correction to Energy=	0.201075
Thermal correction to Enthalpy=	0.202019
Thermal correction to Gibbs Free Energy=	0.158226

Sum of electronic and zero-point Energies=	-366.252871
Sum of electronic and thermal Energies=	-366.244129
Sum of electronic and thermal Enthalpies=	-366.243185
Sum of electronic and thermal Free Energies=	-366.286978

1	N	Isotropic =	200.1550	Anisotropy =	61.0171
2	C	Isotropic =	136.9119	Anisotropy =	58.9024
3	C	Isotropic =	166.9212	Anisotropy =	25.0916
4	C	Isotropic =	167.6301	Anisotropy =	22.7974
5	C	Isotropic =	133.9548	Anisotropy =	64.2891
6	C	Isotropic =	133.8328	Anisotropy =	61.2436
7	C	Isotropic =	126.9139	Anisotropy =	63.5484
8	O	Isotropic =	315.7121	Anisotropy =	99.1199
9	H	Isotropic =	30.1970	Anisotropy =	7.4763
10	H	Isotropic =	28.9913	Anisotropy =	8.0934
11	H	Isotropic =	30.1416	Anisotropy =	10.7050
12	H	Isotropic =	30.1380	Anisotropy =	10.7135
13	H	Isotropic =	30.1979	Anisotropy =	10.8871
14	H	Isotropic =	30.1594	Anisotropy =	10.8403
15	H	Isotropic =	28.9391	Anisotropy =	9.0497
16	H	Isotropic =	29.8737	Anisotropy =	7.6080
17	H	Isotropic =	29.8364	Anisotropy =	5.4829
18	H	Isotropic =	28.9561	Anisotropy =	7.2092
19	H	Isotropic =	27.9503	Anisotropy =	6.0732
20	H	Isotropic =	28.1496	Anisotropy =	4.2580
21	H	Isotropic =	31.2419	Anisotropy =	20.5243

Conformer_8

N	-0.319287759148	1.951004350781	0.556494526483
C	-1.571681508823	1.718579722707	-0.163603176358
C	-2.548540254487	2.730855830384	0.446940219674
C	-1.963726766206	3.036547594402	1.846065683546
C	-0.740108843745	2.124872768421	1.944836976566
C	0.662824216652	0.893693034640	0.401721118420
C	1.218846889300	0.824210843996	-1.008047231876
O	2.236472983921	-0.174258900606	-1.013721860891
H	-1.442765325531	1.848202853132	-1.240980187887
H	-1.924811352920	0.685469093123	0.013970069373
H	-3.559929770959	2.321180659974	0.496527698486
H	-2.592473876014	3.638648946317	-0.160031196210
H	-1.662804090881	4.085108585288	1.916076814753
H	-2.674836512529	2.842464731596	2.652204942996
H	0.071602475218	2.540944285056	2.548251452871
H	-1.024293473289	1.149933948966	2.383423672915

H	1.492344006641	1.088297475061	1.090260519258
H	0.233006053119	-0.089969413171	0.669648658324
H	0.430206813506	0.563653066484	-1.724311572250
H	1.631516841745	1.801580863338	-1.290345056151
H	2.549239254431	-0.277820339890	-1.916082072040

SCF Done: E(RwB97X) = -366.445204184

Zero-point correction=	0.192334
Thermal correction to Energy=	0.201075
Thermal correction to Enthalpy=	0.202019
Thermal correction to Gibbs Free Energy=	0.158226
Sum of electronic and zero-point Energies=	-366.252871
Sum of electronic and thermal Energies=	-366.244129
Sum of electronic and thermal Enthalpies=	-366.243185
Sum of electronic and thermal Free Energies=	-366.286979

1 N	Isotropic = 200.1546	Anisotropy = 61.0172
2 C	Isotropic = 136.9119	Anisotropy = 58.9016
3 C	Isotropic = 166.9209	Anisotropy = 25.0918
4 C	Isotropic = 167.6305	Anisotropy = 22.7973
5 C	Isotropic = 133.9550	Anisotropy = 64.2898
6 C	Isotropic = 133.8330	Anisotropy = 61.2433
7 C	Isotropic = 126.9137	Anisotropy = 63.5480
8 O	Isotropic = 315.7118	Anisotropy = 99.1206
9 H	Isotropic = 28.9913	Anisotropy = 8.0934
10 H	Isotropic = 30.1970	Anisotropy = 7.4764
11 H	Isotropic = 30.1416	Anisotropy = 10.7050
12 H	Isotropic = 30.1380	Anisotropy = 10.7135
13 H	Isotropic = 30.1594	Anisotropy = 10.8403
14 H	Isotropic = 30.1979	Anisotropy = 10.8871
15 H	Isotropic = 28.9390	Anisotropy = 9.0497
16 H	Isotropic = 29.8737	Anisotropy = 7.6080
17 H	Isotropic = 28.9561	Anisotropy = 7.2093
18 H	Isotropic = 29.8364	Anisotropy = 5.4829
19 H	Isotropic = 27.9503	Anisotropy = 6.0731
20 H	Isotropic = 28.1496	Anisotropy = 4.2579
21 H	Isotropic = 31.2420	Anisotropy = 20.5243

Conformer_9

N	-0.696042944094	1.360666564285	0.448707653768
C	-2.018757346695	1.669958192859	-0.090140921271
C	-2.685155090013	2.487751375659	1.016955888453
C	-1.502095512290	3.160416892928	1.752333551310

C	-0.254085123211	2.623677227185	1.041215222548
C	0.203312270961	0.824571353445	-0.556326530191
C	1.515728985139	0.334779212121	0.038186195517
O	2.341100402722	-0.274201202248	-0.950369329250
H	-1.924177568675	2.277378134211	-1.009711660606
H	-2.558198127041	0.753851508111	-0.346565043855
H	-3.394496783714	3.211366074027	0.609040789462
H	-3.236172377478	1.831315720302	1.695454759446
H	-1.544497977667	4.250851666484	1.703943484672
H	-1.494071865027	2.879552048911	2.808502436871
H	0.589780098577	2.473756880608	1.718859992643
H	0.068397811819	3.322456288291	0.246661240505
H	-0.289321426949	-0.021018378854	-1.048230827604
H	0.417166346462	1.582100940668	-1.336821837595
H	1.318362653886	-0.433480467133	0.790500740790
H	2.054588726001	1.155318228231	0.527267934881
H	2.599534847289	0.404631739910	-1.580863740495

SCF Done: E(RwB97X) = -366.445467641

Zero-point correction=	0.192502
Thermal correction to Energy=	0.201190
Thermal correction to Enthalpy=	0.202134
Thermal correction to Gibbs Free Energy=	0.158382
Sum of electronic and zero-point Energies=	-366.252965
Sum of electronic and thermal Energies=	-366.244278
Sum of electronic and thermal Enthalpies=	-366.243333
Sum of electronic and thermal Free Energies=	-366.287085

1 N	Isotropic = 199.5092	Anisotropy = 61.9621
2 C	Isotropic = 133.9441	Anisotropy = 64.3003
3 C	Isotropic = 167.8211	Anisotropy = 22.5817
4 C	Isotropic = 166.8861	Anisotropy = 25.1155
5 C	Isotropic = 137.0219	Anisotropy = 58.8189
6 C	Isotropic = 131.4349	Anisotropy = 63.1465
7 C	Isotropic = 126.6881	Anisotropy = 65.0476
8 O	Isotropic = 309.7013	Anisotropy = 54.0378
9 H	Isotropic = 29.9105	Anisotropy = 7.5780
10 H	Isotropic = 28.9559	Anisotropy = 9.0161
11 H	Isotropic = 30.2153	Anisotropy = 10.8726
12 H	Isotropic = 30.1700	Anisotropy = 10.8738
13 H	Isotropic = 30.1435	Anisotropy = 10.6987
14 H	Isotropic = 30.1349	Anisotropy = 10.7340
15 H	Isotropic = 28.9369	Anisotropy = 8.0274
16 H	Isotropic = 30.2251	Anisotropy = 7.4516
17 H	Isotropic = 28.9478	Anisotropy = 7.0175

18 H	Isotropic =	29.9990	Anisotropy =	5.5236
19 H	Isotropic =	28.3339	Anisotropy =	4.0551
20 H	Isotropic =	27.9343	Anisotropy =	6.2485
21 H	Isotropic =	31.5000	Anisotropy =	17.2036

2-(pyrrolidin-1-yl)ethan-1-ol_protonated

Conformer_1

N	-0.466480405962	1.438252651863	-0.052513631676
C	-0.091609517252	2.042318032923	-1.382351777479
C	-1.207470612452	3.050437053649	-1.704286029003
C	-2.150144805815	3.016810497779	-0.491347796004
C	-1.945158003505	1.625539008001	0.075985736504
C	-0.008456395790	0.038395990924	0.160932688155
C	1.498677482881	-0.022103007136	0.241443475773
O	1.893710251511	0.874558353548	1.274814048046
H	-0.023841711781	2.005382866966	0.677367407224
H	0.896246985061	2.491246981847	-1.287131412945
H	-0.047721975787	1.226642638027	-2.104528522239
H	-0.804621734586	4.048123206809	-1.881145388248
H	-1.734187458896	2.734468368110	-2.606719156452
H	-1.856109989104	3.764353411994	0.251315384273
H	-3.192419316071	3.192458060915	-0.758956454544
H	-2.417963025871	0.857130692491	-0.540608613583
H	-2.230760991960	1.495094949243	1.119345085653
H	-0.457480169131	-0.300311860206	1.097018614909
H	-0.385506053388	-0.568144089937	-0.664038280885
H	1.789663483246	-1.052131887364	0.472491688069
H	1.955140681718	0.258853772382	-0.714153775254
H	2.850593282935	0.965924307170	1.259066709704

SCF Done: E(RwB97X) = -366.921503068

Zero-point correction=	0.208712
Thermal correction to Energy=	0.217267
Thermal correction to Enthalpy=	0.218212
Thermal correction to Gibbs Free Energy=	0.174930
Sum of electronic and zero-point Energies=	-366.712791
Sum of electronic and thermal Energies=	-366.704236
Sum of electronic and thermal Enthalpies=	-366.703292
Sum of electronic and thermal Free Energies=	-366.746573

1 N	Isotropic =	188.3900	Anisotropy =	43.8019
2 C	Isotropic =	137.9342	Anisotropy =	65.9219
3 C	Isotropic =	167.6432	Anisotropy =	22.6046

4	C	Isotropic =	165.5241	Anisotropy =	21.9096
5	C	Isotropic =	133.0390	Anisotropy =	58.9553
6	C	Isotropic =	134.1830	Anisotropy =	46.9084
7	C	Isotropic =	132.1153	Anisotropy =	55.7061
8	O	Isotropic =	321.4119	Anisotropy =	93.3227
9	H	Isotropic =	26.2657	Anisotropy =	12.9069
10	H	Isotropic =	28.0925	Anisotropy =	8.1381
11	H	Isotropic =	28.8645	Anisotropy =	7.5420
12	H	Isotropic =	29.7642	Anisotropy =	11.2798
13	H	Isotropic =	29.6879	Anisotropy =	10.8342
14	H	Isotropic =	29.8735	Anisotropy =	10.4364
15	H	Isotropic =	29.7189	Anisotropy =	11.6108
16	H	Isotropic =	28.7736	Anisotropy =	8.2350
17	H	Isotropic =	28.2991	Anisotropy =	9.1749
18	H	Isotropic =	28.2588	Anisotropy =	9.2322
19	H	Isotropic =	28.8238	Anisotropy =	7.2576
20	H	Isotropic =	27.9048	Anisotropy =	8.6728
21	H	Isotropic =	27.7812	Anisotropy =	5.7888
22	H	Isotropic =	30.8039	Anisotropy =	21.6761

Conformer_10

N	-0.621950635784	1.836634655768	0.008129661731
C	-0.200499935492	2.296478176141	-1.363710306089
C	-1.453978633246	2.931314289539	-1.987229918306
C	-2.566310583363	2.766865510192	-0.937229142798
C	-2.097279030044	1.600961653614	-0.087755441274
C	0.137672943181	0.676711803126	0.540351326373
C	1.606392083085	1.013828938688	0.715251914326
O	2.184986757998	-0.102235486552	1.373759343773
H	-0.486474378543	2.619433232381	0.653843244603
H	0.640412558219	2.979410535610	-1.251762612612
H	0.125466753881	1.407266984627	-1.904445084258
H	-1.286874298661	3.979546742505	-2.236646730557
H	-1.709593621256	2.403390791133	-2.907440726990
H	-2.651258407031	3.663157741722	-0.316455525474
H	-3.541771282012	2.568280699023	-1.382035441516
H	-2.230770879927	0.641098543408	-0.592097932728
H	-2.514708204219	1.554394527822	0.917562700539
H	-0.305658479810	0.415954718774	1.503511127724
H	-0.000933437001	-0.150604963664	-0.158555146258
H	2.083653923437	1.182417845757	-0.256466389126
H	1.710073853545	1.925990416062	1.318231845752
H	3.134902933045	0.037102644324	1.422189233165

SCF Done: E(RwB97X) = -366.917870243

Zero-point correction=	0.208390
Thermal correction to Energy=	0.217095
Thermal correction to Enthalpy=	0.218039
Thermal correction to Gibbs Free Energy=	0.174623
Sum of electronic and zero-point Energies=	-366.709480
Sum of electronic and thermal Energies=	-366.700775
Sum of electronic and thermal Enthalpies=	-366.699831
Sum of electronic and thermal Free Energies=	-366.743247

1	N	Isotropic =	183.9562	Anisotropy =	49.2032
2	C	Isotropic =	136.0511	Anisotropy =	66.3364
3	C	Isotropic =	167.7980	Anisotropy =	23.6280
4	C	Isotropic =	166.2276	Anisotropy =	22.0541
5	C	Isotropic =	132.0985	Anisotropy =	62.4030
6	C	Isotropic =	135.1974	Anisotropy =	59.8938
7	C	Isotropic =	130.4692	Anisotropy =	65.2935
8	O	Isotropic =	319.1635	Anisotropy =	99.0021
9	H	Isotropic =	27.0765	Anisotropy =	12.5878
10	H	Isotropic =	28.3551	Anisotropy =	8.0757
11	H	Isotropic =	28.8926	Anisotropy =	7.2097
12	H	Isotropic =	29.8179	Anisotropy =	11.2131
13	H	Isotropic =	29.6978	Anisotropy =	10.7411
14	H	Isotropic =	29.9342	Anisotropy =	10.6978
15	H	Isotropic =	29.7355	Anisotropy =	11.4654
16	H	Isotropic =	28.7806	Anisotropy =	7.8222
17	H	Isotropic =	28.2306	Anisotropy =	8.9539
18	H	Isotropic =	28.4162	Anisotropy =	7.2432
19	H	Isotropic =	28.7657	Anisotropy =	5.5908
20	H	Isotropic =	27.7737	Anisotropy =	5.8000
21	H	Isotropic =	27.9854	Anisotropy =	4.4525
22	H	Isotropic =	31.0072	Anisotropy =	20.9077

Conformer_11

N	-0.483299927661	2.390412723917	0.049317401329
C	-0.213195110309	2.498138032187	-1.422905083951
C	-1.609229789351	2.657973293508	-1.993874935280
C	-2.423258832725	1.634145687033	-1.192766501977
C	-1.772006684864	1.607945696053	0.196030363350
C	0.648282198974	1.935032413425	0.906989706549
C	1.279762736624	0.631963962794	0.448877132232
O	2.077957618549	0.201412558394	1.542758595538
H	-0.695065298542	3.339904983296	0.361828792377

H	0.242565602733	1.563489819162	-1.752988846104
H	0.470607856596	3.328751872473	-1.595677878516
H	-1.971082897628	3.675020095583	-1.813477356062
H	-1.629354381242	2.469844967136	-3.067740119564
H	-2.343379207117	0.647946055328	-1.655744464420
H	-3.480091931935	1.895987815064	-1.132584944067
H	-2.359155994707	2.104023162034	0.967696497540
H	-1.525439694576	0.601477243655	0.530199257779
H	1.387018090056	2.737986208190	0.914605288370
H	0.247735679359	1.817909588823	1.916023175881
H	1.899523851057	0.792378841579	-0.439377029857
H	0.514511226080	-0.115931003827	0.206474219740
H	2.608794890630	-0.544614015808	1.250036729113

SCF Done: E(RwB97X) = -366.914819906

Zero-point correction=	0.208369
Thermal correction to Energy=	0.216218
Thermal correction to Enthalpy=	0.217162
Thermal correction to Gibbs Free Energy=	0.175818
Sum of electronic and zero-point Energies=	-366.706451
Sum of electronic and thermal Energies=	-366.698602
Sum of electronic and thermal Enthalpies=	-366.697658
Sum of electronic and thermal Free Energies=	-366.739002

1 N	Isotropic =	187.7216	Anisotropy =	43.9984
2 C	Isotropic =	136.5889	Anisotropy =	49.4758
3 C	Isotropic =	163.8912	Anisotropy =	22.1553
4 C	Isotropic =	166.2315	Anisotropy =	23.2075
5 C	Isotropic =	137.5638	Anisotropy =	67.2855
6 C	Isotropic =	140.4214	Anisotropy =	53.3508
7 C	Isotropic =	134.7046	Anisotropy =	69.8002
8 O	Isotropic =	322.0061	Anisotropy =	98.5936
9 H	Isotropic =	26.6155	Anisotropy =	13.8641
10 H	Isotropic =	29.0576	Anisotropy =	7.0382
11 H	Isotropic =	28.4755	Anisotropy =	9.1880
12 H	Isotropic =	29.9606	Anisotropy =	10.7359
13 H	Isotropic =	29.7744	Anisotropy =	11.5379
14 H	Isotropic =	29.8451	Anisotropy =	10.1714
15 H	Isotropic =	29.7905	Anisotropy =	11.5318
16 H	Isotropic =	28.2644	Anisotropy =	9.5314
17 H	Isotropic =	28.4498	Anisotropy =	6.5280
18 H	Isotropic =	28.2303	Anisotropy =	7.9298
19 H	Isotropic =	28.6802	Anisotropy =	7.4066
20 H	Isotropic =	27.7520	Anisotropy =	5.4350
21 H	Isotropic =	27.8898	Anisotropy =	6.3117

22 H Isotropic = 31.0359 Anisotropy = 20.9297

Conformer_13

```
-----  
N      -0.800409064316    1.012011873683   -0.545332040089  
C      -2.211174618872    1.440064681593   -0.256886464034  
C      -2.202116486082    2.948760490053   -0.490668333383  
C      -1.059221985761    3.195984280954   -1.501362056619  
C      -0.436507216815    1.822697671831   -1.757799413846  
C      0.110353671309     1.204500552418    0.620337700060  
C      1.452736871256     0.529058988700    0.402364653742  
O      2.139319801603     0.635657847216    1.639874559319  
H      -0.795197445332     0.018135030434   -0.785549200169  
H      -2.483834595463     1.127986838813    0.750069051033  
H      -2.839251681077     0.921476622971   -0.982333646188  
H      -2.015480246137     3.481123879661    0.443804275262  
H      -3.171403035834     3.273066897439   -0.870444440676  
H      -0.320204055089     3.885891367477   -1.090625706867  
H      -1.420249076874     3.616859693434   -2.440270607047  
H      -0.900474861027     1.318278500835   -2.606065122599  
H      0.643276173265      1.828782892495   -1.892919284810  
H      0.228176686837      2.276176904768    0.791712838528  
H      -0.382425982880      0.757055031866    1.484903169452  
H      2.019013844979      1.017963167301   -0.397274097548  
H      1.296369647999      -0.522477144228    0.126286707786  
H      3.029403654311      0.293143930285    1.519077458693
```

SCF Done: E(RwB97X) = -366.915357848

```
Zero-point correction=          0.208807  
Thermal correction to Energy=      0.217440  
Thermal correction to Enthalpy=     0.218384  
Thermal correction to Gibbs Free Energy= 0.174930  
Sum of electronic and zero-point Energies= -366.706551  
Sum of electronic and thermal Energies= -366.697918  
Sum of electronic and thermal Enthalpies= -366.696973  
Sum of electronic and thermal Free Energies= -366.740428
```

```
1 N Isotropic = 185.3996 Anisotropy = 34.0476  
2 C Isotropic = 131.6085 Anisotropy = 71.4009  
3 C Isotropic = 169.8606 Anisotropy = 26.8064  
4 C Isotropic = 170.3340 Anisotropy = 28.8887  
5 C Isotropic = 137.1066 Anisotropy = 63.8447  
6 C Isotropic = 137.8497 Anisotropy = 58.9604  
7 C Isotropic = 130.7572 Anisotropy = 64.4986
```


8	O	Isotropic =	320.7555	Anisotropy =	100.1094
9	H	Isotropic =	26.7613	Anisotropy =	15.0391
10	H	Isotropic =	28.3935	Anisotropy =	8.9496
11	H	Isotropic =	28.3820	Anisotropy =	10.5208
12	H	Isotropic =	29.7278	Anisotropy =	10.1493
13	H	Isotropic =	29.7142	Anisotropy =	11.5708
14	H	Isotropic =	29.7040	Anisotropy =	10.1611
15	H	Isotropic =	29.7221	Anisotropy =	11.5181
16	H	Isotropic =	28.6525	Anisotropy =	10.6983
17	H	Isotropic =	28.4112	Anisotropy =	8.0921
18	H	Isotropic =	28.4637	Anisotropy =	5.9830
19	H	Isotropic =	28.8810	Anisotropy =	7.2227
20	H	Isotropic =	27.7324	Anisotropy =	5.2314
21	H	Isotropic =	27.9803	Anisotropy =	4.6495
22	H	Isotropic =	31.0243	Anisotropy =	21.0961

Conformer_2

N	-0.145418160139	1.522446808669	-0.494772091144
C	-0.541122301282	1.993386505400	-1.858482880067
C	-1.380692743362	3.218352506068	-1.551731344499
C	-2.205911167050	2.788709027873	-0.328873957553
C	-1.364971816426	1.708791587860	0.372332517707
C	0.449345645342	0.158423428100	-0.469660063197
C	1.025932284853	-0.145864404124	0.892901608931
O	1.955855413186	0.891136828248	1.189175210119
H	0.576573801487	2.162783208975	-0.149825433810
H	-1.132086145957	1.193917361433	-2.312130239461
H	0.357842319125	2.173374513194	-2.447253211910
H	-1.999954669010	3.504742160009	-2.402201067477
H	-0.727234371103	4.060168863244	-1.304416403325
H	-3.159767146405	2.360505347237	-0.642648786888
H	-2.415370641530	3.626053005400	0.337402663536
H	-1.033808646011	1.985954704067	1.372322524375
H	-1.877208268494	0.747323036080	0.416885627766
H	-0.332597676792	-0.554208404003	-0.736792798260
H	1.232258136278	0.142487723294	-1.230840577036
H	0.237508352615	-0.191258084737	1.652366232514
H	1.517459422449	-1.123304018714	0.847869625642
H	2.237068378227	0.805278296427	2.104472844036

SCF Done: E(RwB97X) = -366.921503113

Zero-point correction=	0.208713
Thermal correction to Energy=	0.217267

Thermal correction to Enthalpy=	0.218212
Thermal correction to Gibbs Free Energy=	0.174933
Sum of electronic and zero-point Energies=	-366.712790
Sum of electronic and thermal Energies=	-366.704236
Sum of electronic and thermal Enthalpies=	-366.703292
Sum of electronic and thermal Free Energies=	-366.746570

1 N	Isotropic = 188.3938	Anisotropy = 43.8007
2 C	Isotropic = 133.0390	Anisotropy = 58.9535
3 C	Isotropic = 165.5231	Anisotropy = 21.9077
4 C	Isotropic = 167.6413	Anisotropy = 22.6060
5 C	Isotropic = 137.9356	Anisotropy = 65.9229
6 C	Isotropic = 134.1838	Anisotropy = 46.9092
7 C	Isotropic = 132.1155	Anisotropy = 55.7062
8 O	Isotropic = 321.4119	Anisotropy = 93.3204
9 H	Isotropic = 26.2656	Anisotropy = 12.9072
10 H	Isotropic = 28.7736	Anisotropy = 8.2350
11 H	Isotropic = 28.2990	Anisotropy = 9.1750
12 H	Isotropic = 29.7190	Anisotropy = 11.6110
13 H	Isotropic = 29.8736	Anisotropy = 10.4363
14 H	Isotropic = 29.6879	Anisotropy = 10.8340
15 H	Isotropic = 29.7642	Anisotropy = 11.2800
16 H	Isotropic = 28.0927	Anisotropy = 8.1384
17 H	Isotropic = 28.8642	Anisotropy = 7.5416
18 H	Isotropic = 28.8238	Anisotropy = 7.2575
19 H	Isotropic = 28.2588	Anisotropy = 9.2326
20 H	Isotropic = 27.7812	Anisotropy = 5.7895
21 H	Isotropic = 27.9047	Anisotropy = 8.6726
22 H	Isotropic = 30.8039	Anisotropy = 21.6764

Conformer_3

N	-0.788196867457	0.961824728369	-0.615603974742
C	-1.372469906968	1.779533882028	0.510848489912
C	-1.602354693861	3.176897398953	-0.088825214726
C	-1.112962573592	3.086036284340	-1.545497552152
C	-0.109944842720	1.947478154702	-1.514094195506
C	-0.010569008043	-0.252387780704	-0.208193013826
C	1.421912805372	0.001013625741	0.195532362538
O	1.462619428320	0.851266654548	1.334316074284
H	-1.585696649423	0.603106541780	-1.145782694439
H	-2.280712964139	1.277569389982	0.842286868641
H	-0.641743038995	1.784609463040	1.316533184798
H	-2.651693912947	3.468455205880	-0.032854233167
H	-1.019195125325	3.913354703468	0.467297866884

H	-0.656313079371	4.011439353344	-1.897345921664
H	-1.937130895816	2.834985497164	-2.219550039357
H	0.101026232009	1.474754370491	-2.473071953540
H	0.819693049518	2.253374110547	-1.032000477693
H	-0.572524288146	-0.718582953006	0.603424475330
H	-0.012311504943	-0.927370649088	-1.065889717846
H	1.992340015435	0.430860761758	-0.635453209480
H	1.856326871795	-0.979613430884	0.421611942818
H	2.383700949296	0.993194687549	1.571810932930

SCF Done: E(RwB97X) = -366.916468373

Zero-point correction=	0.208747
Thermal correction to Energy=	0.217277
Thermal correction to Enthalpy=	0.218221
Thermal correction to Gibbs Free Energy=	0.175114
Sum of electronic and zero-point Energies=	-366.707721
Sum of electronic and thermal Energies=	-366.699192
Sum of electronic and thermal Enthalpies=	-366.698247
Sum of electronic and thermal Free Energies=	-366.741354

1 N	Isotropic = 184.5991	Anisotropy = 46.7745
2 C	Isotropic = 134.8811	Anisotropy = 70.4724
3 C	Isotropic = 168.6855	Anisotropy = 22.5515
4 C	Isotropic = 165.5784	Anisotropy = 22.8871
5 C	Isotropic = 139.0952	Anisotropy = 46.2748
6 C	Isotropic = 139.9560	Anisotropy = 40.1257
7 C	Isotropic = 131.5623	Anisotropy = 63.1232
8 O	Isotropic = 313.6797	Anisotropy = 100.0885
9 H	Isotropic = 26.7628	Anisotropy = 13.6029
10 H	Isotropic = 28.2095	Anisotropy = 8.9820
11 H	Isotropic = 27.8806	Anisotropy = 7.1133
12 H	Isotropic = 29.8270	Anisotropy = 11.5487
13 H	Isotropic = 29.7438	Anisotropy = 10.3660
14 H	Isotropic = 29.6343	Anisotropy = 11.3277
15 H	Isotropic = 29.9127	Anisotropy = 10.9078
16 H	Isotropic = 28.5218	Anisotropy = 9.5867
17 H	Isotropic = 28.5264	Anisotropy = 7.2601
18 H	Isotropic = 28.1855	Anisotropy = 9.0869
19 H	Isotropic = 28.6050	Anisotropy = 9.6226
20 H	Isotropic = 27.4914	Anisotropy = 5.5844
21 H	Isotropic = 27.8928	Anisotropy = 8.9467
22 H	Isotropic = 30.9664	Anisotropy = 21.4083

Conformer_4

N	-0.743433546064	0.975693586231	-0.684559770383
C	-1.444248930534	1.689786182325	0.427981239879
C	-1.976743008422	2.923833777655	-0.276947844785
C	-0.821603204726	3.335181520135	-1.207588467665
C	-0.015491220792	2.049409525624	-1.456671585004
C	0.063060996247	-0.236098362822	-0.329401642994
C	0.928005147656	-0.100996715730	0.900572130989
O	1.891381856244	0.926465949396	0.706561059877
H	-1.480682885201	0.633708111765	-1.305269548491
H	-2.195483085869	1.030466573734	0.862216890181
H	-0.696794747061	1.954649717564	1.177230068869
H	-2.869525831468	2.664666598993	-0.853488169639
H	-2.246540500925	3.705134999457	0.434019551122
H	-0.184224739988	4.077813141331	-0.723888207890
H	-1.188111635643	3.764516131708	-2.140645087786
H	0.019542586663	1.735597233223	-2.499274361747
H	0.994376624426	2.104131655740	-1.056315046021
H	-0.647878359970	-1.047345133890	-0.162989471899
H	0.663487051015	-0.473862608453	-1.209635684965
H	0.317178323166	0.096696876131	1.788547845115
H	1.413741306788	-1.073094266256	1.043905041338
H	2.429587804458	0.989045506139	1.501141061900

SCF Done: E(RwB97X) = -366.916468400

Zero-point correction= 0.208747
Thermal correction to Energy= 0.217277
Thermal correction to Enthalpy= 0.218221
Thermal correction to Gibbs Free Energy= 0.175115
Sum of electronic and zero-point Energies= -366.707722
Sum of electronic and thermal Energies= -366.699192
Sum of electronic and thermal Enthalpies= -366.698248
Sum of electronic and thermal Free Energies= -366.741354

1 N Isotropic = 184.5998 Anisotropy = 46.7738
2 C Isotropic = 139.0959 Anisotropy = 46.2738
3 C Isotropic = 165.5782 Anisotropy = 22.8871
4 C Isotropic = 168.6858 Anisotropy = 22.5512
5 C Isotropic = 134.8803 Anisotropy = 70.4738
6 C Isotropic = 139.9569 Anisotropy = 40.1285
7 C Isotropic = 131.5619 Anisotropy = 63.1228
8 O Isotropic = 313.6808 Anisotropy = 100.0846
9 H Isotropic = 26.7629 Anisotropy = 13.6031
10 H Isotropic = 28.5217 Anisotropy = 9.5867
11 H Isotropic = 28.5264 Anisotropy = 7.2599

12	H	Isotropic =	29.9127	Anisotropy =	10.9079
13	H	Isotropic =	29.6343	Anisotropy =	11.3278
14	H	Isotropic =	29.7438	Anisotropy =	10.3659
15	H	Isotropic =	29.8271	Anisotropy =	11.5488
16	H	Isotropic =	28.2095	Anisotropy =	8.9822
17	H	Isotropic =	27.8802	Anisotropy =	7.1132
18	H	Isotropic =	28.6050	Anisotropy =	9.6227
19	H	Isotropic =	28.1856	Anisotropy =	9.0870
20	H	Isotropic =	27.4914	Anisotropy =	5.5850
21	H	Isotropic =	27.8927	Anisotropy =	8.9469
22	H	Isotropic =	30.9663	Anisotropy =	21.4081

Conformer_5

N	-0.826874033258	0.804241258031	-0.872547286361
C	-1.779110673806	1.423823954064	0.127466455524
C	-1.298857309489	2.857685820415	0.268465521808
C	-0.880418878660	3.203216342924	-1.159798706504
C	-0.161941985017	1.943609398473	-1.628232818758
C	0.123008026229	-0.209706365215	-0.303838035578
C	0.929162731076	0.238804004758	0.893627580170
O	1.894976666981	1.209059739383	0.506467674258
H	-1.392292404761	0.286784051421	-1.544843712545
H	-2.772073491146	1.386339142852	-0.322205406296
H	-1.781404577303	0.832792227224	1.041491244131
H	-0.441788794808	2.913739318085	0.947001358894
H	-2.089105929810	3.502623092595	0.655139188374
H	-0.223659220198	4.072304857608	-1.219595101682
H	-1.764468669670	3.394665655451	-1.774783039058
H	-0.252277729805	1.739076311918	-2.694171451211
H	0.886885232546	1.952241901980	-1.342013597318
H	-0.487124559138	-1.065862421492	-0.010652863438
H	0.779886098401	-0.511941114472	-1.122072019741
H	0.281222103198	0.628697192796	1.686966090880
H	1.419589352755	-0.661196041704	1.281900152707
H	2.410468045683	1.445701672908	1.283028771745

SCF Done: E(RwB97X) = -366.916183927

Zero-point correction=	0.208789
Thermal correction to Energy=	0.216298
Thermal correction to Enthalpy=	0.217242
Thermal correction to Gibbs Free Energy=	0.177034
Sum of electronic and zero-point Energies=	-366.707395
Sum of electronic and thermal Energies=	-366.699886

Sum of electronic and thermal Enthalpies= -366.698942
Sum of electronic and thermal Free Energies= -366.739149

1 N	Isotropic =	192.0067	Anisotropy =	35.6563
2 C	Isotropic =	136.2517	Anisotropy =	54.7551
3 C	Isotropic =	163.3220	Anisotropy =	19.9066
4 C	Isotropic =	163.3246	Anisotropy =	24.4670
5 C	Isotropic =	133.3639	Anisotropy =	69.0115
6 C	Isotropic =	134.6683	Anisotropy =	41.2283
7 C	Isotropic =	131.7506	Anisotropy =	61.7743
8 O	Isotropic =	308.7023	Anisotropy =	97.2393
9 H	Isotropic =	26.2819	Anisotropy =	15.5757
10 H	Isotropic =	28.5070	Anisotropy =	10.7955
11 H	Isotropic =	28.3781	Anisotropy =	7.6499
12 H	Isotropic =	29.7804	Anisotropy =	8.3877
13 H	Isotropic =	29.7953	Anisotropy =	12.0072
14 H	Isotropic =	29.6808	Anisotropy =	11.2027
15 H	Isotropic =	29.8972	Anisotropy =	11.2968
16 H	Isotropic =	28.0992	Anisotropy =	9.2419
17 H	Isotropic =	27.7542	Anisotropy =	6.5554
18 H	Isotropic =	28.6607	Anisotropy =	9.7584
19 H	Isotropic =	28.2764	Anisotropy =	9.1465
20 H	Isotropic =	27.4057	Anisotropy =	4.6749
21 H	Isotropic =	27.8784	Anisotropy =	9.0448
22 H	Isotropic =	30.9417	Anisotropy =	20.9229

Conformer_6

N	-0.979598161731	0.778001187422	-0.649447100553
C	-1.562416122622	1.680677879480	0.426007765110
C	-1.550201408610	3.078557897489	-0.180352613665
C	-0.348032650588	3.040672400068	-1.122543269974
C	-0.483761985919	1.671647995214	-1.765939534980
C	0.014969048883	-0.229952974081	-0.150901025312
C	1.363986793444	0.317935211298	0.255349964685
O	1.250479576690	1.078464920349	1.452372495426
H	-1.748177643450	0.224561938930	-1.026863061103
H	-2.552005330421	1.304721901179	0.682126316373
H	-0.907767663032	1.615635700721	1.291631098028
H	-2.467270262486	3.261428593978	-0.747789624762
H	-1.467141496654	3.840212170207	0.596309044108
H	0.587591652915	3.112280364676	-0.558931077782
H	-0.361566156143	3.832668970533	-1.872551453200
H	-1.260285944086	1.674647842890	-2.531807464047
H	0.428490429225	1.253863696649	-2.187860210402

H	-0.460587561700	-0.747330538299	0.684875389121
H	0.160010040809	-0.941451281174	-0.965721724783
H	1.808763269946	0.917748383392	-0.546903715451
H	2.009719668714	-0.553861784030	0.411151665877
H	2.128701906818	1.383069523108	1.698788137285

SCF Done: E(RwB97X) = -366.916187404

Zero-point correction=	0.208778
Thermal correction to Energy=	0.216291
Thermal correction to Enthalpy=	0.217235
Thermal correction to Gibbs Free Energy=	0.177010
Sum of electronic and zero-point Energies=	-366.707409
Sum of electronic and thermal Energies=	-366.699897
Sum of electronic and thermal Enthalpies=	-366.698952
Sum of electronic and thermal Free Energies=	-366.739178

1 N	Isotropic = 191.9982	Anisotropy = 35.7078
2 C	Isotropic = 133.3794	Anisotropy = 68.8457
3 C	Isotropic = 163.3106	Anisotropy = 24.4195
4 C	Isotropic = 163.3160	Anisotropy = 19.9415
5 C	Isotropic = 136.2473	Anisotropy = 54.8369
6 C	Isotropic = 134.6968	Anisotropy = 41.1307
7 C	Isotropic = 131.7471	Anisotropy = 61.7624
8 O	Isotropic = 308.6863	Anisotropy = 97.3800
9 H	Isotropic = 26.2833	Anisotropy = 15.5666
10 H	Isotropic = 28.1015	Anisotropy = 9.2345
11 H	Isotropic = 27.7431	Anisotropy = 6.6095
12 H	Isotropic = 29.8991	Anisotropy = 11.2897
13 H	Isotropic = 29.6822	Anisotropy = 11.2116
14 H	Isotropic = 29.7845	Anisotropy = 8.3946
15 H	Isotropic = 29.7941	Anisotropy = 12.0063
16 H	Isotropic = 28.5057	Anisotropy = 10.7911
17 H	Isotropic = 28.3784	Anisotropy = 7.6369
18 H	Isotropic = 28.2759	Anisotropy = 9.1431
19 H	Isotropic = 28.6596	Anisotropy = 9.7581
20 H	Isotropic = 27.4042	Anisotropy = 4.6632
21 H	Isotropic = 27.8777	Anisotropy = 9.0427
22 H	Isotropic = 30.9420	Anisotropy = 20.9186

Conformer_7

N	-0.821381198540	0.985668458846	-0.560195238911
C	-1.034256152939	2.016628944932	0.507045155831
C	-1.866477291960	3.056188627259	-0.219602289096

C	-1.195494301514	3.143093139025	-1.598523195701
C	-0.578956656979	1.756064530738	-1.835698691797
C	0.165471060589	-0.104353233738	-0.280482394046
C	1.524207836740	0.365128693215	0.185102127577
O	1.466248143516	0.653721575103	1.578121197019
H	-1.721065423417	0.514775460653	-0.677434280104
H	-1.510617665349	1.544940152983	1.366131876053
H	-0.056211088184	2.404281542395	0.792783472855
H	-2.899952647611	2.707891270744	-0.309300459054
H	-1.871484240455	4.009211872241	0.310221760569
H	-0.406198894662	3.897504234589	-1.588927261963
H	-1.903409866806	3.405306835024	-2.385378837083
H	-1.038936110093	1.193633440283	-2.647407191867
H	0.496835225871	1.801117711460	-2.000521699667
H	-0.281021220058	-0.752902155290	0.475550261291
H	0.260323097595	-0.668609229592	-1.209507673063
H	1.863650995702	1.239956794652	-0.382499463367
H	2.229967052431	-0.449961790482	-0.008601963588
H	2.343859346124	0.924913124959	1.863124788112

SCF Done: E(RwB97X) = -366.916716599

Zero-point correction=	0.208649
Thermal correction to Energy=	0.217200
Thermal correction to Enthalpy=	0.218145
Thermal correction to Gibbs Free Energy=	0.174882
Sum of electronic and zero-point Energies=	-366.708068
Sum of electronic and thermal Energies=	-366.699516
Sum of electronic and thermal Enthalpies=	-366.698572
Sum of electronic and thermal Free Energies=	-366.741834

1 N	Isotropic =	184.7874	Anisotropy =	42.6636
2 C	Isotropic =	135.1170	Anisotropy =	46.3242
3 C	Isotropic =	164.4726	Anisotropy =	23.5406
4 C	Isotropic =	167.5468	Anisotropy =	22.0188
5 C	Isotropic =	137.9724	Anisotropy =	65.4850
6 C	Isotropic =	137.2409	Anisotropy =	35.2955
7 C	Isotropic =	133.7918	Anisotropy =	61.1734
8 O	Isotropic =	308.2140	Anisotropy =	113.7750
9 H	Isotropic =	26.6691	Anisotropy =	13.8416
10 H	Isotropic =	28.3995	Anisotropy =	8.5324
11 H	Isotropic =	28.3872	Anisotropy =	7.7847
12 H	Isotropic =	29.9621	Anisotropy =	10.8005
13 H	Isotropic =	29.7075	Anisotropy =	11.3290
14 H	Isotropic =	29.7498	Anisotropy =	10.3743
15 H	Isotropic =	29.7951	Anisotropy =	11.5026

16	H	Isotropic =	28.3682	Anisotropy =	9.7347
17	H	Isotropic =	28.5895	Anisotropy =	6.6493
18	H	Isotropic =	28.3449	Anisotropy =	9.0373
19	H	Isotropic =	28.4926	Anisotropy =	9.2016
20	H	Isotropic =	27.5905	Anisotropy =	4.7832
21	H	Isotropic =	27.9408	Anisotropy =	8.7899
22	H	Isotropic =	31.0848	Anisotropy =	21.2716

Conformer_8

N	-0.717425751354	1.007403829805	-0.715747294393
C	-1.886988669039	1.526753764664	0.085273575588
C	-2.049705140144	2.995509959388	-0.334816566148
C	-1.019585735121	3.211924888555	-1.453378466785
C	0.073896187997	2.215947466082	-1.116316638559
C	0.027315966652	-0.128511375640	-0.086998068571
C	0.910922394425	0.251322307090	1.078477469512
O	2.141421957437	0.767973804518	0.582404086170
H	-1.108995156634	0.630150404641	-1.581350518114
H	-2.744816008649	0.896408780040	-0.146196471568
H	-1.643283711851	1.420201882506	1.141577455875
H	-1.829096626422	3.645498103032	0.514340057120
H	-3.067269853915	3.205914199858	-0.665471954283
H	-0.637515754760	4.232680147361	-1.486143315425
H	-1.449257699328	2.974673449621	-2.431399499069
H	0.739707258803	1.948327646994	-1.936387201505
H	0.659175795407	2.529995451663	-0.251843992364
H	-0.731691441244	-0.843726987255	0.233696135329
H	0.628875822206	-0.589534648782	-0.872580401020
H	0.418297224957	0.976979252910	1.736854264005
H	1.084667855638	-0.660084272155	1.660833361164
H	2.701351084939	0.978891945105	1.335373983042

SCF Done: E(RwB97X) = -366.916716620

Zero-point correction=	0.208648
Thermal correction to Energy=	0.217200
Thermal correction to Enthalpy=	0.218144
Thermal correction to Gibbs Free Energy=	0.174882
Sum of electronic and zero-point Energies=	-366.708069
Sum of electronic and thermal Energies=	-366.699517
Sum of electronic and thermal Enthalpies=	-366.698572
Sum of electronic and thermal Free Energies=	-366.741834

1	N	Isotropic =	184.7886	Anisotropy =	42.6652

2 C	Isotropic =	137.9731	Anisotropy =	65.4858
3 C	Isotropic =	167.5426	Anisotropy =	22.0199
4 C	Isotropic =	164.4703	Anisotropy =	23.5371
5 C	Isotropic =	135.1147	Anisotropy =	46.3249
6 C	Isotropic =	137.2393	Anisotropy =	35.2937
7 C	Isotropic =	133.7909	Anisotropy =	61.1734
8 O	Isotropic =	308.2134	Anisotropy =	113.7608
9 H	Isotropic =	26.6688	Anisotropy =	13.8419
10 H	Isotropic =	28.3681	Anisotropy =	9.7351
11 H	Isotropic =	28.5894	Anisotropy =	6.6491
12 H	Isotropic =	29.7498	Anisotropy =	10.3735
13 H	Isotropic =	29.7951	Anisotropy =	11.5027
14 H	Isotropic =	29.7075	Anisotropy =	11.3294
15 H	Isotropic =	29.9621	Anisotropy =	10.8003
16 H	Isotropic =	28.3995	Anisotropy =	8.5325
17 H	Isotropic =	28.3867	Anisotropy =	7.7858
18 H	Isotropic =	28.4926	Anisotropy =	9.2018
19 H	Isotropic =	28.3448	Anisotropy =	9.0375
20 H	Isotropic =	27.5904	Anisotropy =	4.7838
21 H	Isotropic =	27.9408	Anisotropy =	8.7897
22 H	Isotropic =	31.0846	Anisotropy =	21.2723

Conformer_9

N	-0.701594460027	1.401006362426	-0.299882986361
C	-2.040152562267	1.913165919515	0.132883839547
C	-2.623729187388	2.453199551178	-1.158909168324
C	-1.422158067430	3.105936656942	-1.863884016269
C	-0.177014517376	2.425332161845	-1.272820569731
C	0.211929659316	1.082480529132	0.826941548720
C	1.506631171655	0.468042442048	0.329373819532
O	2.215132338690	0.062711961968	1.490293543767
H	-0.867668147350	0.534771866780	-0.819615363973
H	-1.853729467740	2.702486620848	0.864822905748
H	-2.597725700958	1.099915958988	0.596365856017
H	-3.434252275314	3.156555319687	-0.966156128725
H	-3.023489286884	1.627996955494	-1.754853673622
H	-1.470448678230	2.976687545533	-2.945498565838
H	-1.385462510028	4.176285744679	-1.654498615112
H	0.438120625344	3.117058216832	-0.696220208806
H	0.445300493046	1.913409529736	-2.005436258073
H	0.394600639962	2.012100694928	1.369686229261
H	-0.312243000489	0.379600311244	1.477647373151
H	1.286465479289	-0.390563216796	-0.319236474420
H	2.086771924824	1.198815826171	-0.244945365336

H 3.082215529355 -0.250996959178 1.218542278846

SCF Done: E(RwB97X) = -366.917870247

Zero-point correction= 0.208390
Thermal correction to Energy= 0.217095
Thermal correction to Enthalpy= 0.218039
Thermal correction to Gibbs Free Energy= 0.174621
Sum of electronic and zero-point Energies= -366.709480
Sum of electronic and thermal Energies= -366.700775
Sum of electronic and thermal Enthalpies= -366.699831
Sum of electronic and thermal Free Energies= -366.743249

1 N	Isotropic =	183.9559	Anisotropy =	49.2064
2 C	Isotropic =	132.0977	Anisotropy =	62.4035
3 C	Isotropic =	166.2276	Anisotropy =	22.0547
4 C	Isotropic =	167.7979	Anisotropy =	23.6283
5 C	Isotropic =	136.0511	Anisotropy =	66.3397
6 C	Isotropic =	135.1957	Anisotropy =	59.8952
7 C	Isotropic =	130.4698	Anisotropy =	65.2925
8 O	Isotropic =	319.1646	Anisotropy =	99.0046
9 H	Isotropic =	27.0766	Anisotropy =	12.5881
10 H	Isotropic =	28.7806	Anisotropy =	7.8218
11 H	Isotropic =	28.2305	Anisotropy =	8.9538
12 H	Isotropic =	29.7355	Anisotropy =	11.4654
13 H	Isotropic =	29.9342	Anisotropy =	10.6978
14 H	Isotropic =	29.8178	Anisotropy =	11.2131
15 H	Isotropic =	29.6978	Anisotropy =	10.7411
16 H	Isotropic =	28.8926	Anisotropy =	7.2097
17 H	Isotropic =	28.3550	Anisotropy =	8.0758
18 H	Isotropic =	28.7656	Anisotropy =	5.5906
19 H	Isotropic =	28.4163	Anisotropy =	7.2430
20 H	Isotropic =	27.9854	Anisotropy =	4.4527
21 H	Isotropic =	27.7737	Anisotropy =	5.7988
22 H	Isotropic =	31.0073	Anisotropy =	20.9080

2,3,4,6,7,8,9,10-octahydropyrimido[1,2-a]azepine_neutral
Conformer_1

N -1.958511186229 -0.511145548006 -0.128194835915
C -1.980148283453 -1.885488815451 0.359206573995
C -0.603457474319 -2.531732003321 0.312599838532
C 0.362691968039 -1.679040476859 1.112433915690
N 0.217827240312 -0.267222231556 0.757703061348
C -0.894942180043 0.185305944935 0.110900808225
C -0.861556241607 1.607219230387 -0.403174351122

C	0.212355235623	1.870620252660	-1.470441765587
C	1.611005340543	2.141242498577	-0.916777943064
C	2.208706826936	1.005573974164	-0.089426211540
C	1.341493003502	0.600840483363	1.102452825061
H	-2.694022791012	-2.453816577250	-0.244771690398
H	-2.357309000222	-1.905611408887	1.392378741003
H	-0.267049937792	-2.595961868667	-0.728626626996
H	-0.627245805052	-3.546503172702	0.718879495748
H	1.396659772435	-1.976821257143	0.910148673495
H	0.188334552398	-1.809190343497	2.188828971082
H	-1.851583138251	1.795443784381	-0.821471692569
H	-0.728108988751	2.305337538989	0.432087797121
H	0.241266626577	1.027370502738	-2.172474308422
H	-0.099914819621	2.743656136507	-2.053053420595
H	2.284863462648	2.375625742537	-1.748555604329
H	1.566883943292	3.041902691458	-0.289424720385
H	2.379664309156	0.120792862799	-0.716146563428
H	3.187669243237	1.321808866148	0.288052251838
H	0.978643049394	1.494612366653	1.622741298819
H	1.944385272259	0.047480827044	1.826125482397

SCF Done: E(RwB97X) = -462.118412703

Zero-point correction=	0.248268
Thermal correction to Energy=	0.257903
Thermal correction to Enthalpy=	0.258847
Thermal correction to Gibbs Free Energy=	0.213391
Sum of electronic and zero-point Energies=	-461.870145
Sum of electronic and thermal Energies=	-461.860510
Sum of electronic and thermal Enthalpies=	-461.859565
Sum of electronic and thermal Free Energies=	-461.905021

1 N	Isotropic =	55.6847	Anisotropy =	263.4504
2 C	Isotropic =	145.4708	Anisotropy =	28.9936
3 C	Isotropic =	167.6279	Anisotropy =	9.8140
4 C	Isotropic =	142.8105	Anisotropy =	34.9995
5 N	Isotropic =	154.7383	Anisotropy =	67.4231
6 C	Isotropic =	20.0208	Anisotropy =	147.5937
7 C	Isotropic =	150.7335	Anisotropy =	27.5934
8 C	Isotropic =	163.4872	Anisotropy =	9.4502
9 C	Isotropic =	160.2036	Anisotropy =	3.5916
10 C	Isotropic =	161.0251	Anisotropy =	9.6024
11 C	Isotropic =	138.9679	Anisotropy =	43.2102
12 H	Isotropic =	28.5805	Anisotropy =	8.4488
13 H	Isotropic =	28.8006	Anisotropy =	8.7323
14 H	Isotropic =	30.3251	Anisotropy =	8.3896

15	H	Isotropic =	30.1823	Anisotropy =	10.3275
16	H	Isotropic =	28.7895	Anisotropy =	6.3027
17	H	Isotropic =	28.6513	Anisotropy =	9.3607
18	H	Isotropic =	29.9266	Anisotropy =	7.7155
19	H	Isotropic =	29.3347	Anisotropy =	5.0028
20	H	Isotropic =	30.5307	Anisotropy =	6.9470
21	H	Isotropic =	30.0971	Anisotropy =	10.4052
22	H	Isotropic =	30.0886	Anisotropy =	10.2931
23	H	Isotropic =	30.4645	Anisotropy =	8.7313
24	H	Isotropic =	30.5387	Anisotropy =	6.8183
25	H	Isotropic =	30.2723	Anisotropy =	10.3216
26	H	Isotropic =	28.4665	Anisotropy =	6.0399
27	H	Isotropic =	29.0674	Anisotropy =	6.9826

Conformer_10

N	-1.903025476093	-0.479223061598	-0.218946598792
C	-1.858568884831	-1.878860953861	0.187600427196
C	-0.440216293206	-2.431617956988	0.162911082547
C	0.427725163432	-1.591721671985	1.082809109316
N	0.162608932929	-0.164665714842	0.885695178446
C	-0.912497181221	0.262213659494	0.154437981474
C	-0.914328142982	1.723736273865	-0.234066860702
C	0.201307667135	2.125692307142	-1.232283474079
C	1.422490077273	1.202291159862	-1.277159455989
C	2.178930552018	1.057110439474	0.043394521256
C	1.249149098190	0.748311982818	1.225273267988
H	-2.510968505897	-2.452836001242	-0.477043839328
H	-2.270837440193	-1.982840874072	1.202538487891
H	-0.054624054738	-2.385186737237	-0.862030490120
H	-0.415477391458	-3.477020183061	0.481837755648
H	1.488752041477	-1.774265006214	0.882132565982
H	0.242248419782	-1.854894159910	2.131807893106
H	-1.892667050768	1.931340701107	-0.669684380026
H	-0.844044149199	2.327143859245	0.675396160360
H	-0.229218487186	2.151976376975	-2.238377571277
H	0.522411787903	3.149157773472	-1.008105203628
H	1.101773188870	0.208176503087	-1.611694070664
H	2.110491242884	1.567927759881	-2.046902952098
H	2.926360917404	0.262564075299	-0.063113731732
H	2.727709916326	1.977705989727	0.274418829540
H	0.827601204614	1.673753514202	1.622490662945
H	1.812312847533	0.294629945358	2.045164704738

SCF Done: E(RwB97X) = -462.113608228

Zero-point correction=	0.248815
Thermal correction to Energy=	0.258405
Thermal correction to Enthalpy=	0.259350
Thermal correction to Gibbs Free Energy=	0.213900
Sum of electronic and zero-point Energies=	-461.864793
Sum of electronic and thermal Energies=	-461.855203
Sum of electronic and thermal Enthalpies=	-461.854259
Sum of electronic and thermal Free Energies=	-461.899708

1 N	Isotropic =	53.3236	Anisotropy =	271.4933
2 C	Isotropic =	145.1132	Anisotropy =	29.4113
3 C	Isotropic =	168.2035	Anisotropy =	11.3938
4 C	Isotropic =	144.6943	Anisotropy =	34.3318
5 N	Isotropic =	161.0576	Anisotropy =	81.6772
6 C	Isotropic =	22.0873	Anisotropy =	143.6833
7 C	Isotropic =	155.6140	Anisotropy =	30.3636
8 C	Isotropic =	168.9487	Anisotropy =	8.7802
9 C	Isotropic =	167.8570	Anisotropy =	14.0672
10 C	Isotropic =	165.9347	Anisotropy =	17.4492
11 C	Isotropic =	143.1502	Anisotropy =	44.1530
12 H	Isotropic =	28.5261	Anisotropy =	8.5289
13 H	Isotropic =	28.8044	Anisotropy =	8.9255
14 H	Isotropic =	30.3145	Anisotropy =	8.2239
15 H	Isotropic =	30.2038	Anisotropy =	10.5740
16 H	Isotropic =	28.7847	Anisotropy =	6.3977
17 H	Isotropic =	28.6580	Anisotropy =	9.9704
18 H	Isotropic =	29.9872	Anisotropy =	8.1137
19 H	Isotropic =	29.1457	Anisotropy =	6.5131
20 H	Isotropic =	30.1757	Anisotropy =	10.4765
21 H	Isotropic =	30.3614	Anisotropy =	9.8578
22 H	Isotropic =	30.4999	Anisotropy =	6.3767
23 H	Isotropic =	30.3906	Anisotropy =	10.8508
24 H	Isotropic =	29.9874	Anisotropy =	9.1240
25 H	Isotropic =	30.5497	Anisotropy =	10.4429
26 H	Isotropic =	28.3351	Anisotropy =	7.0945
27 H	Isotropic =	29.0203	Anisotropy =	7.8489

Conformer_11

N	-1.977198751606	-0.434063513444	0.086080922242
C	-2.063341220186	-1.716992904727	0.766922006614
C	-0.867153534365	-2.593151733989	0.434878752729
C	0.387091041232	-1.854077918540	0.853647278407
N	0.352644445257	-0.446111780237	0.443024696445

C	-0.809087401400	0.116436014851	-0.011761618419
C	-0.785270754394	1.471464745579	-0.702174762317
C	0.435205416710	1.766365671644	-1.574547939526
C	1.588221908852	2.369571294569	-0.772947768446
C	1.762587509252	1.677772505771	0.578149229413
C	1.689423027468	0.159654292736	0.498206118112
H	-2.999662697192	-2.202214828787	0.475837375379
H	-2.110045823166	-1.564298861248	1.856025848478
H	-0.850908519198	-2.787315573329	-0.643614911320
H	-0.915587425897	-3.557125324108	0.948503654649
H	0.515959873391	-1.905175049312	1.942937704616
H	1.273134601423	-2.313382468586	0.400988344598
H	-1.696605180031	1.491903246558	-1.301724776524
H	-0.902196179916	2.257424878345	0.053635411240
H	0.761893996838	0.841570469435	-2.064704012130
H	0.146565202992	2.451237054592	-2.377479633611
H	2.516765240251	2.294843307473	-1.350442867648
H	1.405216049707	3.437567604173	-0.607324050523
H	2.739196034675	1.937260451449	0.998692871040
H	1.017200134967	2.035452125827	1.296596967160
H	2.154459804492	-0.253038164936	1.399841795651
H	2.287293199841	-0.200575541758	-0.352146636308

SCF Done: E(RwB97X) = -462.110668528

Zero-point correction=	0.248085
Thermal correction to Energy=	0.257849
Thermal correction to Enthalpy=	0.258793
Thermal correction to Gibbs Free Energy=	0.213136
Sum of electronic and zero-point Energies=	-461.862584
Sum of electronic and thermal Energies=	-461.852820
Sum of electronic and thermal Enthalpies=	-461.851876
Sum of electronic and thermal Free Energies=	-461.897532

1 N	Isotropic = 53.4698	Anisotropy = 264.7778
2 C	Isotropic = 145.5545	Anisotropy = 28.1082
3 C	Isotropic = 167.7091	Anisotropy = 8.3636
4 C	Isotropic = 141.5160	Anisotropy = 37.8242
5 N	Isotropic = 155.1206	Anisotropy = 77.6499
6 C	Isotropic = 22.2720	Anisotropy = 140.7872
7 C	Isotropic = 154.0077	Anisotropy = 36.4424
8 C	Isotropic = 168.7794	Anisotropy = 15.5542
9 C	Isotropic = 164.2200	Anisotropy = 6.9634
10 C	Isotropic = 165.7004	Anisotropy = 18.4856
11 C	Isotropic = 138.8958	Anisotropy = 45.3404
12 H	Isotropic = 28.5802	Anisotropy = 8.5670

13	H	Isotropic =	28.8852	Anisotropy =	8.5924
14	H	Isotropic =	30.3863	Anisotropy =	8.9981
15	H	Isotropic =	30.1762	Anisotropy =	10.4386
16	H	Isotropic =	28.7469	Anisotropy =	8.7523
17	H	Isotropic =	28.9083	Anisotropy =	6.8557
18	H	Isotropic =	29.6411	Anisotropy =	7.3676
19	H	Isotropic =	29.3840	Anisotropy =	5.4625
20	H	Isotropic =	30.1990	Anisotropy =	6.2606
21	H	Isotropic =	30.2571	Anisotropy =	10.8823
22	H	Isotropic =	30.3262	Anisotropy =	10.1826
23	H	Isotropic =	30.3632	Anisotropy =	10.3754
24	H	Isotropic =	30.1001	Anisotropy =	10.7304
25	H	Isotropic =	29.8885	Anisotropy =	6.4510
26	H	Isotropic =	28.8685	Anisotropy =	6.7129
27	H	Isotropic =	28.6815	Anisotropy =	6.6001

Conformer_12

N	-1.797747498831	-0.731343599346	-0.492191346760
C	-1.861977318778	-2.050570483977	0.118044502454
C	-1.192089459644	-2.054901129255	1.481863885964
C	0.248951179639	-1.625259839777	1.298734260258
N	0.362258913802	-0.462053456953	0.412010969529
C	-0.710540426913	-0.046823953380	-0.329339545784
C	-0.687265928138	1.309108441831	-1.017994140331
C	0.031615513076	2.434906293552	-0.274117584035
C	1.528537708640	2.468426956348	-0.580658762718
C	2.132327753329	1.065278143703	-0.613269316285
C	1.677020862620	0.180182839923	0.538133687452
H	-1.369426204295	-2.791164224674	-0.530460037718
H	-2.912322671559	-2.346909715943	0.194373208382
H	-1.225431298888	-3.043876598704	1.946855509318
H	-1.715672295162	-1.354825968089	2.142823572657
H	0.695338105609	-1.356265401642	2.262743967271
H	0.844511900895	-2.449441234489	0.884241570192
H	-0.258518811654	1.191158208348	-2.020449856649
H	-1.738290766340	1.560948618031	-1.167431576247
H	-0.421830273295	3.392781170717	-0.546006833708
H	-0.128434208395	2.316398258174	0.804105255861
H	1.697464189244	2.953443507771	-1.549039463264
H	2.044651857647	3.076893195507	0.170788157011
H	1.904098982577	0.566278925832	-1.561222673497
H	3.223374724103	1.135196426278	-0.561471555658
H	1.717846459136	0.742705825906	1.482705109406
H	2.390749011575	-0.644471205690	0.638429036899

SCF Done: E(RwB97X) = -462.110668528

Zero-point correction=	0.248085
Thermal correction to Energy=	0.257849
Thermal correction to Enthalpy=	0.258793
Thermal correction to Gibbs Free Energy=	0.213136
Sum of electronic and zero-point Energies=	-461.862584
Sum of electronic and thermal Energies=	-461.852820
Sum of electronic and thermal Enthalpies=	-461.851876
Sum of electronic and thermal Free Energies=	-461.897532

1	N	Isotropic =	53.4695	Anisotropy =	264.7783
2	C	Isotropic =	145.5545	Anisotropy =	28.1082
3	C	Isotropic =	167.7091	Anisotropy =	8.3635
4	C	Isotropic =	141.5160	Anisotropy =	37.8243
5	N	Isotropic =	155.1206	Anisotropy =	77.6499
6	C	Isotropic =	22.2718	Anisotropy =	140.7872
7	C	Isotropic =	154.0078	Anisotropy =	36.4423
8	C	Isotropic =	168.7794	Anisotropy =	15.5543
9	C	Isotropic =	164.2200	Anisotropy =	6.9634
10	C	Isotropic =	165.7004	Anisotropy =	18.4856
11	C	Isotropic =	138.8958	Anisotropy =	45.3404
12	H	Isotropic =	28.8852	Anisotropy =	8.5924
13	H	Isotropic =	28.5802	Anisotropy =	8.5670
14	H	Isotropic =	30.1762	Anisotropy =	10.4386
15	H	Isotropic =	30.3863	Anisotropy =	8.9981
16	H	Isotropic =	28.9083	Anisotropy =	6.8557
17	H	Isotropic =	28.7469	Anisotropy =	8.7523
18	H	Isotropic =	29.3840	Anisotropy =	5.4625
19	H	Isotropic =	29.6411	Anisotropy =	7.3676
20	H	Isotropic =	30.2571	Anisotropy =	10.8823
21	H	Isotropic =	30.1990	Anisotropy =	6.2606
22	H	Isotropic =	30.3632	Anisotropy =	10.3754
23	H	Isotropic =	30.3262	Anisotropy =	10.1826
24	H	Isotropic =	29.8885	Anisotropy =	6.4510
25	H	Isotropic =	30.1001	Anisotropy =	10.7304
26	H	Isotropic =	28.6815	Anisotropy =	6.6001
27	H	Isotropic =	28.8685	Anisotropy =	6.7129

Conformer_13

N	-1.930158997082	-0.484798212693	-0.181586351703
C	-1.871709509701	-1.906209329767	0.138463452209
C	-0.456560653901	-2.455671860235	0.022796426413

C	0.449796688926	-1.671731634572	0.954948175232
N	0.179645945436	-0.235579553193	0.854145571293
C	-0.923713044286	0.233544508457	0.194317927366
C	-0.938495412676	1.715617287892	-0.106054279000
C	0.135760642763	2.176430035843	-1.124053047842
C	1.352360741560	1.257991967353	-1.273660592246
C	2.162058861459	1.035205497442	0.003759180127
C	1.281037215629	0.656120623146	1.202381575572
H	-2.551795366914	-2.439817087946	-0.532038063565
H	-2.242350801773	-2.070885701297	1.161389927696
H	-0.113060121113	-2.347867586246	-1.012446054413
H	-0.420755342623	-3.518246541613	0.277449192475
H	1.501403468401	-1.841471441538	0.700644844678
H	0.306658368859	-1.997112468374	1.993070256828
H	-0.829227985954	2.263774717385	0.834020300778
H	-1.933565048891	1.948588770682	-0.487593559078
H	0.467679585490	3.185084754063	-0.853334491466
H	-0.335822467842	2.261732786629	-2.108228816993
H	2.008894638418	1.668999078621	-2.047987352121
H	1.016334703371	0.285283369307	-1.653072527618
H	2.721426078381	1.940856068284	0.266306141352
H	2.903150912163	0.248950064331	-0.180351679394
H	0.878014059625	1.556127181059	1.670863726119
H	1.876492842274	0.154784706980	1.970050117302

SCF Done: E(RwB97X) = -462.113608227

Zero-point correction=	0.248812
Thermal correction to Energy=	0.258402
Thermal correction to Enthalpy=	0.259346
Thermal correction to Gibbs Free Energy=	0.213898
Sum of electronic and zero-point Energies=	-461.864797
Sum of electronic and thermal Energies=	-461.855206
Sum of electronic and thermal Enthalpies=	-461.854262
Sum of electronic and thermal Free Energies=	-461.899711

1 N	Isotropic =	53.3295	Anisotropy =	271.5056
2 C	Isotropic =	145.1110	Anisotropy =	29.4088
3 C	Isotropic =	168.2032	Anisotropy =	11.4025
4 C	Isotropic =	144.6921	Anisotropy =	34.3325
5 N	Isotropic =	161.0591	Anisotropy =	81.6751
6 C	Isotropic =	22.0899	Anisotropy =	143.6863
7 C	Isotropic =	155.6126	Anisotropy =	30.3501
8 C	Isotropic =	168.9424	Anisotropy =	8.7821
9 C	Isotropic =	167.8579	Anisotropy =	14.0681
10 C	Isotropic =	165.9375	Anisotropy =	17.4435

11	C	Isotropic =	143.1483	Anisotropy =	44.1541
12	H	Isotropic =	28.5260	Anisotropy =	8.5288
13	H	Isotropic =	28.8041	Anisotropy =	8.9254
14	H	Isotropic =	30.3145	Anisotropy =	8.2228
15	H	Isotropic =	30.2039	Anisotropy =	10.5738
16	H	Isotropic =	28.7847	Anisotropy =	6.3981
17	H	Isotropic =	28.6578	Anisotropy =	9.9707
18	H	Isotropic =	29.1455	Anisotropy =	6.5117
19	H	Isotropic =	29.9876	Anisotropy =	8.1152
20	H	Isotropic =	30.3612	Anisotropy =	9.8590
21	H	Isotropic =	30.1758	Anisotropy =	10.4758
22	H	Isotropic =	30.3905	Anisotropy =	10.8507
23	H	Isotropic =	30.4999	Anisotropy =	6.3771
24	H	Isotropic =	30.5496	Anisotropy =	10.4421
25	H	Isotropic =	29.9875	Anisotropy =	9.1253
26	H	Isotropic =	28.3346	Anisotropy =	7.0933
27	H	Isotropic =	29.0200	Anisotropy =	7.8496

Conformer_14

N	-1.883149699485	-0.560937721600	-0.328767595042
C	-2.035915767168	-1.638195088631	0.642023962096
C	-1.024324343022	-1.528484771164	1.774506713491
C	0.374318979613	-1.550445085456	1.184333525677
N	0.453303207051	-0.684604077763	0.005468238057
C	-0.675333696857	-0.172481114311	-0.574860018992
C	-0.461249654099	0.936315793965	-1.580687288871
C	0.090593283510	2.253651521012	-0.978433155235
C	0.826771105303	2.120735995525	0.358119830554
C	2.054908480247	1.210562909351	0.338406235803
C	1.771782880390	-0.148637263971	-0.316666414139
H	-1.913944666962	-2.609500116733	0.139463676634
H	-3.058345626752	-1.611322324665	1.030274127275
H	-1.138065121072	-2.347459786719	2.489724078926
H	-1.189185215045	-0.588333702070	2.313281688487
H	1.106478461672	-1.197783490942	1.918464116881
H	0.656917386833	-2.573093677380	0.904364581404
H	0.205482666447	0.570948818803	-2.366902864401
H	-1.426677619379	1.121778145054	-2.053509163409
H	0.748377523566	2.729049266136	-1.714747025105
H	-0.747696582314	2.940898345615	-0.826024063516
H	1.125102432098	3.119291156876	0.694908345113
H	0.123679536276	1.748935693661	1.113412028290
H	2.876741223633	1.686896634528	-0.209063565840
H	2.403582840142	1.065425026292	1.367318546880

H	2.511364712021	-0.887540419966	0.003086172342
H	1.870683273353	-0.070170665450	-1.401094713360

SCF Done: E(RwB97X) = -462.113608224

Zero-point correction=	0.248813
Thermal correction to Energy=	0.258404
Thermal correction to Enthalpy=	0.259348
Thermal correction to Gibbs Free Energy=	0.213898
Sum of electronic and zero-point Energies=	-461.864795
Sum of electronic and thermal Energies=	-461.855205
Sum of electronic and thermal Enthalpies=	-461.854260
Sum of electronic and thermal Free Energies=	-461.899710

1 N	Isotropic = 53.3215	Anisotropy = 271.5042
2 C	Isotropic = 145.1139	Anisotropy = 29.4126
3 C	Isotropic = 168.2036	Anisotropy = 11.3889
4 C	Isotropic = 144.6966	Anisotropy = 34.3292
5 N	Isotropic = 161.0543	Anisotropy = 81.6848
6 C	Isotropic = 22.0837	Anisotropy = 143.6855
7 C	Isotropic = 155.6142	Anisotropy = 30.3569
8 C	Isotropic = 168.9466	Anisotropy = 8.7800
9 C	Isotropic = 167.8577	Anisotropy = 14.0680
10 C	Isotropic = 165.9382	Anisotropy = 17.4502
11 C	Isotropic = 143.1507	Anisotropy = 44.1462
12 H	Isotropic = 28.8044	Anisotropy = 8.9253
13 H	Isotropic = 28.5260	Anisotropy = 8.5289
14 H	Isotropic = 30.2037	Anisotropy = 10.5742
15 H	Isotropic = 30.3145	Anisotropy = 8.2242
16 H	Isotropic = 28.7846	Anisotropy = 6.3982
17 H	Isotropic = 28.6581	Anisotropy = 9.9704
18 H	Isotropic = 29.1454	Anisotropy = 6.5116
19 H	Isotropic = 29.9874	Anisotropy = 8.1145
20 H	Isotropic = 30.3612	Anisotropy = 9.8588
21 H	Isotropic = 30.1758	Anisotropy = 10.4756
22 H	Isotropic = 30.3905	Anisotropy = 10.8503
23 H	Isotropic = 30.4998	Anisotropy = 6.3773
24 H	Isotropic = 30.5495	Anisotropy = 10.4427
25 H	Isotropic = 29.9874	Anisotropy = 9.1241
26 H	Isotropic = 29.0203	Anisotropy = 7.8490
27 H	Isotropic = 28.3347	Anisotropy = 7.0942

Conformer_15

N	-1.918874100373	-0.537726203700	-0.179991513844

C	-2.031685233520	-1.933168214792	0.228622275638
C	-1.045757924738	-2.304998126358	1.321127448710
C	0.338430969566	-1.881345093892	0.875692332465
N	0.350952106691	-0.465916762601	0.504617694845
C	-0.790463161091	0.076131935395	-0.045840123747
C	-0.786302157297	1.532600083113	-0.478225560439
C	0.331085944363	1.941368762154	-1.444057791714
C	1.603116899945	2.394280773150	-0.726397897038
C	1.920949474784	1.538115311098	0.500606873794
C	1.711836660161	0.042934609108	0.284214592766
H	-1.872821414313	-2.576415078060	-0.647991031918
H	-3.060827890523	-2.108919518847	0.557840071378
H	-1.061985486510	-3.380220820732	1.519268092127
H	-1.306692467368	-1.788657550139	2.252160482121
H	1.065183784839	-2.020817632905	1.681068576682
H	0.667651578607	-2.498518136878	0.026282420685
H	-1.759326805662	1.688586910309	-0.944898346841
H	-0.759687203906	2.170789438772	0.413167456113
H	0.554274932674	1.102021689100	-2.113113560551
H	-0.032703691222	2.749234938864	-2.086090484923
H	2.445213989051	2.361989668866	-1.427159652622
H	1.498540604759	3.439390362727	-0.412826049459
H	2.966694207141	1.691441823833	0.785541423526
H	1.321670661031	1.854268571647	1.361208771738
H	2.335179002043	-0.495901759071	1.001503344039
H	2.067146720869	-0.248549980159	-0.716129843529

SCF Done: E(RwB97X) = -462.110400697

Zero-point correction=	0.248106
Thermal correction to Energy=	0.257873
Thermal correction to Enthalpy=	0.258817
Thermal correction to Gibbs Free Energy=	0.213088
Sum of electronic and zero-point Energies=	-461.862295
Sum of electronic and thermal Energies=	-461.852527
Sum of electronic and thermal Enthalpies=	-461.851583
Sum of electronic and thermal Free Energies=	-461.897313

1 N	Isotropic =	43.0890	Anisotropy =	274.7085
2 C	Isotropic =	144.9207	Anisotropy =	29.3217
3 C	Isotropic =	167.4589	Anisotropy =	6.8423
4 C	Isotropic =	140.2885	Anisotropy =	38.6302
5 N	Isotropic =	153.6768	Anisotropy =	50.7841
6 C	Isotropic =	22.1992	Anisotropy =	143.0388
7 C	Isotropic =	152.2279	Anisotropy =	35.6493
8 C	Isotropic =	169.0650	Anisotropy =	18.5351

9	C	Isotropic =	165.0517	Anisotropy =	7.6174
10	C	Isotropic =	164.3900	Anisotropy =	21.5047
11	C	Isotropic =	139.0007	Anisotropy =	49.1270
12	H	Isotropic =	28.6808	Anisotropy =	8.1563
13	H	Isotropic =	28.6271	Anisotropy =	8.2835
14	H	Isotropic =	30.1762	Anisotropy =	10.2512
15	H	Isotropic =	30.0733	Anisotropy =	8.3947
16	H	Isotropic =	28.9058	Anisotropy =	6.7673
17	H	Isotropic =	28.6910	Anisotropy =	8.2204
18	H	Isotropic =	29.8255	Anisotropy =	7.3304
19	H	Isotropic =	29.2686	Anisotropy =	4.9646
20	H	Isotropic =	30.2241	Anisotropy =	6.5690
21	H	Isotropic =	30.2020	Anisotropy =	10.6947
22	H	Isotropic =	30.3313	Anisotropy =	10.1647
23	H	Isotropic =	30.3240	Anisotropy =	10.1913
24	H	Isotropic =	30.0357	Anisotropy =	10.3268
25	H	Isotropic =	29.8785	Anisotropy =	6.4514
26	H	Isotropic =	29.0970	Anisotropy =	6.5040
27	H	Isotropic =	28.6223	Anisotropy =	6.1359

Conformer_16

N	-1.914479643924	-0.545985864822	-0.194343795355
C	-2.136055760129	-1.747188848146	0.602504584653
C	-0.883356492883	-2.591548569118	0.749806738577
C	0.236255294124	-1.698056046894	1.241748765392
N	0.389660949298	-0.533958363210	0.368464569614
C	-0.734028539692	-0.024461987431	-0.245868616082
C	-0.605250237412	1.209575256675	-1.122682749987
C	0.055411171134	2.428733835709	-0.470266208325
C	1.575718426848	2.441458159984	-0.633701597434
C	2.194748722506	1.052044148306	-0.472665906648
C	1.602180215053	0.238357359873	0.673179282744
H	-2.939812774511	-2.323259728103	0.132904990827
H	-2.504193981049	-1.454601106947	1.595640851317
H	-0.608943243749	-3.025909199490	-0.218461393706
H	-1.041320658862	-3.414234274900	1.452560494846
H	0.035221670762	-1.373508445687	2.273757064920
H	1.188182084522	-2.236613706876	1.248919903207
H	-0.068460922220	0.942193528610	-2.040798287578
H	-1.626848017747	1.451121419747	-1.417446058119
H	-0.366161278971	3.338086721625	-0.909070722406
H	-0.209631657317	2.456469067054	0.593187399956
H	1.837986926085	2.834686941599	-1.622692312085
H	2.013053669753	3.127713479702	0.100485284718

H	2.099154230523	0.474107793971	-1.398179826121
H	3.268819512636	1.155566961824	-0.288456456849
H	1.428996248496	0.884902877011	1.547178920262
H	2.341154086728	-0.504791410068	0.981495079660

SCF Done: E(RwB97X) = -462.110400697

Zero-point correction=	0.248106
Thermal correction to Energy=	0.257873
Thermal correction to Enthalpy=	0.258818
Thermal correction to Gibbs Free Energy=	0.213089
Sum of electronic and zero-point Energies=	-461.862295
Sum of electronic and thermal Energies=	-461.852527
Sum of electronic and thermal Enthalpies=	-461.851583
Sum of electronic and thermal Free Energies=	-461.897312

1 N	Isotropic = 43.0867	Anisotropy = 274.7162
2 C	Isotropic = 144.9213	Anisotropy = 29.3226
3 C	Isotropic = 167.4595	Anisotropy = 6.8397
4 C	Isotropic = 140.2890	Anisotropy = 38.6312
5 N	Isotropic = 153.6802	Anisotropy = 50.7892
6 C	Isotropic = 22.1996	Anisotropy = 143.0386
7 C	Isotropic = 152.2295	Anisotropy = 35.6475
8 C	Isotropic = 169.0651	Anisotropy = 18.5375
9 C	Isotropic = 165.0522	Anisotropy = 7.6181
10 C	Isotropic = 164.3896	Anisotropy = 21.5046
11 C	Isotropic = 138.9999	Anisotropy = 49.1287
12 H	Isotropic = 28.6271	Anisotropy = 8.2834
13 H	Isotropic = 28.6808	Anisotropy = 8.1563
14 H	Isotropic = 30.0732	Anisotropy = 8.3949
15 H	Isotropic = 30.1763	Anisotropy = 10.2512
16 H	Isotropic = 28.6910	Anisotropy = 8.2200
17 H	Isotropic = 28.9057	Anisotropy = 6.7675
18 H	Isotropic = 29.2687	Anisotropy = 4.9642
19 H	Isotropic = 29.8256	Anisotropy = 7.3306
20 H	Isotropic = 30.2020	Anisotropy = 10.6947
21 H	Isotropic = 30.2243	Anisotropy = 6.5687
22 H	Isotropic = 30.3240	Anisotropy = 10.1912
23 H	Isotropic = 30.3312	Anisotropy = 10.1647
24 H	Isotropic = 29.8784	Anisotropy = 6.4517
25 H	Isotropic = 30.0357	Anisotropy = 10.3268
26 H	Isotropic = 28.6224	Anisotropy = 6.1362
27 H	Isotropic = 29.0969	Anisotropy = 6.5041

Conformer_17

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N   -1.874460234273   -0.279591562395   0.021857270734
C   -2.010305432360   -1.301551318996   1.057989989517
C   -0.894891537557   -2.336948439606   1.048676152628
C    0.440914162831   -1.617385834917   1.008164112789
N    0.455576810359   -0.694730871981   -0.120197720276
C   -0.703404482095   -0.044312681054   -0.466609532171
C   -0.563719451635    1.041609769657   -1.510164168439
C    0.186375079558    2.303480748884   -1.005575240501
C    0.997480359890    2.114717775330    0.280195222832
C    2.156057014185    1.122135612793    0.165725817323
C    1.751520723779   -0.175290061768   -0.543813813784
H   -2.982573610030   -1.788417122307    0.929580084537
H   -2.041544287095   -0.805519305341    2.037854366686
H   -0.986144491061   -2.979173732877    0.165326964079
H   -0.953831279206   -2.977014517138    1.933401620447
H    0.609036598397   -1.077513890802    1.951887047462
H    1.265847230796   -2.323779260514    0.881016095270
H   -0.061170280741    0.626256028288   -2.388206095063
H   -1.574044240373    1.308539411829   -1.822250294374
H    0.844009872427    2.672389957103   -1.800771113531
H   -0.549028249071    3.093118020311   -0.823583549127
H    1.386671773513    3.087085394032    0.599828973843
H    0.320878560983    1.786878121944    1.079267357607
H    2.985591030502    1.568227779472   -0.395824945331
H    2.537226564505    0.898430243097    1.168519412172
H    2.492867970500   -0.956367084793   -0.356955426370
H    1.737163823271   -0.017573178251   -1.624838588957

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SCF Done: E(RwB97X) = -462.113266813

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Zero-point correction=          0.248246
Thermal correction to Energy=      0.257995
Thermal correction to Enthalpy=     0.258939
Thermal correction to Gibbs Free Energy= 0.213010
Sum of electronic and zero-point Energies= -461.865021
Sum of electronic and thermal Energies= -461.855272
Sum of electronic and thermal Enthalpies= -461.854328
Sum of electronic and thermal Free Energies= -461.900256

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1 N  Isotropic =  51.0305  Anisotropy = 276.2036
2 C  Isotropic = 144.7781  Anisotropy =  29.5828
3 C  Isotropic = 167.2195  Anisotropy =   7.3515
4 C  Isotropic = 144.2734  Anisotropy =  34.1364
5 N  Isotropic = 159.0475  Anisotropy =  73.7999
6 C  Isotropic =  22.5371  Anisotropy = 144.0563

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7 C	Isotropic = 155.3149	Anisotropy = 31.0400
8 C	Isotropic = 169.2988	Anisotropy = 7.6550
9 C	Isotropic = 168.4237	Anisotropy = 15.0515
10 C	Isotropic = 164.5922	Anisotropy = 16.4738
11 C	Isotropic = 141.6766	Anisotropy = 46.3825
12 H	Isotropic = 28.5701	Anisotropy = 8.3823
13 H	Isotropic = 28.5938	Anisotropy = 7.9757
14 H	Isotropic = 30.0253	Anisotropy = 8.8179
15 H	Isotropic = 30.1391	Anisotropy = 10.2269
16 H	Isotropic = 28.5004	Anisotropy = 7.8484
17 H	Isotropic = 28.8998	Anisotropy = 7.5260
18 H	Isotropic = 29.1004	Anisotropy = 6.3800
19 H	Isotropic = 29.9248	Anisotropy = 7.8678
20 H	Isotropic = 30.3722	Anisotropy = 9.6386
21 H	Isotropic = 30.1635	Anisotropy = 10.5966
22 H	Isotropic = 30.3753	Anisotropy = 10.9163
23 H	Isotropic = 30.5726	Anisotropy = 6.3112
24 H	Isotropic = 30.5594	Anisotropy = 10.5067
25 H	Isotropic = 29.9620	Anisotropy = 8.7485
26 H	Isotropic = 29.0846	Anisotropy = 7.6560
27 H	Isotropic = 28.1649	Anisotropy = 6.7618

Conformer_18

N	-1.756092151193	-0.500882706241	-0.429268965484
C	-1.663913905517	-1.950043061284	-0.262353594099
C	-0.873801763302	-2.377214305268	0.966275377505
C	0.447042742292	-1.629643562277	0.983409023173
N	0.189963733253	-0.197846650742	0.890814914648
C	-0.857619717938	0.244540803068	0.120656678547
C	-0.936667262739	1.740399154027	-0.088868820743
C	0.185359400068	2.306042650606	-1.000276160262
C	1.389083807739	1.382008273835	-1.209892850334
C	2.184205701689	1.069390772263	0.059226538748
C	1.282216286156	0.702900332210	1.243506145331
H	-1.201388779521	-2.378007434662	-1.162395435867
H	-2.681276745666	-2.352488530664	-0.219431128591
H	-0.698225918477	-3.456561211248	0.957281430080
H	-1.436051791427	-2.138018131641	1.876081266099
H	0.994879691425	-1.817851849475	1.910838567804
H	1.082095018265	-1.963659559759	0.149454229375
H	-1.913135508592	1.944214989848	-0.529747164142
H	-0.920532900951	2.235758753175	0.886009890220
H	-0.244097587560	2.523116302169	-1.983083991078
H	0.527878145714	3.264955359107	-0.595208210766

H	1.039253179195	0.442414010199	-1.655498542038
H	2.057066730195	1.832663673974	-1.951407382218
H	2.883012369136	0.250994427041	-0.147718920645
H	2.789326960002	1.935575421226	0.352511106022
H	0.867356520898	1.610542807870	1.688222289265
H	1.866463746858	0.215499272644	2.028163709449

SCF Done: E(RwB97X) = -462.113266796

Zero-point correction=	0.248246
Thermal correction to Energy=	0.257995
Thermal correction to Enthalpy=	0.258939
Thermal correction to Gibbs Free Energy=	0.213011
Sum of electronic and zero-point Energies=	-461.865021
Sum of electronic and thermal Energies=	-461.855272
Sum of electronic and thermal Enthalpies=	-461.854328
Sum of electronic and thermal Free Energies=	-461.900256

1 N	Isotropic = 51.0331	Anisotropy = 276.2018
2 C	Isotropic = 144.7785	Anisotropy = 29.5823
3 C	Isotropic = 167.2199	Anisotropy = 7.3513
4 C	Isotropic = 144.2729	Anisotropy = 34.1364
5 N	Isotropic = 159.0479	Anisotropy = 73.7974
6 C	Isotropic = 22.5365	Anisotropy = 144.0592
7 C	Isotropic = 155.3156	Anisotropy = 31.0380
8 C	Isotropic = 169.2977	Anisotropy = 7.6561
9 C	Isotropic = 168.4237	Anisotropy = 15.0512
10 C	Isotropic = 164.5927	Anisotropy = 16.4748
11 C	Isotropic = 141.6771	Anisotropy = 46.3836
12 H	Isotropic = 28.5938	Anisotropy = 7.9756
13 H	Isotropic = 28.5701	Anisotropy = 8.3824
14 H	Isotropic = 30.1391	Anisotropy = 10.2269
15 H	Isotropic = 30.0253	Anisotropy = 8.8181
16 H	Isotropic = 28.8998	Anisotropy = 7.5262
17 H	Isotropic = 28.5004	Anisotropy = 7.8485
18 H	Isotropic = 29.9249	Anisotropy = 7.8681
19 H	Isotropic = 29.1004	Anisotropy = 6.3797
20 H	Isotropic = 30.1635	Anisotropy = 10.5965
21 H	Isotropic = 30.3721	Anisotropy = 9.6389
22 H	Isotropic = 30.5726	Anisotropy = 6.3111
23 H	Isotropic = 30.3753	Anisotropy = 10.9162
24 H	Isotropic = 29.9619	Anisotropy = 8.7489
25 H	Isotropic = 30.5593	Anisotropy = 10.5066
26 H	Isotropic = 28.1649	Anisotropy = 6.7623
27 H	Isotropic = 29.0846	Anisotropy = 7.6558

Conformer_2

N	-1.906485392508	-0.599111279812	-0.301928408566
C	-2.018050423358	-1.821407785611	0.485721746795
C	-0.991161658797	-1.876172162812	1.607140452545
C	0.394263021438	-1.732448138298	1.006971041569
N	0.428987539849	-0.624277568827	0.052611876339
C	-0.721327293707	-0.108256446154	-0.468818527440
C	-0.600731744315	1.166203990436	-1.274071358121
C	-0.085460961498	2.374212884361	-0.475988683554
C	1.434142654055	2.440309564897	-0.326194116887
C	2.064431932182	1.249528985420	0.392330458644
C	1.751914119791	-0.093146117525	-0.267973239419
H	-1.889784411431	-2.696185170167	-0.168810177760
H	-3.033596581525	-1.879622528330	0.889058162126
H	-1.059662422267	-2.815348770336	2.162698378305
H	-1.177344370878	-1.056734209734	2.310919984869
H	1.133349557886	-1.531617350899	1.789339246002
H	0.692747754028	-2.662151674321	0.504452990295
H	0.043893180119	0.999972186430	-2.145659515940
H	-1.602540722624	1.374357199693	-1.653024272998
H	-0.418634462738	3.282602543208	-0.988789101097
H	-0.562783773214	2.386950831004	0.512321212638
H	1.877988847360	2.515866668080	-1.328191777458
H	1.700914081565	3.363038913041	0.201326510724
H	3.152157770882	1.381852720613	0.406642493671
H	1.734380222690	1.211903777980	1.438510532375
H	1.870314165021	-0.013116350272	-1.354603400967
H	2.471779371993	-0.844304712068	0.065107493310

SCF Done: E(RwB97X) = -462.118412703

Zero-point correction=	0.248268
Thermal correction to Energy=	0.257903
Thermal correction to Enthalpy=	0.258847
Thermal correction to Gibbs Free Energy=	0.213391
Sum of electronic and zero-point Energies=	-461.870145
Sum of electronic and thermal Energies=	-461.860510
Sum of electronic and thermal Enthalpies=	-461.859565
Sum of electronic and thermal Free Energies=	-461.905021

1	N	Isotropic =	55.6848	Anisotropy =	263.4503
2	C	Isotropic =	145.4708	Anisotropy =	28.9936
3	C	Isotropic =	167.6279	Anisotropy =	9.8142
4	C	Isotropic =	142.8104	Anisotropy =	34.9996

5	N	Isotropic =	154.7383	Anisotropy =	67.4225
6	C	Isotropic =	20.0208	Anisotropy =	147.5937
7	C	Isotropic =	150.7335	Anisotropy =	27.5933
8	C	Isotropic =	163.4872	Anisotropy =	9.4502
9	C	Isotropic =	160.2036	Anisotropy =	3.5916
10	C	Isotropic =	161.0251	Anisotropy =	9.6024
11	C	Isotropic =	138.9678	Anisotropy =	43.2104
12	H	Isotropic =	28.8006	Anisotropy =	8.7323
13	H	Isotropic =	28.5805	Anisotropy =	8.4487
14	H	Isotropic =	30.1823	Anisotropy =	10.3275
15	H	Isotropic =	30.3250	Anisotropy =	8.3896
16	H	Isotropic =	28.7895	Anisotropy =	6.3027
17	H	Isotropic =	28.6513	Anisotropy =	9.3607
18	H	Isotropic =	29.3347	Anisotropy =	5.0028
19	H	Isotropic =	29.9266	Anisotropy =	7.7155
20	H	Isotropic =	30.0971	Anisotropy =	10.4052
21	H	Isotropic =	30.5307	Anisotropy =	6.9470
22	H	Isotropic =	30.4645	Anisotropy =	8.7313
23	H	Isotropic =	30.0886	Anisotropy =	10.2931
24	H	Isotropic =	30.2723	Anisotropy =	10.3216
25	H	Isotropic =	30.5387	Anisotropy =	6.8183
26	H	Isotropic =	28.4665	Anisotropy =	6.0399
27	H	Isotropic =	29.0674	Anisotropy =	6.9825

Conformer_3

N	-1.886403995519	-0.466654337271	-0.141352266340
C	-2.092676400472	-1.518677582498	0.849052064254
C	-0.909018176272	-2.466048470723	0.964229686084
C	0.348961766791	-1.649965536714	1.193925954828
N	0.454877895969	-0.599070047086	0.184047965281
C	-0.675800474588	-0.084530902725	-0.386490934747
C	-0.498322630527	1.050398310019	-1.371112601449
C	-0.088783533894	2.377366399403	-0.714216467608
C	1.399436803512	2.493564275075	-0.391007828246
C	1.943222523913	1.406172031970	0.532930049307
C	1.777850006862	-0.010657372796	-0.019913034073
H	-3.000238584708	-2.068831207914	0.580518760338
H	-2.288052670209	-1.057429190237	1.827612613016
H	-1.051500205270	-3.172936196390	1.786270650806
H	-0.806132291342	-3.044842672507	0.039173152955
H	0.338588455259	-1.209436205577	2.200899346449
H	1.238136480103	-2.282094314674	1.121600697107
H	0.232135215960	0.779055463562	-2.142462268631
H	-1.463402399265	1.171161746462	-1.865440074343

H	-0.358580610663	3.191243663340	-1.395361742762
H	-0.684609443029	2.527398458200	0.195279564058
H	1.965634514281	2.462229003057	-1.331929439043
H	1.591802187425	3.475977017454	0.054494775966
H	3.012565105534	1.585321526055	0.692199173360
H	1.463822333916	1.460941373501	1.518710239506
H	2.483813479457	-0.677764793992	0.478461778854
H	2.036074646774	-0.024790436995	-1.085719814928

SCF Done: E(RwB97X) = -462.117664154

Zero-point correction=	0.248142
Thermal correction to Energy=	0.257835
Thermal correction to Enthalpy=	0.258780
Thermal correction to Gibbs Free Energy=	0.213135
Sum of electronic and zero-point Energies=	-461.869523
Sum of electronic and thermal Energies=	-461.859829
Sum of electronic and thermal Enthalpies=	-461.858885
Sum of electronic and thermal Free Energies=	-461.904529

1 N	Isotropic =	55.1315	Anisotropy =	266.9709
2 C	Isotropic =	144.7583	Anisotropy =	29.7497
3 C	Isotropic =	167.5787	Anisotropy =	8.5476
4 C	Isotropic =	141.9871	Anisotropy =	36.6073
5 N	Isotropic =	154.1586	Anisotropy =	71.6248
6 C	Isotropic =	20.6766	Anisotropy =	147.1137
7 C	Isotropic =	151.3420	Anisotropy =	27.1387
8 C	Isotropic =	163.7442	Anisotropy =	8.5724
9 C	Isotropic =	160.2547	Anisotropy =	3.3780
10 C	Isotropic =	160.7733	Anisotropy =	10.1574
11 C	Isotropic =	137.4321	Anisotropy =	44.3019
12 H	Isotropic =	28.5774	Anisotropy =	8.3290
13 H	Isotropic =	28.7111	Anisotropy =	8.1274
14 H	Isotropic =	30.2039	Anisotropy =	10.1971
15 H	Isotropic =	30.1525	Anisotropy =	8.7998
16 H	Isotropic =	28.4535	Anisotropy =	8.2159
17 H	Isotropic =	28.8721	Anisotropy =	7.0109
18 H	Isotropic =	29.3282	Anisotropy =	4.7543
19 H	Isotropic =	29.9209	Anisotropy =	7.6082
20 H	Isotropic =	30.0941	Anisotropy =	10.3378
21 H	Isotropic =	30.6141	Anisotropy =	7.2703
22 H	Isotropic =	30.4825	Anisotropy =	8.6843
23 H	Isotropic =	30.1206	Anisotropy =	10.3344
24 H	Isotropic =	30.2310	Anisotropy =	10.1918
25 H	Isotropic =	30.4982	Anisotropy =	6.7921
26 H	Isotropic =	29.0460	Anisotropy =	6.5418

27 H Isotropic = 28.2599 Anisotropy = 5.9087

Conformer_4

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-----
N    -1.829433790191  -0.559854056798  -0.324982233497
C    -1.797077705030  -2.002123613927  -0.103593424904
C    -0.949372388422  -2.400074050809   1.094261263500
C     0.424804711005  -1.774019966697   0.949488613417
N     0.297185440156  -0.341197907041   0.692218532582
C    -0.814511066337   0.142290555846   0.060501128377
C    -0.849628424383   1.624892639417  -0.239000088162
C     0.111467006431   2.049843077400  -1.359621200188
C     1.563190323405   2.225731358890  -0.918794712874
C     2.200217960489   0.985860847112  -0.295334607058
C     1.475353829870   0.484026368329   0.954914484469
H    -1.408778424281  -2.495410495288  -1.006031626793
H    -2.826621924165  -2.352789785267   0.020986033628
H    -0.859195238727  -3.487451721060   1.166515372446
H    -1.419819798840  -2.041237826926   2.016884499878
H     1.007289796386  -1.904586581016   1.865519661833
H     0.979997717366  -2.258418547859   0.133837003710
H    -1.875944772644   1.845798216414  -0.535981535151
H    -0.639788007069   2.204969512154   0.667451111893
H     0.052216246892   1.322360574725  -2.179352586769
H    -0.242870890285   3.001974270557  -1.768321980280
H     2.160947533401   2.545164282840  -1.779759747900
H     1.610232018774   3.043422535118  -0.186631206485
H     3.232138023518   1.226213731563  -0.015466459383
H     2.253642474690   0.169250840654  -1.026690121758
H     1.204984054255   1.334354563782   1.592618357062
H     2.154175293735  -0.138688822116   1.540765468407
```

SCF Done: E(RwB97X) = -462.117664152

```
Zero-point correction=          0.248142
Thermal correction to Energy=      0.257835
Thermal correction to Enthalpy=     0.258780
Thermal correction to Gibbs Free Energy= 0.213135
Sum of electronic and zero-point Energies= -461.869523
Sum of electronic and thermal Energies= -461.859829
Sum of electronic and thermal Enthalpies= -461.858885
Sum of electronic and thermal Free Energies= -461.904529
```

1 N Isotropic = 55.1319 Anisotropy = 266.9699

2 C Isotropic = 144.7584 Anisotropy = 29.7498

3 C	Isotropic =	167.5788	Anisotropy =	8.5476
4 C	Isotropic =	141.9871	Anisotropy =	36.6075
5 N	Isotropic =	154.1587	Anisotropy =	71.6254
6 C	Isotropic =	20.6767	Anisotropy =	147.1138
7 C	Isotropic =	151.3420	Anisotropy =	27.1387
8 C	Isotropic =	163.7442	Anisotropy =	8.5724
9 C	Isotropic =	160.2547	Anisotropy =	3.3780
10 C	Isotropic =	160.7732	Anisotropy =	10.1574
11 C	Isotropic =	137.4321	Anisotropy =	44.3021
12 H	Isotropic =	28.7111	Anisotropy =	8.1274
13 H	Isotropic =	28.5774	Anisotropy =	8.3290
14 H	Isotropic =	30.2039	Anisotropy =	10.1971
15 H	Isotropic =	30.1526	Anisotropy =	8.7999
16 H	Isotropic =	28.8721	Anisotropy =	7.0109
17 H	Isotropic =	28.4535	Anisotropy =	8.2160
18 H	Isotropic =	29.9208	Anisotropy =	7.6082
19 H	Isotropic =	29.3282	Anisotropy =	4.7543
20 H	Isotropic =	30.6141	Anisotropy =	7.2703
21 H	Isotropic =	30.0941	Anisotropy =	10.3378
22 H	Isotropic =	30.1206	Anisotropy =	10.3344
23 H	Isotropic =	30.4825	Anisotropy =	8.6843
24 H	Isotropic =	30.2310	Anisotropy =	10.1918
25 H	Isotropic =	30.4982	Anisotropy =	6.7921
26 H	Isotropic =	28.2599	Anisotropy =	5.9087
27 H	Isotropic =	29.0460	Anisotropy =	6.5418

Conformer_5

N	-1.911005388053	-0.540688485195	-0.165497790987
C	-2.003018278906	-1.942897772911	0.224775867592
C	-0.987861234988	-2.322851760377	1.287298017482
C	0.381724718158	-1.881400385161	0.814816990206
N	0.374154456781	-0.460521987537	0.465054725173
C	-0.784484201362	0.080272628763	-0.049495962021
C	-0.802118445858	1.542967604699	-0.460043654188
C	0.288262804477	1.974996081507	-1.446452229533
C	1.573879717561	2.427615595690	-0.753227923153
C	1.927997786043	1.556168475091	0.452855404857
C	1.725268250038	0.062669576603	0.219392117064
H	-1.860667678195	-2.571784364749	-0.664992690490
H	-3.022422665415	-2.131807401385	0.576250931517
H	-0.990891659790	-3.400989663456	1.469607803397
H	-1.230020201834	-1.822509471517	2.232038389154
H	0.694865592961	-2.483079124355	-0.051623994937
H	1.128997023305	-2.027025214164	1.600075813564

H	-0.758856143746	2.168172683819	0.439848640639
H	-1.787364205775	1.697851208358	-0.900733816684
H	-0.097308297002	2.789235266329	-2.067375269994
H	0.501579920682	1.147399036533	-2.133137034040
H	1.468954248263	3.467155171374	-0.421770697026
H	2.398892413524	2.412296064114	-1.474584427769
H	1.347293068591	1.854818029864	1.332238976591
H	2.979118235686	1.713751614921	0.714754837048
H	2.370093305264	-0.481548069625	0.913245984189
H	2.058336859589	-0.211165337237	-0.793519007650

SCF Done: E(RwB97X) = -462.110400728

Zero-point correction=	0.248106
Thermal correction to Energy=	0.257873
Thermal correction to Enthalpy=	0.258817
Thermal correction to Gibbs Free Energy=	0.213089
Sum of electronic and zero-point Energies=	-461.862295
Sum of electronic and thermal Energies=	-461.852528
Sum of electronic and thermal Enthalpies=	-461.851584
Sum of electronic and thermal Free Energies=	-461.897312

1	N	Isotropic =	43.0852	Anisotropy =	274.7180
2	C	Isotropic =	144.9197	Anisotropy =	29.3218
3	C	Isotropic =	167.4580	Anisotropy =	6.8418
4	C	Isotropic =	140.2905	Anisotropy =	38.6289
5	N	Isotropic =	153.6747	Anisotropy =	50.7757
6	C	Isotropic =	22.2000	Anisotropy =	143.0320
7	C	Isotropic =	152.2285	Anisotropy =	35.6543
8	C	Isotropic =	169.0631	Anisotropy =	18.5360
9	C	Isotropic =	165.0544	Anisotropy =	7.6115
10	C	Isotropic =	164.3912	Anisotropy =	21.5038
11	C	Isotropic =	138.9978	Anisotropy =	49.1249
12	H	Isotropic =	28.6807	Anisotropy =	8.1563
13	H	Isotropic =	28.6271	Anisotropy =	8.2833
14	H	Isotropic =	30.1762	Anisotropy =	10.2511
15	H	Isotropic =	30.0731	Anisotropy =	8.3943
16	H	Isotropic =	28.6911	Anisotropy =	8.2200
17	H	Isotropic =	28.9058	Anisotropy =	6.7675
18	H	Isotropic =	29.2685	Anisotropy =	4.9653
19	H	Isotropic =	29.8256	Anisotropy =	7.3302
20	H	Isotropic =	30.2019	Anisotropy =	10.6946
21	H	Isotropic =	30.2240	Anisotropy =	6.5686
22	H	Isotropic =	30.3240	Anisotropy =	10.1918
23	H	Isotropic =	30.3313	Anisotropy =	10.1641
24	H	Isotropic =	29.8784	Anisotropy =	6.4508

25	H	Isotropic =	30.0358	Anisotropy =	10.3273
26	H	Isotropic =	29.0969	Anisotropy =	6.5044
27	H	Isotropic =	28.6224	Anisotropy =	6.1349

Conformer_6

N	-1.880813476375	-0.590623073960	-0.262953992883
C	-2.109449397783	-1.766787693612	0.568510526568
C	-0.841935715479	-2.564255915673	0.816130360191
C	0.221973237315	-1.617067562954	1.330732392957
N	0.387918655886	-0.483272106959	0.420646597703
C	-0.715403073213	-0.034003115505	-0.272537316854
C	-0.576046968367	1.168949583956	-1.190045649886
C	0.011556630715	2.432811835323	-0.552898933026
C	1.537454330227	2.487894192740	-0.635587556088
C	2.187906401275	1.126174378620	-0.386413022634
C	1.558474078126	0.338650224092	0.758036188676
H	-2.868797766444	-2.385955362030	0.080219302267
H	-2.539788105328	-1.448170831181	1.528063515940
H	-0.502277351733	-3.026519337342	-0.117926629108
H	-1.013268989915	-3.363936532637	1.541928681410
H	-0.044697701184	-1.259457906177	2.336613308556
H	1.187749309547	-2.124199585623	1.410404172082
H	0.017453543514	0.883797228428	-2.066974620777
H	-1.586930200786	1.366246930793	-1.547948999936
H	-0.412472273355	3.310674402099	-1.049641070977
H	-0.311660418580	2.492900742325	0.492986891385
H	1.841305493559	2.851119032615	-1.624151140016
H	1.913505387020	3.215372153250	0.092833519548
H	2.159905492294	0.510386931446	-1.291811667735
H	3.246837585583	1.270836856569	-0.149737092656
H	1.318720024762	1.012538581524	1.594876458360
H	2.301481268719	-0.368004050126	1.134845776933

SCF Done: E(RwB97X) = -462.110400728

Zero-point correction=	0.248106
Thermal correction to Energy=	0.257873
Thermal correction to Enthalpy=	0.258817
Thermal correction to Gibbs Free Energy=	0.213089
Sum of electronic and zero-point Energies=	-461.862295
Sum of electronic and thermal Energies=	-461.852528
Sum of electronic and thermal Enthalpies=	-461.851584
Sum of electronic and thermal Free Energies=	-461.897312

1 N	Isotropic =	43.0852	Anisotropy =	274.7181
2 C	Isotropic =	144.9197	Anisotropy =	29.3218
3 C	Isotropic =	167.4580	Anisotropy =	6.8418
4 C	Isotropic =	140.2905	Anisotropy =	38.6289
5 N	Isotropic =	153.6747	Anisotropy =	50.7757
6 C	Isotropic =	22.2000	Anisotropy =	143.0320
7 C	Isotropic =	152.2285	Anisotropy =	35.6543
8 C	Isotropic =	169.0631	Anisotropy =	18.5360
9 C	Isotropic =	165.0544	Anisotropy =	7.6115
10 C	Isotropic =	164.3912	Anisotropy =	21.5038
11 C	Isotropic =	138.9978	Anisotropy =	49.1248
12 H	Isotropic =	28.6271	Anisotropy =	8.2833
13 H	Isotropic =	28.6807	Anisotropy =	8.1563
14 H	Isotropic =	30.0731	Anisotropy =	8.3943
15 H	Isotropic =	30.1762	Anisotropy =	10.2511
16 H	Isotropic =	28.6911	Anisotropy =	8.2200
17 H	Isotropic =	28.9058	Anisotropy =	6.7675
18 H	Isotropic =	29.2685	Anisotropy =	4.9653
19 H	Isotropic =	29.8256	Anisotropy =	7.3302
20 H	Isotropic =	30.2019	Anisotropy =	10.6946
21 H	Isotropic =	30.2240	Anisotropy =	6.5686
22 H	Isotropic =	30.3240	Anisotropy =	10.1918
23 H	Isotropic =	30.3313	Anisotropy =	10.1641
24 H	Isotropic =	29.8784	Anisotropy =	6.4508
25 H	Isotropic =	30.0358	Anisotropy =	10.3273
26 H	Isotropic =	28.6224	Anisotropy =	6.1349
27 H	Isotropic =	29.0969	Anisotropy =	6.5044

Conformer_7

N	-1.764202738214	-0.513079962605	-0.400750406102
C	-1.673362087556	-1.963372186276	-0.243184971575
C	-0.819940710667	-2.399973809063	0.938892467346
C	0.505099494284	-1.661573876149	0.885528518510
N	0.253383457992	-0.227745185872	0.811485250198
C	-0.831661947480	0.224337444241	0.101168857089
C	-0.911532394209	1.721398344768	-0.099335267989
C	0.162970410330	2.282468917554	-1.068942395608
C	1.346804856885	1.350824197230	-1.347013932766
C	2.208026462276	1.028438218425	-0.124326232905
C	1.369597643218	0.664324378132	1.106465255703
H	-1.264133684390	-2.391705663686	-1.168506075120
H	-2.689679644861	-2.358828291579	-0.145465919496
H	-0.652762454786	-3.480472597313	0.917149182467
H	-1.329604883015	-2.159873026321	1.878934204649

H	1.090954804275	-1.997151775150	0.016909807524
H	1.101761655907	-1.856662188401	1.780851606810
H	-1.909131924095	1.933368736484	-0.485687838715
H	-0.838848083343	2.213333263624	0.874698633905
H	-0.318028626130	2.506039786563	-2.026083760510
H	0.533944483097	3.237534558012	-0.680167783364
H	0.966398090725	0.415169545816	-1.775540515726
H	1.976317578544	1.799316976231	-2.122709657810
H	2.888594890883	0.205890464439	-0.371658630912
H	2.834469600683	1.889395660159	0.137941766737
H	0.986051540478	1.573380038664	1.575718541429
H	1.992414209168	0.170418032075	1.856629296233

SCF Done: E(RwB97X) = -462.113266833

Zero-point correction=	0.248246
Thermal correction to Energy=	0.257995
Thermal correction to Enthalpy=	0.258939
Thermal correction to Gibbs Free Energy=	0.213011
Sum of electronic and zero-point Energies=	-461.865021
Sum of electronic and thermal Energies=	-461.855272
Sum of electronic and thermal Enthalpies=	-461.854327
Sum of electronic and thermal Free Energies=	-461.900256

1 N	Isotropic = 51.0316	Anisotropy = 276.2058
2 C	Isotropic = 144.7782	Anisotropy = 29.5849
3 C	Isotropic = 167.2185	Anisotropy = 7.3507
4 C	Isotropic = 144.2751	Anisotropy = 34.1372
5 N	Isotropic = 159.0493	Anisotropy = 73.7998
6 C	Isotropic = 22.5367	Anisotropy = 144.0557
7 C	Isotropic = 155.3137	Anisotropy = 31.0413
8 C	Isotropic = 169.3002	Anisotropy = 7.6581
9 C	Isotropic = 168.4232	Anisotropy = 15.0530
10 C	Isotropic = 164.5917	Anisotropy = 16.4731
11 C	Isotropic = 141.6766	Anisotropy = 46.3825
12 H	Isotropic = 28.5938	Anisotropy = 7.9759
13 H	Isotropic = 28.5702	Anisotropy = 8.3823
14 H	Isotropic = 30.1390	Anisotropy = 10.2268
15 H	Isotropic = 30.0253	Anisotropy = 8.8177
16 H	Isotropic = 28.5006	Anisotropy = 7.8483
17 H	Isotropic = 28.8999	Anisotropy = 7.5256
18 H	Isotropic = 29.9247	Anisotropy = 7.8679
19 H	Isotropic = 29.1005	Anisotropy = 6.3802
20 H	Isotropic = 30.1635	Anisotropy = 10.5971
21 H	Isotropic = 30.3722	Anisotropy = 9.6383
22 H	Isotropic = 30.5726	Anisotropy = 6.3106

23	H	Isotropic =	30.3753	Anisotropy =	10.9164
24	H	Isotropic =	29.9621	Anisotropy =	8.7486
25	H	Isotropic =	30.5595	Anisotropy =	10.5069
26	H	Isotropic =	28.1650	Anisotropy =	6.7614
27	H	Isotropic =	29.0847	Anisotropy =	7.6566

Conformer_8

N	-1.857579951981	-0.358326021117	-0.090474905162
C	-2.033098023416	-1.367843316810	0.951873545951
C	-0.861511820092	-2.331190383916	1.076735463646
C	0.425661308586	-1.530103386994	1.149172460870
N	0.495937273918	-0.629404442212	0.005272727159
C	-0.660398526693	-0.059103286391	-0.468009665679
C	-0.484246750326	1.014291550729	-1.518979000846
C	0.134586133292	2.329543004646	-0.974338238758
C	0.824431524307	2.215250244117	0.388669104206
C	2.046627612208	1.295305453415	0.411893204447
C	1.793545542490	-0.037481304192	-0.302250004755
H	-2.956536974587	-1.917017899490	0.740910724117
H	-2.191277412323	-0.857044405005	1.911674912720
H	-0.825819377599	-2.993992805050	0.204667478991
H	-0.968758277438	-2.957343235611	1.966865636372
H	1.300410937328	-2.185590509609	1.120564070669
H	0.466531673915	-0.963386500212	2.091247335739
H	-1.473067638972	1.211833273642	-1.934451174922
H	0.126724880794	0.615270147521	-2.333545938167
H	-0.661592709962	3.074819123394	-0.884185802366
H	0.844124464476	2.724354293813	-1.710272612071
H	0.093194467780	1.860144565332	1.125546991761
H	1.120444815344	3.215719261326	0.721191955768
H	2.339544648388	1.114068057587	1.452222813949
H	2.899130660670	1.782240528546	-0.076569890212
H	2.558733518651	-0.767099813392	-0.025237650942
H	1.876558001241	0.099587805933	-1.382993542485

SCF Done: E(RwB97X) = -462.113266811

Zero-point correction=	0.248248
Thermal correction to Energy=	0.257996
Thermal correction to Enthalpy=	0.258940
Thermal correction to Gibbs Free Energy=	0.213014
Sum of electronic and zero-point Energies=	-461.865019
Sum of electronic and thermal Energies=	-461.855271
Sum of electronic and thermal Enthalpies=	-461.854326

Sum of electronic and thermal Free Energies= -461.900252

1	N	Isotropic =	51.0073	Anisotropy =	276.2447
2	C	Isotropic =	144.7778	Anisotropy =	29.5864
3	C	Isotropic =	167.2174	Anisotropy =	7.3433
4	C	Isotropic =	144.2774	Anisotropy =	34.1321
5	N	Isotropic =	159.0472	Anisotropy =	73.7926
6	C	Isotropic =	22.5329	Anisotropy =	144.0604
7	C	Isotropic =	155.3156	Anisotropy =	31.0394
8	C	Isotropic =	169.3012	Anisotropy =	7.6565
9	C	Isotropic =	168.4246	Anisotropy =	15.0542
10	C	Isotropic =	164.5936	Anisotropy =	16.4818
11	C	Isotropic =	141.6785	Anisotropy =	46.3764
12	H	Isotropic =	28.5700	Anisotropy =	8.3821
13	H	Isotropic =	28.5936	Anisotropy =	7.9756
14	H	Isotropic =	30.0249	Anisotropy =	8.8174
15	H	Isotropic =	30.1390	Anisotropy =	10.2269
16	H	Isotropic =	28.9001	Anisotropy =	7.5261
17	H	Isotropic =	28.5007	Anisotropy =	7.8467
18	H	Isotropic =	29.9247	Anisotropy =	7.8685
19	H	Isotropic =	29.1005	Anisotropy =	6.3806
20	H	Isotropic =	30.1635	Anisotropy =	10.5971
21	H	Isotropic =	30.3721	Anisotropy =	9.6384
22	H	Isotropic =	30.5725	Anisotropy =	6.3102
23	H	Isotropic =	30.3753	Anisotropy =	10.9164
24	H	Isotropic =	29.9620	Anisotropy =	8.7478
25	H	Isotropic =	30.5595	Anisotropy =	10.5071
26	H	Isotropic =	29.0848	Anisotropy =	7.6574
27	H	Isotropic =	28.1651	Anisotropy =	6.7615

Conformer_9

N	-1.892659349333	-0.496639389570	-0.253684236461
C	-1.986641277107	-1.661960216253	0.617761220129
C	-0.889763636828	-1.670503042521	1.673591657717
C	0.459237266322	-1.644650042648	0.977500202404
N	0.460405464007	-0.669195503369	-0.115298676174
C	-0.701646956169	-0.094893786654	-0.554231242200
C	-0.548894203728	1.104833289562	-1.462162233754
C	0.066860311900	2.353405448636	-0.780564899243
C	0.900721858544	2.085873666411	0.476053167209
C	2.110322080517	1.173144692203	0.273656298725
C	1.758125466519	-0.113897365338	-0.485427353830
H	-1.918111057948	-2.580673565314	0.015972521646
H	-2.975796285371	-1.665329610038	1.085074162372

H	-0.960427783412	-2.554587320544	2.312805951482
H	-0.999142343680	-0.786327537446	2.312019980829
H	1.250213648007	-1.369757058979	1.683311082763
H	0.705111284064	-2.637230531025	0.579527382601
H	0.050033651181	0.812784581779	-2.329424126139
H	-1.544901833093	1.342380374538	-1.838393359912
H	0.673681075548	2.893030413918	-1.516375005259
H	-0.746989592905	3.028954420403	-0.498522281952
H	1.238475086354	3.044742221536	0.883526054129
H	0.251873727898	1.647431901096	1.244034432779
H	2.894717820854	1.694570731815	-0.287475158677
H	2.534537348661	0.926236334761	1.253638735194
H	2.509097908142	-0.885635433162	-0.296577885592
H	1.775060321057	0.068892326202	-1.561636390789

SCF Done: E(RwB97X) = -462.113608142

Zero-point correction=	0.248813
Thermal correction to Energy=	0.258404
Thermal correction to Enthalpy=	0.259348
Thermal correction to Gibbs Free Energy=	0.213897
Sum of electronic and zero-point Energies=	-461.864795
Sum of electronic and thermal Energies=	-461.855204
Sum of electronic and thermal Enthalpies=	-461.854260
Sum of electronic and thermal Free Energies=	-461.899711

1 N	Isotropic =	53.3239	Anisotropy =	271.5243
2 C	Isotropic =	145.1219	Anisotropy =	29.4286
3 C	Isotropic =	168.2109	Anisotropy =	11.3519
4 C	Isotropic =	144.7045	Anisotropy =	34.3495
5 N	Isotropic =	161.0636	Anisotropy =	81.6837
6 C	Isotropic =	22.0882	Anisotropy =	143.6836
7 C	Isotropic =	155.6146	Anisotropy =	30.3662
8 C	Isotropic =	168.9487	Anisotropy =	8.7821
9 C	Isotropic =	167.8582	Anisotropy =	14.0679
10 C	Isotropic =	165.9347	Anisotropy =	17.4630
11 C	Isotropic =	143.1532	Anisotropy =	44.1474
12 H	Isotropic =	28.8043	Anisotropy =	8.9264
13 H	Isotropic =	28.5260	Anisotropy =	8.5289
14 H	Isotropic =	30.2038	Anisotropy =	10.5748
15 H	Isotropic =	30.3142	Anisotropy =	8.2268
16 H	Isotropic =	28.7846	Anisotropy =	6.3969
17 H	Isotropic =	28.6583	Anisotropy =	9.9705
18 H	Isotropic =	29.1457	Anisotropy =	6.5135
19 H	Isotropic =	29.9872	Anisotropy =	8.1143
20 H	Isotropic =	30.3614	Anisotropy =	9.8577

21	H	Isotropic =	30.1757	Anisotropy =	10.4769
22	H	Isotropic =	30.3907	Anisotropy =	10.8513
23	H	Isotropic =	30.5003	Anisotropy =	6.3761
24	H	Isotropic =	30.5496	Anisotropy =	10.4425
25	H	Isotropic =	29.9871	Anisotropy =	9.1243
26	H	Isotropic =	29.0205	Anisotropy =	7.8490
27	H	Isotropic =	28.3351	Anisotropy =	7.0954

2,3,4,6,7,8,9,10-octahydropyrimido[1,2-a]azepine_protonated

Conformer_1

C	10.299906343278	-7.680704578838	-2.036763954804
C	10.483874022744	-6.183910101943	-2.189719896415
N	9.353366171219	-5.652526210375	-2.945658227657
C	8.146442614538	-6.195840935045	-2.969397798199
C	7.082363561946	-5.486037477181	-3.755535663321
C	6.006778846274	-4.844537073871	-2.864674180477
C	4.960526211600	-5.825895326501	-2.342865706161
C	5.516581972865	-6.972141860505	-1.501454783777
C	6.515692340764	-7.859598516450	-2.238838480033
N	7.877924714608	-7.301303381640	-2.300319283819
C	8.912813590250	-7.972687867361	-1.495458384244
H	10.430275426372	-8.171024196193	-3.006230694788
H	11.047485196496	-8.081743547560	-1.350386613286
H	11.394890586469	-5.942907310795	-2.738204302194
H	10.526979116008	-5.692815356137	-1.212695188345
H	9.486891268696	-4.807889305126	-3.482800208760
H	6.623168700867	-6.193927725568	-4.453227305824
H	7.572743423085	-4.716498597479	-4.354788311487
H	5.503690104082	-4.079692874731	-3.462896945351
H	6.490391769899	-4.320334509811	-2.031925393329
H	4.420441825459	-6.251445845363	-3.198675948245
H	4.223361615184	-5.273214835961	-1.751384243601
H	4.684961750853	-7.610069461772	-1.185382294573
H	5.987182310306	-6.591264713134	-0.586796331915
H	6.170019842349	-8.075549731093	-3.254770299470
H	6.613108730261	-8.814642848115	-1.723365629435
H	8.816299965718	-7.639892562813	-0.456442050516
H	8.707037977811	-9.043103248637	-1.530541879970

SCF Done: E(RwB97X) = -462.605564968

Zero-point correction=	0.262869
Thermal correction to Energy=	0.272651

Thermal correction to Enthalpy=	0.273595
Thermal correction to Gibbs Free Energy=	0.228130
Sum of electronic and zero-point Energies=	-462.342696
Sum of electronic and thermal Energies=	-462.332914
Sum of electronic and thermal Enthalpies=	-462.331970
Sum of electronic and thermal Free Energies=	-462.377435

1 C	Isotropic =	170.2275	Anisotropy =	8.0269
2 C	Isotropic =	150.5590	Anisotropy =	27.3521
3 N	Isotropic =	140.5627	Anisotropy =	73.1561
4 C	Isotropic =	15.5075	Anisotropy =	172.1955
5 C	Isotropic =	155.1469	Anisotropy =	23.0726
6 C	Isotropic =	166.2025	Anisotropy =	7.6379
7 C	Isotropic =	160.8015	Anisotropy =	3.3928
8 C	Isotropic =	162.6788	Anisotropy =	9.0786
9 C	Isotropic =	135.6002	Anisotropy =	48.9874
10 N	Isotropic =	122.8029	Anisotropy =	113.2509
11 C	Isotropic =	140.9671	Anisotropy =	40.5538
12 H	Isotropic =	29.9190	Anisotropy =	9.6281
13 H	Isotropic =	29.8966	Anisotropy =	11.0934
14 H	Isotropic =	28.4644	Anisotropy =	9.7268
15 H	Isotropic =	28.5718	Anisotropy =	9.6743
16 H	Isotropic =	25.8700	Anisotropy =	8.9313
17 H	Isotropic =	29.0474	Anisotropy =	5.7817
18 H	Isotropic =	29.5473	Anisotropy =	8.0449
19 H	Isotropic =	30.0050	Anisotropy =	10.7776
20 H	Isotropic =	30.4643	Anisotropy =	7.5348
21 H	Isotropic =	30.3290	Anisotropy =	8.7010
22 H	Isotropic =	30.0309	Anisotropy =	10.5529
23 H	Isotropic =	30.1224	Anisotropy =	10.5468
24 H	Isotropic =	30.3567	Anisotropy =	6.9562
25 H	Isotropic =	28.0159	Anisotropy =	5.9683
26 H	Isotropic =	28.6555	Anisotropy =	6.7513
27 H	Isotropic =	28.2413	Anisotropy =	8.0981
28 H	Isotropic =	28.5716	Anisotropy =	7.0577

Conformer_10

C	10.215673878777	-7.626292526086	-1.916974596752
C	10.388388806126	-6.128502165982	-2.083350727054
N	9.295880522791	-5.613248914560	-2.906785429740
C	8.113853243371	-6.192856349781	-3.029473905665
C	7.078571454519	-5.546904639285	-3.904286878690
C	5.823497050419	-5.047172621771	-3.139387561397
C	5.656786497461	-5.577245177952	-1.713435388489

C	5.475067448665	-7.092150104302	-1.606422753182
C	6.473167653281	-7.876469531600	-2.460888009289
N	7.829309756844	-7.316913823340	-2.394488864875
C	8.795834938259	-7.932656211810	-1.474619911612
H	10.423286720518	-8.132906888704	-2.864329314744
H	10.919226940932	-8.000069611635	-1.171320376149
H	11.326264891066	-5.886133548537	-2.584226911699
H	10.373351420784	-5.623124325655	-1.113077804356
H	9.440935641902	-4.753803293705	-3.417077565595
H	6.799915816055	-6.280430125399	-4.665093469915
H	7.551091744081	-4.716996396822	-4.432099849780
H	4.938926204421	-5.300063195714	-3.732073650406
H	5.867034199455	-3.956185118625	-3.091754854956
H	4.793865974154	-5.082635388395	-1.257519562442
H	6.523576141344	-5.273023250698	-1.114068785740
H	4.469724961322	-7.379106487756	-1.932785304887
H	5.567980696981	-7.390826048535	-0.557320307868
H	6.155751594206	-7.895567111818	-3.505268873242
H	6.538050014784	-8.913279633431	-2.129907935432
H	8.610183291763	-7.556967839293	-0.462289250389
H	8.610402495719	-9.007369668810	-1.479572155653

SCF Done: E(RwB97X) = -462.600474582

Zero-point correction=	0.262753
Thermal correction to Energy=	0.272711
Thermal correction to Enthalpy=	0.273655
Thermal correction to Gibbs Free Energy=	0.227329
Sum of electronic and zero-point Energies=	-462.337721
Sum of electronic and thermal Energies=	-462.327764
Sum of electronic and thermal Enthalpies=	-462.326819
Sum of electronic and thermal Free Energies=	-462.373145

1 C	Isotropic =	170.3933	Anisotropy =	8.4645
2 C	Isotropic =	150.2830	Anisotropy =	27.4082
3 N	Isotropic =	139.2511	Anisotropy =	79.7588
4 C	Isotropic =	17.7564	Anisotropy =	168.6653
5 C	Isotropic =	158.7573	Anisotropy =	28.1637
6 C	Isotropic =	170.8987	Anisotropy =	6.6947
7 C	Isotropic =	168.8795	Anisotropy =	13.8099
8 C	Isotropic =	166.6364	Anisotropy =	12.4146
9 C	Isotropic =	139.5801	Anisotropy =	51.7504
10 N	Isotropic =	130.4524	Anisotropy =	102.9365
11 C	Isotropic =	142.6090	Anisotropy =	39.6797
12 H	Isotropic =	29.8691	Anisotropy =	9.7267
13 H	Isotropic =	29.8481	Anisotropy =	11.1687

14	H	Isotropic =	28.4547	Anisotropy =	9.8304
15	H	Isotropic =	28.4926	Anisotropy =	9.5689
16	H	Isotropic =	25.8313	Anisotropy =	9.2181
17	H	Isotropic =	28.8664	Anisotropy =	7.5678
18	H	Isotropic =	29.4958	Anisotropy =	8.3243
19	H	Isotropic =	30.2252	Anisotropy =	9.9679
20	H	Isotropic =	30.0513	Anisotropy =	10.8610
21	H	Isotropic =	30.2266	Anisotropy =	11.2253
22	H	Isotropic =	30.6208	Anisotropy =	6.6605
23	H	Isotropic =	30.4004	Anisotropy =	10.7738
24	H	Isotropic =	29.9306	Anisotropy =	9.3881
25	H	Isotropic =	28.0392	Anisotropy =	6.9022
26	H	Isotropic =	28.6544	Anisotropy =	7.6599
27	H	Isotropic =	28.2617	Anisotropy =	8.0937
28	H	Isotropic =	28.5488	Anisotropy =	7.4746

Conformer_11

C	9.843922875362	-7.981814166917	-2.672675661526
C	10.442109895372	-6.594875427511	-2.821881110318
N	9.351820065989	-5.633013010616	-2.953823586335
C	8.160692871249	-5.796501964909	-2.403441219735
C	7.117697129909	-4.734774361737	-2.601751669161
C	5.851876198447	-5.210303480875	-3.363826667646
C	5.658308466957	-6.725277063131	-3.470690513440
C	5.496625988100	-7.453168289036	-2.135255486484
C	6.541976298719	-7.032870565606	-1.099508708299
N	7.875835004395	-6.871597768022	-1.691611461650
C	8.828423909806	-7.982792631862	-1.544133769898
H	10.628932491224	-8.707734617914	-2.454734758545
H	9.359805836066	-8.274206273249	-3.609556104585
H	11.064993387156	-6.517831926522	-3.713155712161
H	11.050263612896	-6.335478201985	-1.949717013136
H	9.500948210433	-4.792618987755	-3.493782225794
H	7.583716248728	-3.902226020133	-3.131068833191
H	6.851885566832	-4.360461965028	-1.609681269298
H	4.976626933437	-4.760685423946	-2.884839803934
H	5.895290032115	-4.805684938553	-4.378206655227
H	6.505667525294	-7.157412604555	-4.016452206986
H	4.777704917805	-6.918365512948	-4.090696307095
H	5.556107117738	-8.532983390260	-2.307233967359
H	4.509460274825	-7.251282712251	-1.706073163822
H	6.632871466427	-7.776291022972	-0.306328885346
H	6.258284079842	-6.093536061430	-0.622117965876
H	9.319541675200	-7.890870072261	-0.570184959514

H 8.248511919678 -8.907741538017 -1.547870313639

SCF Done: E(RwB97X) = -462.600862088

Zero-point correction= 0.263160
Thermal correction to Energy= 0.272997
Thermal correction to Enthalpy= 0.273941
Thermal correction to Gibbs Free Energy= 0.228030
Sum of electronic and zero-point Energies= -462.337702
Sum of electronic and thermal Energies= -462.327865
Sum of electronic and thermal Enthalpies= -462.326921
Sum of electronic and thermal Free Energies= -462.372832

1	C	Isotropic =	170.2236	Anisotropy =	10.5881
2	C	Isotropic =	150.4454	Anisotropy =	27.2778
3	N	Isotropic =	140.1200	Anisotropy =	71.8709
4	C	Isotropic =	18.2098	Anisotropy =	167.5992
5	C	Isotropic =	159.0622	Anisotropy =	27.6273
6	C	Isotropic =	171.0529	Anisotropy =	7.2943
7	C	Isotropic =	168.5293	Anisotropy =	13.3043
8	C	Isotropic =	167.4537	Anisotropy =	12.9693
9	C	Isotropic =	140.7060	Anisotropy =	49.4416
10	N	Isotropic =	130.7800	Anisotropy =	107.9751
11	C	Isotropic =	143.1949	Anisotropy =	37.7218
12	H	Isotropic =	29.8654	Anisotropy =	11.3226
13	H	Isotropic =	29.9220	Anisotropy =	8.8175
14	H	Isotropic =	28.4063	Anisotropy =	9.6959
15	H	Isotropic =	28.5921	Anisotropy =	10.3865
16	H	Isotropic =	25.8054	Anisotropy =	9.3302
17	H	Isotropic =	29.5438	Anisotropy =	8.4930
18	H	Isotropic =	28.8895	Anisotropy =	7.7863
19	H	Isotropic =	30.2213	Anisotropy =	10.0817
20	H	Isotropic =	30.0728	Anisotropy =	10.8747
21	H	Isotropic =	30.5608	Anisotropy =	6.5651
22	H	Isotropic =	30.2521	Anisotropy =	11.1866
23	H	Isotropic =	29.9788	Anisotropy =	9.4713
24	H	Isotropic =	30.4151	Anisotropy =	10.8635
25	H	Isotropic =	28.6513	Anisotropy =	7.7953
26	H	Isotropic =	28.2289	Anisotropy =	7.0698
27	H	Isotropic =	28.4054	Anisotropy =	9.7548
28	H	Isotropic =	28.4700	Anisotropy =	6.5846

Conformer_12

C 9.916417301075 -7.141256663791 -1.224643033982

C	10.463355833074	-6.348815449123	-2.397927610987
N	9.345279523149	-5.709195219471	-3.085059838088
C	8.124514586777	-6.215703442023	-3.125626913916
C	7.054120714256	-5.470921296273	-3.869950181660
C	5.870698020414	-4.991726259537	-2.987299782158
C	5.751761545191	-5.643330006814	-1.606959943437
C	5.522482130264	-7.155495036055	-1.622369853038
C	6.467972375645	-7.889781474758	-2.575806205439
N	7.834137258494	-7.354475082556	-2.523493834248
C	8.820343360225	-8.075797545149	-1.704346601388
H	10.713678149157	-7.724939971825	-0.761622564099
H	9.516863567289	-6.453451675833	-0.473055913427
H	10.992777828153	-7.002275113191	-3.098291187002
H	11.147180800897	-5.565047468524	-2.071762870703
H	9.497756768545	-4.830095917488	-3.558345559652
H	6.698762439155	-6.133292160729	-4.663667142249
H	7.521799319305	-4.618705240879	-4.365430904294
H	5.972233294100	-3.913350611329	-2.841107765423
H	4.943356170361	-5.145561708905	-3.547677861492
H	4.929228608243	-5.163657816480	-1.067973521519
H	6.655553099522	-5.421690436175	-1.026751534163
H	4.498082489288	-7.384362608415	-1.934899277671
H	5.641792205054	-7.545504881492	-0.606115389714
H	6.108721195607	-7.824408954888	-3.604102359195
H	6.531466452583	-8.950617387978	-2.329471901210
H	9.232753439632	-8.895631994766	-2.301011821482
H	8.283011524545	-8.506908575551	-0.857428628365

SCF Done: E(RwB97X) = -462.600862080

Zero-point correction=	0.263161
Thermal correction to Energy=	0.272996
Thermal correction to Enthalpy=	0.273940
Thermal correction to Gibbs Free Energy=	0.228032
Sum of electronic and zero-point Energies=	-462.337701
Sum of electronic and thermal Energies=	-462.327866
Sum of electronic and thermal Enthalpies=	-462.326922
Sum of electronic and thermal Free Energies=	-462.372830

1 C	Isotropic =	170.2229	Anisotropy =	10.5888
2 C	Isotropic =	150.4435	Anisotropy =	27.2799
3 N	Isotropic =	140.1177	Anisotropy =	71.8774
4 C	Isotropic =	18.2081	Anisotropy =	167.5995
5 C	Isotropic =	159.0617	Anisotropy =	27.6257
6 C	Isotropic =	171.0528	Anisotropy =	7.2901
7 C	Isotropic =	168.5289	Anisotropy =	13.3075

8	C	Isotropic =	167.4536	Anisotropy =	12.9722
9	C	Isotropic =	140.7068	Anisotropy =	49.4318
10	N	Isotropic =	130.7767	Anisotropy =	107.9820
11	C	Isotropic =	143.1953	Anisotropy =	37.7202
12	H	Isotropic =	29.8653	Anisotropy =	11.3225
13	H	Isotropic =	29.9222	Anisotropy =	8.8173
14	H	Isotropic =	28.5921	Anisotropy =	10.3865
15	H	Isotropic =	28.4062	Anisotropy =	9.6958
16	H	Isotropic =	25.8053	Anisotropy =	9.3301
17	H	Isotropic =	28.8890	Anisotropy =	7.7859
18	H	Isotropic =	29.5435	Anisotropy =	8.4934
19	H	Isotropic =	30.0727	Anisotropy =	10.8744
20	H	Isotropic =	30.2210	Anisotropy =	10.0816
21	H	Isotropic =	30.2521	Anisotropy =	11.1864
22	H	Isotropic =	30.5608	Anisotropy =	6.5654
23	H	Isotropic =	30.4151	Anisotropy =	10.8639
24	H	Isotropic =	29.9787	Anisotropy =	9.4703
25	H	Isotropic =	28.2289	Anisotropy =	7.0693
26	H	Isotropic =	28.6514	Anisotropy =	7.7956
27	H	Isotropic =	28.4054	Anisotropy =	9.7550
28	H	Isotropic =	28.4699	Anisotropy =	6.5841

Conformer_14

C	10.202470331512	-7.637951773949	-1.852242063904
C	10.384447472982	-6.144162876782	-2.042912426550
N	9.313166767628	-5.641196840306	-2.901108288343
C	8.132148157561	-6.219170506588	-3.040082277161
C	7.119661417077	-5.586692083325	-3.950708878514
C	5.849102618830	-5.068465556072	-3.224674853054
C	5.647764551834	-5.570516540111	-1.793069388267
C	5.458107383056	-7.082521885674	-1.661352881374
C	6.472566194655	-7.886249908906	-2.477626469693
N	7.828909410578	-7.330011618507	-2.390644343084
C	8.771686130490	-7.931284725239	-1.437172643574
H	10.430060549774	-8.163155853654	-2.784768521063
H	10.887230366766	-7.999745563236	-1.083537854621
H	11.334532705344	-5.914365891568	-2.526399915869
H	10.348793223873	-5.620365993021	-1.083002078577
H	9.473145085881	-4.792115569508	-3.424129341467
H	6.855979397142	-6.333690704709	-4.703704791593
H	7.607230515438	-4.768521552419	-4.483132607986
H	4.977501790902	-5.329945305815	-3.832655028349
H	5.895379799564	-3.976907646505	-3.196921296675
H	4.776449590657	-5.064426047110	-1.366679727671

H	6.501712138115	-5.257627831437	-1.179886455810
H	4.459448202015	-7.372477749046	-2.005130114444
H	5.525986638147	-7.361365589966	-0.604901027863
H	6.179125858686	-7.924118052248	-3.528493239777
H	6.525924835157	-8.916783964896	-2.125666886855
H	8.564067251162	-7.535863026899	-0.436693645951
H	8.582501615173	-9.005299342504	-1.426102951909

SCF Done: E(RwB97X) = -462.600474593

Zero-point correction=	0.262753
Thermal correction to Energy=	0.272711
Thermal correction to Enthalpy=	0.273655
Thermal correction to Gibbs Free Energy=	0.227332
Sum of electronic and zero-point Energies=	-462.337721
Sum of electronic and thermal Energies=	-462.327764
Sum of electronic and thermal Enthalpies=	-462.326820
Sum of electronic and thermal Free Energies=	-462.373143

1 C	Isotropic =	170.3935	Anisotropy =	8.4632
2 C	Isotropic =	150.2828	Anisotropy =	27.4081
3 N	Isotropic =	139.2528	Anisotropy =	79.7594
4 C	Isotropic =	17.7567	Anisotropy =	168.6632
5 C	Isotropic =	158.7582	Anisotropy =	28.1643
6 C	Isotropic =	170.9001	Anisotropy =	6.6936
7 C	Isotropic =	168.8785	Anisotropy =	13.8103
8 C	Isotropic =	166.6362	Anisotropy =	12.4162
9 C	Isotropic =	139.5797	Anisotropy =	51.7471
10 N	Isotropic =	130.4488	Anisotropy =	102.9420
11 C	Isotropic =	142.6103	Anisotropy =	39.6770
12 H	Isotropic =	29.8691	Anisotropy =	9.7267
13 H	Isotropic =	29.8481	Anisotropy =	11.1686
14 H	Isotropic =	28.4547	Anisotropy =	9.8303
15 H	Isotropic =	28.4925	Anisotropy =	9.5686
16 H	Isotropic =	25.8314	Anisotropy =	9.2186
17 H	Isotropic =	28.8663	Anisotropy =	7.5684
18 H	Isotropic =	29.4958	Anisotropy =	8.3246
19 H	Isotropic =	30.2253	Anisotropy =	9.9676
20 H	Isotropic =	30.0514	Anisotropy =	10.8614
21 H	Isotropic =	30.2266	Anisotropy =	11.2254
22 H	Isotropic =	30.6209	Anisotropy =	6.6602
23 H	Isotropic =	30.4004	Anisotropy =	10.7743
24 H	Isotropic =	29.9307	Anisotropy =	9.3875
25 H	Isotropic =	28.0391	Anisotropy =	6.9017
26 H	Isotropic =	28.6545	Anisotropy =	7.6602
27 H	Isotropic =	28.2617	Anisotropy =	8.0934

28 H Isotropic = 28.5489 Anisotropy = 7.4749

Conformer_2

C	10.308401632459	-7.596451477128	-1.886898994710
C	10.432324365667	-6.695538313682	-3.099595048230
N	9.346589867300	-5.719897562698	-3.065456470655
C	8.173819777144	-5.924286189612	-2.486446856945
C	7.148165193973	-4.833208606034	-2.594519683349
C	5.970317223192	-5.206547940195	-3.508483375212
C	4.931728175774	-6.111797154598	-2.851329148393
C	5.468157510481	-7.452715831750	-2.356117851626
C	6.568607517630	-7.334578031535	-1.305123690079
N	7.902525085176	-7.057255047413	-1.866288383960
C	8.895664237074	-8.142879730827	-1.798121857238
H	11.012751977551	-8.426430077172	-1.963361008728
H	10.545093118171	-7.031745793528	-0.980058455188
H	10.367575110519	-7.274663070169	-4.025895000984
H	11.374382669171	-6.146544482070	-3.100325777276
H	9.484809412826	-4.828687719566	-3.519771856333
H	7.650467170295	-3.945398898259	-2.983432426741
H	6.785319876062	-4.584962456958	-1.591793901533
H	6.354735332266	-5.666742766803	-4.426406951050
H	5.484122170724	-4.274078146703	-3.808599771846
H	4.120655253912	-6.292552662099	-3.564214738656
H	4.488332206127	-5.577845871819	-2.000746288880
H	5.839500931550	-8.056737342981	-3.193013357311
H	4.644242837605	-8.014133287561	-1.903988944068
H	6.667398508534	-8.275963064774	-0.765358574824
H	6.322315503465	-6.564392553597	-0.567291423851
H	8.745599412550	-8.660437081470	-0.849977186281
H	8.694297922803	-8.850528838999	-2.609482976056

SCF Done: E(RwB97X) = -462.605564970

Zero-point correction=	0.262869
Thermal correction to Energy=	0.272651
Thermal correction to Enthalpy=	0.273595
Thermal correction to Gibbs Free Energy=	0.228130
Sum of electronic and zero-point Energies=	-462.342696
Sum of electronic and thermal Energies=	-462.332914
Sum of electronic and thermal Enthalpies=	-462.331970
Sum of electronic and thermal Free Energies=	-462.377435

1 C Isotropic = 170.2276 Anisotropy = 8.0270

2	C	Isotropic =	150.5590	Anisotropy =	27.3521
3	N	Isotropic =	140.5628	Anisotropy =	73.1561
4	C	Isotropic =	15.5076	Anisotropy =	172.1954
5	C	Isotropic =	155.1469	Anisotropy =	23.0725
6	C	Isotropic =	166.2025	Anisotropy =	7.6379
7	C	Isotropic =	160.8016	Anisotropy =	3.3930
8	C	Isotropic =	162.6789	Anisotropy =	9.0785
9	C	Isotropic =	135.6003	Anisotropy =	48.9876
10	N	Isotropic =	122.8033	Anisotropy =	113.2503
11	C	Isotropic =	140.9671	Anisotropy =	40.5539
12	H	Isotropic =	29.8966	Anisotropy =	11.0934
13	H	Isotropic =	29.9190	Anisotropy =	9.6281
14	H	Isotropic =	28.5718	Anisotropy =	9.6743
15	H	Isotropic =	28.4644	Anisotropy =	9.7268
16	H	Isotropic =	25.8700	Anisotropy =	8.9313
17	H	Isotropic =	29.5473	Anisotropy =	8.0449
18	H	Isotropic =	29.0474	Anisotropy =	5.7817
19	H	Isotropic =	30.4643	Anisotropy =	7.5347
20	H	Isotropic =	30.0050	Anisotropy =	10.7776
21	H	Isotropic =	30.0309	Anisotropy =	10.5529
22	H	Isotropic =	30.3290	Anisotropy =	8.7010
23	H	Isotropic =	30.3567	Anisotropy =	6.9562
24	H	Isotropic =	30.1224	Anisotropy =	10.5468
25	H	Isotropic =	28.6555	Anisotropy =	6.7513
26	H	Isotropic =	28.0159	Anisotropy =	5.9683
27	H	Isotropic =	28.5716	Anisotropy =	7.0577
28	H	Isotropic =	28.2412	Anisotropy =	8.0981

Conformer_3

C	10.022248229209	-7.935540256613	-2.612999686168
C	10.546878746327	-6.514715457877	-2.695758763129
N	9.413984204882	-5.615811808521	-2.894335549375
C	8.191301268526	-5.856713006281	-2.448895758508
C	7.125379807227	-4.845001969677	-2.752252101904
C	6.004260625700	-5.390432338235	-3.650777411368
C	4.958231524957	-6.226849369587	-2.916782057958
C	5.498573587657	-7.481686299495	-2.235332471560
C	6.580682687044	-7.198690914504	-1.198300562209
N	7.909709288706	-6.962155435643	-1.786432466168
C	8.919845011079	-8.012564588090	-1.573704262535
H	9.634947321038	-8.242596754725	-3.589286009964
H	10.826911726226	-8.618937591853	-2.336754662951
H	11.228284786005	-6.383661479397	-3.536586319400
H	11.072587293817	-6.237938936730	-1.776663938561

H	9.553853773720	-4.766621037620	-3.422346487960
H	7.609591934173	-3.993980669360	-3.234637932099
H	6.709895396261	-4.481164823011	-1.806433251429
H	6.445081725700	-5.966007413226	-4.473293254596
H	5.506805345940	-4.529186138095	-4.105861324755
H	4.175640692264	-6.514011948987	-3.626659864206
H	4.477098777754	-5.596227928394	-2.157854352846
H	5.894433512086	-8.186906964836	-2.976415656412
H	4.673734079039	-7.988022027157	-1.723916692982
H	6.699933237399	-8.053561308169	-0.532135642066
H	6.308272394341	-6.342550528649	-0.573496490139
H	9.322890318702	-7.904318785985	-0.561378920514
H	8.403242704222	-8.972244219281	-1.633208108240

SCF Done: E(RwB97X) = -462.606175603

Zero-point correction=	0.263051
Thermal correction to Energy=	0.272757
Thermal correction to Enthalpy=	0.273701
Thermal correction to Gibbs Free Energy=	0.228496
Sum of electronic and zero-point Energies=	-462.343124
Sum of electronic and thermal Energies=	-462.333419
Sum of electronic and thermal Enthalpies=	-462.332475
Sum of electronic and thermal Free Energies=	-462.377680

1 C	Isotropic = 169.8966	Anisotropy = 9.6049
2 C	Isotropic = 150.8613	Anisotropy = 27.3322
3 N	Isotropic = 140.9723	Anisotropy = 68.3316
4 C	Isotropic = 15.1545	Anisotropy = 172.5084
5 C	Isotropic = 154.9498	Anisotropy = 23.7873
6 C	Isotropic = 165.4084	Anisotropy = 8.3145
7 C	Isotropic = 160.7217	Anisotropy = 3.4613
8 C	Isotropic = 163.1572	Anisotropy = 8.5742
9 C	Isotropic = 136.1961	Anisotropy = 48.3551
10 N	Isotropic = 123.0897	Anisotropy = 110.7298
11 C	Isotropic = 141.5168	Anisotropy = 38.9960
12 H	Isotropic = 29.9787	Anisotropy = 9.0732
13 H	Isotropic = 29.8727	Anisotropy = 11.1515
14 H	Isotropic = 28.4541	Anisotropy = 9.6484
15 H	Isotropic = 28.6228	Anisotropy = 10.2499
16 H	Isotropic = 25.8383	Anisotropy = 9.0717
17 H	Isotropic = 29.5735	Anisotropy = 8.1273
18 H	Isotropic = 29.0245	Anisotropy = 6.0024
19 H	Isotropic = 30.4141	Anisotropy = 7.2224
20 H	Isotropic = 29.9963	Anisotropy = 10.8584
21 H	Isotropic = 30.0120	Anisotropy = 10.5262

22	H	Isotropic =	30.3249	Anisotropy =	8.7506
23	H	Isotropic =	30.4075	Anisotropy =	6.9375
24	H	Isotropic =	30.1601	Anisotropy =	10.6523
25	H	Isotropic =	28.6636	Anisotropy =	6.9246
26	H	Isotropic =	28.2139	Anisotropy =	6.0250
27	H	Isotropic =	28.4176	Anisotropy =	9.1919
28	H	Isotropic =	28.4824	Anisotropy =	6.3723

Conformer_4

C	10.092454982863	-7.191514051840	-1.325511297493
C	10.554519998936	-6.433770894843	-2.555613519006
N	9.400493493763	-5.758871178162	-3.141824527094
C	8.158259959089	-6.206838692319	-3.054706693759
C	7.074137395721	-5.388068117562	-3.691940644808
C	6.057041154829	-4.831325651183	-2.683325943856
C	4.995207364873	-5.835074324438	-2.238895479502
C	5.536700667458	-7.077582756674	-1.536102828574
C	6.516034212065	-7.883542498316	-2.383344299394
N	7.875983510806	-7.319409606951	-2.404589162398
C	8.913783080251	-8.076556221634	-1.684388403232
H	10.903213442544	-7.810239865403	-0.937341767855
H	9.801018388860	-6.482864779457	-0.544293290053
H	10.989836633122	-7.114657452153	-3.293585927718
H	11.295331658792	-5.673422276341	-2.307524269815
H	9.542791369959	-4.884071841331	-3.625519827627
H	6.566171054854	-6.004092442002	-4.441648765961
H	7.555433067328	-4.568035690692	-4.227941139495
H	5.558329979566	-3.983482253295	-3.161611331298
H	6.590152683130	-4.429043430432	-1.813783743415
H	4.424557408837	-6.152937531054	-3.121201997664
H	4.287562570100	-5.328154558696	-1.574735680691
H	4.697674095478	-7.734173148791	-1.284695788933
H	6.024517701076	-6.808450736286	-0.591196743597
H	6.153492872013	-7.982449219809	-3.411130636760
H	6.620698670545	-8.892842543820	-1.984397847608
H	8.449575964952	-8.480943808382	-0.783063514163
H	9.227326618189	-8.916584428133	-2.312884928231

SCF Done: E(RwB97X) = -462.606175599

Zero-point correction=	0.263051
Thermal correction to Energy=	0.272757
Thermal correction to Enthalpy=	0.273701
Thermal correction to Gibbs Free Energy=	0.228496

Sum of electronic and zero-point Energies=	-462.343124
Sum of electronic and thermal Energies=	-462.333419
Sum of electronic and thermal Enthalpies=	-462.332475
Sum of electronic and thermal Free Energies=	-462.377680

1	C	Isotropic =	169.8965	Anisotropy =	9.6049
2	C	Isotropic =	150.8613	Anisotropy =	27.3321
3	N	Isotropic =	140.9727	Anisotropy =	68.3308
4	C	Isotropic =	15.1547	Anisotropy =	172.5082
5	C	Isotropic =	154.9499	Anisotropy =	23.7874
6	C	Isotropic =	165.4084	Anisotropy =	8.3146
7	C	Isotropic =	160.7217	Anisotropy =	3.4613
8	C	Isotropic =	163.1573	Anisotropy =	8.5742
9	C	Isotropic =	136.1962	Anisotropy =	48.3550
10	N	Isotropic =	123.0894	Anisotropy =	110.7308
11	C	Isotropic =	141.5168	Anisotropy =	38.9959
12	H	Isotropic =	29.8727	Anisotropy =	11.1515
13	H	Isotropic =	29.9787	Anisotropy =	9.0732
14	H	Isotropic =	28.6228	Anisotropy =	10.2499
15	H	Isotropic =	28.4541	Anisotropy =	9.6484
16	H	Isotropic =	25.8383	Anisotropy =	9.0717
17	H	Isotropic =	29.0245	Anisotropy =	6.0025
18	H	Isotropic =	29.5734	Anisotropy =	8.1273
19	H	Isotropic =	29.9963	Anisotropy =	10.8584
20	H	Isotropic =	30.4141	Anisotropy =	7.2224
21	H	Isotropic =	30.3249	Anisotropy =	8.7506
22	H	Isotropic =	30.0120	Anisotropy =	10.5262
23	H	Isotropic =	30.1601	Anisotropy =	10.6523
24	H	Isotropic =	30.4075	Anisotropy =	6.9375
25	H	Isotropic =	28.2139	Anisotropy =	6.0250
26	H	Isotropic =	28.6636	Anisotropy =	6.9246
27	H	Isotropic =	28.4824	Anisotropy =	6.3723
28	H	Isotropic =	28.4176	Anisotropy =	9.1919

Conformer_5

C	10.317117788295	-7.275604084713	-1.538890621465
C	10.550270084257	-6.694686770785	-2.918559369947
N	9.392902775715	-5.878009194626	-3.263217933797
C	8.152245690454	-6.117497276663	-2.857815816711
C	7.110890844247	-5.148024882421	-3.363584990219
C	5.941681251222	-4.870991544072	-2.419379556100
C	4.840855597836	-5.923742811824	-2.525072580289
C	5.409602389657	-7.339057276942	-2.604871374606
C	6.551019615722	-7.596991437912	-1.632862225909

N	7.891235027622	-7.137546217239	-2.060909929226
C	8.975608968677	-7.978918143909	-1.515802770750
H	11.101851530801	-7.991711196331	-1.289142065760
H	10.336700273153	-6.475213319273	-0.793172696803
H	10.674144872371	-7.488457282953	-3.662107195849
H	11.430730952824	-6.052653119902	-2.946989776406
H	9.535221016971	-5.063450836523	-3.842447446860
H	6.749569287111	-5.521474825779	-4.328350016511
H	7.644119684607	-4.218673397412	-3.576632810347
H	5.537032104635	-3.883654363475	-2.656304695931
H	6.313017396980	-4.809989955437	-1.390660101330
H	4.229878254143	-5.733855429092	-3.414214798280
H	4.175892381349	-5.838856941580	-1.659064975829
H	5.751215402211	-7.566936781180	-3.620431329901
H	4.623485635353	-8.065432928339	-2.379900938327
H	6.662320234780	-8.675033754831	-1.500350943392
H	6.339679768066	-7.169688021786	-0.646136135974
H	8.694439665612	-8.231694179692	-0.491577619899
H	9.005271505328	-8.906054025310	-2.097649283584

SCF Done: E(RwB97X) = -462.599533960

Zero-point correction=	0.262898
Thermal correction to Energy=	0.272733
Thermal correction to Enthalpy=	0.273677
Thermal correction to Gibbs Free Energy=	0.228142
Sum of electronic and zero-point Energies=	-462.336635
Sum of electronic and thermal Energies=	-462.326801
Sum of electronic and thermal Enthalpies=	-462.325857
Sum of electronic and thermal Free Energies=	-462.371392

1 C	Isotropic =	170.0156	Anisotropy =	8.1136
2 C	Isotropic =	151.0050	Anisotropy =	26.7037
3 N	Isotropic =	141.4045	Anisotropy =	63.8850
4 C	Isotropic =	17.7722	Anisotropy =	166.3407
5 C	Isotropic =	157.8022	Anisotropy =	32.2818
6 C	Isotropic =	169.1852	Anisotropy =	15.8093
7 C	Isotropic =	165.3657	Anisotropy =	6.9937
8 C	Isotropic =	165.5067	Anisotropy =	19.1624
9 C	Isotropic =	136.9091	Anisotropy =	50.8732
10 N	Isotropic =	123.4432	Anisotropy =	114.0335
11 C	Isotropic =	140.4747	Anisotropy =	40.4210
12 H	Isotropic =	29.9013	Anisotropy =	11.1687
13 H	Isotropic =	30.0052	Anisotropy =	9.5545
14 H	Isotropic =	28.6613	Anisotropy =	10.1000
15 H	Isotropic =	28.4847	Anisotropy =	9.7238

16	H	Isotropic =	26.0407	Anisotropy =	8.6574
17	H	Isotropic =	29.0632	Anisotropy =	6.5477
18	H	Isotropic =	29.4017	Anisotropy =	7.7715
19	H	Isotropic =	30.1067	Anisotropy =	11.3648
20	H	Isotropic =	29.9825	Anisotropy =	6.5767
21	H	Isotropic =	30.2901	Anisotropy =	10.4635
22	H	Isotropic =	30.2644	Anisotropy =	10.4450
23	H	Isotropic =	29.8667	Anisotropy =	6.2881
24	H	Isotropic =	29.9814	Anisotropy =	10.9397
25	H	Isotropic =	28.5938	Anisotropy =	6.4204
26	H	Isotropic =	28.2408	Anisotropy =	6.5588
27	H	Isotropic =	28.5465	Anisotropy =	6.6706
28	H	Isotropic =	28.4711	Anisotropy =	8.5676

Conformer_6

C	10.262664905968	-7.812107327068	-2.482442610561
C	10.585944222313	-6.343207905518	-2.300410243041
N	9.423975893567	-5.571885812039	-2.724842427364
C	8.166123611006	-5.980782494674	-2.617387180439
C	7.126043914130	-4.998773269263	-3.101113572402
C	5.866853251809	-5.608304340690	-3.716120305747
C	4.832825573742	-6.002877986656	-2.664278189342
C	5.475669753155	-6.688090043899	-1.460039187366
C	6.539548629350	-7.709983702748	-1.831603561578
N	7.887549068925	-7.173852043594	-2.124775177280
C	8.960672689086	-8.126047056255	-1.774567162045
H	10.177678520270	-8.042034597144	-3.548751592173
H	11.057153099604	-8.432086014344	-2.063627945963
H	11.432699451846	-6.033292166138	-2.912933433674
H	10.813151165417	-6.118844148989	-1.253358244872
H	9.575680673520	-4.664870862950	-3.141467168037
H	7.629159611645	-4.366147872720	-3.836012374903
H	6.868945675272	-4.345324217615	-2.259867758964
H	6.143807099795	-6.477229454690	-4.322866674491
H	5.436008838735	-4.879090372365	-4.407010490410
H	4.091658084865	-6.668816670445	-3.118752928024
H	4.292879360646	-5.113140103454	-2.322592668744
H	4.709858095475	-7.214380831519	-0.883182758777
H	5.915195613418	-5.951255572714	-0.778949942036
H	6.222285923973	-8.326322907131	-2.680338777206
H	6.692088347170	-8.381676026506	-0.984441640816
H	9.086669256009	-8.103996376275	-0.687072415531
H	8.604309669288	-9.119679822594	-2.053293568215

SCF Done: E(RwB97X) = -462.599533960

Zero-point correction=	0.262898
Thermal correction to Energy=	0.272733
Thermal correction to Enthalpy=	0.273677
Thermal correction to Gibbs Free Energy=	0.228142
Sum of electronic and zero-point Energies=	-462.336635
Sum of electronic and thermal Energies=	-462.326801
Sum of electronic and thermal Enthalpies=	-462.325857
Sum of electronic and thermal Free Energies=	-462.371392

1	C	Isotropic =	170.0156	Anisotropy =	8.1136
2	C	Isotropic =	151.0050	Anisotropy =	26.7037
3	N	Isotropic =	141.4045	Anisotropy =	63.8850
4	C	Isotropic =	17.7722	Anisotropy =	166.3407
5	C	Isotropic =	157.8022	Anisotropy =	32.2818
6	C	Isotropic =	169.1852	Anisotropy =	15.8093
7	C	Isotropic =	165.3657	Anisotropy =	6.9937
8	C	Isotropic =	165.5067	Anisotropy =	19.1624
9	C	Isotropic =	136.9091	Anisotropy =	50.8732
10	N	Isotropic =	123.4432	Anisotropy =	114.0336
11	C	Isotropic =	140.4747	Anisotropy =	40.4210
12	H	Isotropic =	30.0052	Anisotropy =	9.5545
13	H	Isotropic =	29.9013	Anisotropy =	11.1687
14	H	Isotropic =	28.4847	Anisotropy =	9.7238
15	H	Isotropic =	28.6613	Anisotropy =	10.1000
16	H	Isotropic =	26.0407	Anisotropy =	8.6574
17	H	Isotropic =	29.4017	Anisotropy =	7.7715
18	H	Isotropic =	29.0632	Anisotropy =	6.5477
19	H	Isotropic =	29.9825	Anisotropy =	6.5767
20	H	Isotropic =	30.1067	Anisotropy =	11.3648
21	H	Isotropic =	30.2644	Anisotropy =	10.4450
22	H	Isotropic =	30.2901	Anisotropy =	10.4635
23	H	Isotropic =	29.9814	Anisotropy =	10.9397
24	H	Isotropic =	29.8667	Anisotropy =	6.2881
25	H	Isotropic =	28.2408	Anisotropy =	6.5588
26	H	Isotropic =	28.5938	Anisotropy =	6.4204
27	H	Isotropic =	28.4711	Anisotropy =	8.5676
28	H	Isotropic =	28.5465	Anisotropy =	6.6706

Conformer_7

C	10.235936780310	-7.840426633974	-2.194418643301
C	10.612753415617	-6.431312273333	-2.596982613663
N	9.413120809728	-5.742296440882	-3.065638999013

C	8.161212428831	-6.076341611670	-2.781601554968
C	7.105702233913	-5.231735280257	-3.451762650441
C	5.890976650558	-4.886359006740	-2.588740895993
C	4.823089265856	-5.977584529755	-2.618166711082
C	5.429027257113	-7.378138292512	-2.544260897524
C	6.551590001852	-7.512861540460	-1.524777449995
N	7.897351701483	-7.089643927033	-1.973305560075
C	9.009386751565	-7.791091805500	-1.304513869314
H	10.020904448435	-8.442854398000	-3.082203351563
H	11.059509850322	-8.311259615413	-1.655160462605
H	11.340325035184	-6.422710987034	-3.409622079848
H	11.033964996320	-5.880626095490	-1.750704335021
H	9.540041543846	-4.951186017331	-3.680607214432
H	6.796979712787	-5.749677694286	-4.366388001325
H	7.604309432279	-4.315440444078	-3.772166826729
H	5.471617309151	-3.943834449198	-2.949669089125
H	6.218663703166	-4.700799425731	-1.559992801708
H	4.232212220990	-5.893308953647	-3.536690617571
H	4.131308270690	-5.827375780465	-1.782548413987
H	5.801282758861	-7.696457677025	-3.523993873396
H	4.654217540693	-8.098139207236	-2.265956956189
H	6.663054491779	-8.566164839293	-1.266583068619
H	6.310635994423	-6.977412995469	-0.599049805698
H	9.228631542780	-7.279015768529	-0.361239681586
H	8.664993851465	-8.798244309657	-1.071653575228

SCF Done: E(RwB97X) = -462.598407412

Zero-point correction=	0.262663
Thermal correction to Energy=	0.272719
Thermal correction to Enthalpy=	0.273663
Thermal correction to Gibbs Free Energy=	0.227046
Sum of electronic and zero-point Energies=	-462.335745
Sum of electronic and thermal Energies=	-462.325689
Sum of electronic and thermal Enthalpies=	-462.324745
Sum of electronic and thermal Free Energies=	-462.371362

1 C	Isotropic =	170.5363	Anisotropy =	9.8552
2 C	Isotropic =	150.2647	Anisotropy =	27.2717
3 N	Isotropic =	138.7895	Anisotropy =	81.6535
4 C	Isotropic =	17.7672	Anisotropy =	166.0327
5 C	Isotropic =	157.0621	Anisotropy =	32.5590
6 C	Isotropic =	169.5963	Anisotropy =	17.0032
7 C	Isotropic =	165.5333	Anisotropy =	7.3075
8 C	Isotropic =	165.2924	Anisotropy =	19.7235
9 C	Isotropic =	135.3970	Anisotropy =	55.2451

10	N	Isotropic =	124.6762	Anisotropy =	102.7587
11	C	Isotropic =	139.5480	Anisotropy =	45.4061
12	H	Isotropic =	29.8974	Anisotropy =	9.1799
13	H	Isotropic =	29.9069	Anisotropy =	11.1605
14	H	Isotropic =	28.5259	Anisotropy =	9.6184
15	H	Isotropic =	28.5738	Anisotropy =	9.9799
16	H	Isotropic =	26.0415	Anisotropy =	8.5645
17	H	Isotropic =	28.9530	Anisotropy =	6.1582
18	H	Isotropic =	29.5107	Anisotropy =	7.7362
19	H	Isotropic =	30.0826	Anisotropy =	11.3212
20	H	Isotropic =	30.0073	Anisotropy =	6.7978
21	H	Isotropic =	30.2834	Anisotropy =	10.4205
22	H	Isotropic =	30.2758	Anisotropy =	10.4307
23	H	Isotropic =	29.7829	Anisotropy =	6.2209
24	H	Isotropic =	29.9720	Anisotropy =	10.8462
25	H	Isotropic =	28.6454	Anisotropy =	6.4867
26	H	Isotropic =	28.1092	Anisotropy =	6.3456
27	H	Isotropic =	28.3489	Anisotropy =	8.6856
28	H	Isotropic =	28.5969	Anisotropy =	6.3008

Conformer_8

C	10.266171650858	-7.541165618699	-1.663290327836
C	10.607396846631	-6.484237619869	-2.690967486440
N	9.420583272407	-5.668309395944	-2.934349049725
C	8.166558822447	-6.023327224716	-2.687523454103
C	7.132972246120	-4.961675493315	-2.972429733692
C	5.833042653741	-5.459670265544	-3.606333599361
C	4.825929937924	-5.949383879073	-2.568100880737
C	5.490546855067	-6.769175785494	-1.463383980180
C	6.526269003046	-7.763484059867	-1.969619593135
N	7.883534359882	-7.226369793490	-2.216002098057
C	8.966532240573	-8.215256437660	-2.057407486285
H	11.062087535128	-8.285765902587	-1.609961173464
H	10.157985251155	-7.086098099048	-0.674084053856
H	10.926841129566	-6.940773392719	-3.632451343645
H	11.401032422973	-5.821752634050	-2.343011275700
H	9.561466773084	-4.738950457262	-3.303935636073
H	7.612247440809	-4.236679039912	-3.632383976172
H	6.929757964565	-4.435289416681	-2.033422276203
H	6.061434976129	-6.256958550334	-4.322086444734
H	5.401075279375	-4.641902463320	-4.188694252831
H	4.058221159488	-6.550745503159	-3.066467200183
H	4.313031342041	-5.093233049849	-2.116586760453
H	4.730518804873	-7.342900483302	-0.925441727083

H	5.960885121563	-6.116638589780	-0.719908917259
H	6.180695473427	-8.263566315429	-2.881887312292
H	6.666089426866	-8.536171315685	-1.213351628602
H	8.652675891827	-8.920225588314	-1.288187553466
H	9.078516118431	-8.764793624894	-2.998430778433

SCF Done: E(RwB97X) = -462.598407411

Zero-point correction=	0.262663
Thermal correction to Energy=	0.272719
Thermal correction to Enthalpy=	0.273663
Thermal correction to Gibbs Free Energy=	0.227046
Sum of electronic and zero-point Energies=	-462.335745
Sum of electronic and thermal Energies=	-462.325689
Sum of electronic and thermal Enthalpies=	-462.324745
Sum of electronic and thermal Free Energies=	-462.371362

1 C	Isotropic = 170.5363	Anisotropy = 9.8552
2 C	Isotropic = 150.2647	Anisotropy = 27.2717
3 N	Isotropic = 138.7895	Anisotropy = 81.6533
4 C	Isotropic = 17.7672	Anisotropy = 166.0327
5 C	Isotropic = 157.0621	Anisotropy = 32.5589
6 C	Isotropic = 169.5963	Anisotropy = 17.0032
7 C	Isotropic = 165.5333	Anisotropy = 7.3075
8 C	Isotropic = 165.2925	Anisotropy = 19.7234
9 C	Isotropic = 135.3970	Anisotropy = 55.2451
10 N	Isotropic = 124.6763	Anisotropy = 102.7587
11 C	Isotropic = 139.5481	Anisotropy = 45.4061
12 H	Isotropic = 29.9069	Anisotropy = 11.1605
13 H	Isotropic = 29.8974	Anisotropy = 9.1799
14 H	Isotropic = 28.5738	Anisotropy = 9.9799
15 H	Isotropic = 28.5259	Anisotropy = 9.6184
16 H	Isotropic = 26.0415	Anisotropy = 8.5645
17 H	Isotropic = 29.5107	Anisotropy = 7.7362
18 H	Isotropic = 28.9529	Anisotropy = 6.1581
19 H	Isotropic = 30.0073	Anisotropy = 6.7978
20 H	Isotropic = 30.0826	Anisotropy = 11.3212
21 H	Isotropic = 30.2758	Anisotropy = 10.4307
22 H	Isotropic = 30.2834	Anisotropy = 10.4205
23 H	Isotropic = 29.9720	Anisotropy = 10.8462
24 H	Isotropic = 29.7829	Anisotropy = 6.2210
25 H	Isotropic = 28.1092	Anisotropy = 6.3456
26 H	Isotropic = 28.6454	Anisotropy = 6.4867
27 H	Isotropic = 28.5969	Anisotropy = 6.3008
28 H	Isotropic = 28.3489	Anisotropy = 8.6856

Conformer_9

C	10.212608574156	-7.657951377325	-1.972887182593
C	10.328321034317	-6.751990506567	-3.183974680824
N	9.284547429939	-5.730817319226	-3.114354272466
C	8.145016759419	-5.869222493754	-2.458229584436
C	7.156344915025	-4.739417723055	-2.478940570882
C	5.820524858820	-5.077952168065	-3.193779025992
C	5.561765962498	-6.563589308964	-3.454614280535
C	5.442783134382	-7.427142651992	-2.197821016741
C	6.543457929584	-7.146571924542	-1.172507897302
N	7.861896692415	-6.978456061455	-1.797078999561
C	8.776996330885	-8.128045375059	-1.819563577899
H	10.521040933390	-7.117897790526	-1.072635127090
H	10.868981815716	-8.521508205077	-2.091799766110
H	10.209766782273	-7.321288482493	-4.110747095722
H	11.291950904127	-6.242273927821	-3.212914874910
H	9.430883724007	-4.858106558748	-3.601229458374
H	7.631497165933	-3.882223374202	-2.958584033072
H	6.975913819955	-4.453203945422	-1.439680454534
H	5.808994461607	-4.558687925800	-4.155366162848
H	5.000601176411	-4.659702691221	-2.601758300988
H	6.361040636764	-6.960280468929	-4.092510598355
H	4.642046395776	-6.658647697113	-4.039601221508
H	5.462740625113	-8.483182683219	-2.485635725464
H	4.482267143462	-7.248723664017	-1.702699114672
H	6.629178878450	-7.967007138648	-0.459576822081
H	6.314456880865	-6.247800686678	-0.596645195088
H	8.642991336564	-8.668825189493	-0.882003673934
H	8.491183698150	-8.792182660589	-2.642761286021

SCF Done: E(RwB97X) = -462.600474582

Zero-point correction=	0.262753
Thermal correction to Energy=	0.272711
Thermal correction to Enthalpy=	0.273655
Thermal correction to Gibbs Free Energy=	0.227329
Sum of electronic and zero-point Energies=	-462.337721
Sum of electronic and thermal Energies=	-462.327764
Sum of electronic and thermal Enthalpies=	-462.326819
Sum of electronic and thermal Free Energies=	-462.373145

1 C	Isotropic =	170.3933	Anisotropy =	8.4645
2 C	Isotropic =	150.2830	Anisotropy =	27.4082
3 N	Isotropic =	139.2511	Anisotropy =	79.7588

4 C	Isotropic =	17.7564	Anisotropy =	168.6653
5 C	Isotropic =	158.7573	Anisotropy =	28.1637
6 C	Isotropic =	170.8987	Anisotropy =	6.6947
7 C	Isotropic =	168.8795	Anisotropy =	13.8099
8 C	Isotropic =	166.6364	Anisotropy =	12.4146
9 C	Isotropic =	139.5801	Anisotropy =	51.7504
10 N	Isotropic =	130.4525	Anisotropy =	102.9365
11 C	Isotropic =	142.6090	Anisotropy =	39.6797
12 H	Isotropic =	29.8691	Anisotropy =	9.7267
13 H	Isotropic =	29.8481	Anisotropy =	11.1687
14 H	Isotropic =	28.4926	Anisotropy =	9.5689
15 H	Isotropic =	28.4547	Anisotropy =	9.8304
16 H	Isotropic =	25.8313	Anisotropy =	9.2181
17 H	Isotropic =	29.4958	Anisotropy =	8.3243
18 H	Isotropic =	28.8664	Anisotropy =	7.5678
19 H	Isotropic =	30.0513	Anisotropy =	10.8610
20 H	Isotropic =	30.2252	Anisotropy =	9.9679
21 H	Isotropic =	30.6208	Anisotropy =	6.6605
22 H	Isotropic =	30.2266	Anisotropy =	11.2253
23 H	Isotropic =	29.9306	Anisotropy =	9.3881
24 H	Isotropic =	30.4004	Anisotropy =	10.7738
25 H	Isotropic =	28.6544	Anisotropy =	7.6599
26 H	Isotropic =	28.0392	Anisotropy =	6.9022
27 H	Isotropic =	28.5488	Anisotropy =	7.4746
28 H	Isotropic =	28.2617	Anisotropy =	8.0937

4-amino-butan-1-ol_neutral

Conformer_1

C	0.958913405060	-0.640124576070	1.737677001922
C	0.494486389665	0.484369342846	0.818121963956
C	1.404562398899	0.830943447915	-0.365980153516
C	1.467559490506	-0.180194889812	-1.508200492411
O	0.830890787592	-1.940236330775	1.187121828275
N	2.222032834992	-1.386535230443	-1.138119364907
H	0.351980514393	-0.630020253595	2.648567880085
H	2.001207581291	-0.452371693606	2.043235333510
H	0.398048715354	1.383796985557	1.439234160281
H	-0.513986604510	0.247593720644	0.453581789322
H	1.057716659175	1.779169451290	-0.791977368365
H	2.425292090655	1.017144939685	-0.002514319398
H	0.452485104117	-0.489683398255	-1.781462328780
H	1.903440474814	0.310076632693	-2.388648590019
H	1.362251659629	-1.937818196499	0.360810404638
H	2.213752568019	-2.051858926841	-1.904711449171

H 3.196665930348 -1.144751024734 -0.981336295424

SCF Done: E(RwB97X) = -289.047323200

Zero-point correction= 0.157768
Thermal correction to Energy= 0.164727
Thermal correction to Enthalpy= 0.165671
Thermal correction to Gibbs Free Energy= 0.127206
Sum of electronic and zero-point Energies= -288.889555
Sum of electronic and thermal Energies= -288.882596
Sum of electronic and thermal Enthalpies= -288.881652
Sum of electronic and thermal Free Energies= -288.920117

1	C	Isotropic =	127.3500	Anisotropy =	45.6538
2	C	Isotropic =	155.1292	Anisotropy =	10.6848
3	C	Isotropic =	157.7643	Anisotropy =	11.0745
4	C	Isotropic =	147.6685	Anisotropy =	20.8664
5	O	Isotropic =	287.2382	Anisotropy =	39.6563
6	N	Isotropic =	230.4726	Anisotropy =	32.4755
7	H	Isotropic =	28.3167	Anisotropy =	7.3222
8	H	Isotropic =	28.4429	Anisotropy =	7.3089
9	H	Isotropic =	30.2151	Anisotropy =	9.2060
10	H	Isotropic =	30.4643	Anisotropy =	7.6594
11	H	Isotropic =	30.1008	Anisotropy =	9.6020
12	H	Isotropic =	30.6069	Anisotropy =	7.4839
13	H	Isotropic =	29.5289	Anisotropy =	7.3466
14	H	Isotropic =	28.7820	Anisotropy =	9.1626
15	H	Isotropic =	24.9694	Anisotropy =	29.3680
16	H	Isotropic =	30.4952	Anisotropy =	16.1609
17	H	Isotropic =	30.9567	Anisotropy =	13.3183

Conformer_10

C	0.622397109863	-0.706630102611	1.637027052946
C	0.865063103640	0.638863387862	0.961389530739
C	0.879842848149	0.651299661337	-0.571621824316
C	2.081218635776	0.004387979817	-1.256533740626
O	1.724219251217	-1.597237208700	1.585615054318
N	2.050820896628	-1.462070628657	-1.157877513573
H	0.409851661090	-0.540065550440	2.697808260586
H	-0.273309134492	-1.176684454110	1.199177327914
H	0.062909043749	1.310300649768	1.292724412584
H	1.803506392391	1.061322963675	1.344535637012
H	0.843371195897	1.695854076372	-0.901012938301
H	-0.038513709771	0.181285966309	-0.951581083400

H	3.005965597352	0.353658037548	-0.783573230627
H	2.109505751740	0.334686331120	-2.303285815608
H	1.921730662976	-1.728482635479	0.632292293884
H	1.256809473157	-1.822903574422	-1.679701352199
H	2.879311220636	-1.857984899389	-1.590582071333

SCF Done: E(RwB97X) = -289.047323192

Zero-point correction=	0.157768
Thermal correction to Energy=	0.164727
Thermal correction to Enthalpy=	0.165672
Thermal correction to Gibbs Free Energy=	0.127205
Sum of electronic and zero-point Energies=	-288.889555
Sum of electronic and thermal Energies=	-288.882596
Sum of electronic and thermal Enthalpies=	-288.881652
Sum of electronic and thermal Free Energies=	-288.920119

1 C	Isotropic = 127.3506	Anisotropy = 45.6643
2 C	Isotropic = 155.1300	Anisotropy = 10.6890
3 C	Isotropic = 157.7638	Anisotropy = 11.0741
4 C	Isotropic = 147.6743	Anisotropy = 20.8687
5 O	Isotropic = 287.2585	Anisotropy = 39.5926
6 N	Isotropic = 230.4826	Anisotropy = 32.5016
7 H	Isotropic = 28.3169	Anisotropy = 7.3219
8 H	Isotropic = 28.4433	Anisotropy = 7.3069
9 H	Isotropic = 30.2150	Anisotropy = 9.2052
10 H	Isotropic = 30.4644	Anisotropy = 7.6593
11 H	Isotropic = 30.1008	Anisotropy = 9.6013
12 H	Isotropic = 30.6069	Anisotropy = 7.4846
13 H	Isotropic = 29.5285	Anisotropy = 7.3470
14 H	Isotropic = 28.7821	Anisotropy = 9.1638
15 H	Isotropic = 24.9782	Anisotropy = 29.3481
16 H	Isotropic = 30.9575	Anisotropy = 13.3143
17 H	Isotropic = 30.4954	Anisotropy = 16.1619

Conformer_11

C	0.681724979503	-0.694431776525	1.661148800235
C	0.519039023982	0.568133868621	0.821399936656
C	1.534361351333	0.784979422670	-0.306693663367
C	1.421604192927	-0.130482148207	-1.523275637326
O	0.292488250926	-1.890025017266	1.006249519740
N	1.872971919198	-1.498465562540	-1.229845502587
H	1.725325196395	-0.767847031144	2.008246120909
H	0.053013529994	-0.613015932756	2.553488241077

H	0.597374081122	1.419688680554	1.508983292433
H	-0.499856104612	0.590330471635	0.412356017814
H	2.554040690725	0.710956465314	0.097572254385
H	1.425453353386	1.814722037852	-0.665412024869
H	0.376125999415	-0.184093737503	-1.847216548090
H	1.993382237802	0.310993719071	-2.350169210228
H	0.846756913646	-1.948228199391	0.197262291036
H	1.751603035542	-2.088543760186	-2.046831256439
H	2.868991348716	-1.493271500200	-1.027662631379

SCF Done: E(RwB97X) = -289.047323203

Zero-point correction=	0.157769
Thermal correction to Energy=	0.164728
Thermal correction to Enthalpy=	0.165672
Thermal correction to Gibbs Free Energy=	0.127206
Sum of electronic and zero-point Energies=	-288.889555
Sum of electronic and thermal Energies=	-288.882595
Sum of electronic and thermal Enthalpies=	-288.881651
Sum of electronic and thermal Free Energies=	-288.920117

1 C	Isotropic = 127.3485	Anisotropy = 45.6588
2 C	Isotropic = 155.1277	Anisotropy = 10.6866
3 C	Isotropic = 157.7642	Anisotropy = 11.0740
4 C	Isotropic = 147.6699	Anisotropy = 20.8603
5 O	Isotropic = 287.2641	Anisotropy = 39.6052
6 N	Isotropic = 230.4771	Anisotropy = 32.5106
7 H	Isotropic = 28.4430	Anisotropy = 7.3075
8 H	Isotropic = 28.3168	Anisotropy = 7.3220
9 H	Isotropic = 30.2149	Anisotropy = 9.2055
10 H	Isotropic = 30.4644	Anisotropy = 7.6588
11 H	Isotropic = 30.6073	Anisotropy = 7.4836
12 H	Isotropic = 30.1007	Anisotropy = 9.6014
13 H	Isotropic = 29.5287	Anisotropy = 7.3453
14 H	Isotropic = 28.7819	Anisotropy = 9.1634
15 H	Isotropic = 24.9772	Anisotropy = 29.3513
16 H	Isotropic = 30.4954	Anisotropy = 16.1621
17 H	Isotropic = 30.9574	Anisotropy = 13.3151

Conformer_12

C	0.636377225516	-0.585632413972	1.578486333954
C	1.386139924411	-0.971454933120	0.314854180120
C	1.505542251381	0.194622175599	-0.661009606788
C	2.267132443013	-0.173378101735	-1.925957761837

O	0.553717765689	-1.652951983845	2.520996249344
N	2.382585021607	0.983287465215	-2.818312924843
H	1.155905530990	0.226962732866	2.094775588628
H	-0.370762981290	-0.226881756189	1.324955610676
H	0.864416487880	-1.807652690097	-0.170524103309
H	2.384082344178	-1.332375079897	0.592004990860
H	2.018920745627	1.031622201450	-0.168339134404
H	0.507234741731	0.555866873268	-0.938093200195
H	3.247952838743	-0.586957752542	-1.645131531718
H	1.728531099785	-0.963733849774	-2.460656569187
H	0.079466058783	-2.377912554414	2.103228271408
H	2.954515556447	1.697268627961	-2.376775092255
H	2.869042945508	0.719001039225	-3.668601300455

SCF Done: E(RwB97X) = -289.040941920

Zero-point correction=	0.156379
Thermal correction to Energy=	0.164368
Thermal correction to Enthalpy=	0.165312
Thermal correction to Gibbs Free Energy=	0.124257
Sum of electronic and zero-point Energies=	-288.884563
Sum of electronic and thermal Energies=	-288.876574
Sum of electronic and thermal Enthalpies=	-288.875630
Sum of electronic and thermal Free Energies=	-288.916685

1 C	Isotropic = 124.8962	Anisotropy = 67.2407
2 C	Isotropic = 156.9057	Anisotropy = 34.0466
3 C	Isotropic = 160.6344	Anisotropy = 29.6385
4 C	Isotropic = 146.2033	Anisotropy = 37.7037
5 O	Isotropic = 296.8731	Anisotropy = 45.4313
6 N	Isotropic = 234.8833	Anisotropy = 39.0441
7 H	Isotropic = 28.4028	Anisotropy = 4.4704
8 H	Isotropic = 28.1275	Anisotropy = 4.9694
9 H	Isotropic = 30.5238	Anisotropy = 5.5873
10 H	Isotropic = 30.3443	Anisotropy = 5.5519
11 H	Isotropic = 30.7302	Anisotropy = 5.6185
12 H	Isotropic = 30.5768	Anisotropy = 5.9033
13 H	Isotropic = 29.0163	Anisotropy = 6.5502
14 H	Isotropic = 29.3688	Anisotropy = 5.9204
15 H	Isotropic = 31.5020	Anisotropy = 16.2948
16 H	Isotropic = 31.1811	Anisotropy = 12.8757
17 H	Isotropic = 30.7297	Anisotropy = 15.8664

Conformer_13

C	1.078123581303	-0.734247819100	1.695355129384
C	0.906110110115	-0.809926184200	0.187889172955
C	1.923238553093	0.054091306524	-0.550505306636
C	1.753784865840	-0.000646182848	-2.061738940240
O	0.106713865487	-1.502529338487	2.402769504259
N	2.730951474454	0.866073228269	-2.726152377397
H	0.950773847912	0.296001898741	2.040525588414
H	2.090809622203	-1.055103208095	1.976122163060
H	-0.112021000110	-0.492500963957	-0.068265627923
H	1.007727991149	-1.855859921047	-0.132595637498
H	1.824578309665	1.097024738189	-0.219738453141
H	2.941776027681	-0.263269974855	-0.294079588108
H	1.915175134703	-1.026531360104	-2.411266223514
H	0.715881900893	0.265016838044	-2.314920106884
H	0.208594363222	-2.421340764957	2.137404426163
H	2.625009671975	0.801108814557	-3.733145378020
H	2.544771680416	1.835138893327	-2.485158344876

SCF Done: E(RwB97X) = -289.040941920

Zero-point correction=	0.156379
Thermal correction to Energy=	0.164368
Thermal correction to Enthalpy=	0.165312
Thermal correction to Gibbs Free Energy=	0.124257
Sum of electronic and zero-point Energies=	-288.884563
Sum of electronic and thermal Energies=	-288.876574
Sum of electronic and thermal Enthalpies=	-288.875630
Sum of electronic and thermal Free Energies=	-288.916685

1 C	Isotropic =	124.8962	Anisotropy =	67.2407
2 C	Isotropic =	156.9057	Anisotropy =	34.0465
3 C	Isotropic =	160.6344	Anisotropy =	29.6385
4 C	Isotropic =	146.2033	Anisotropy =	37.7037
5 O	Isotropic =	296.8731	Anisotropy =	45.4315
6 N	Isotropic =	234.8833	Anisotropy =	39.0441
7 H	Isotropic =	28.4028	Anisotropy =	4.4704
8 H	Isotropic =	28.1275	Anisotropy =	4.9694
9 H	Isotropic =	30.3443	Anisotropy =	5.5519
10 H	Isotropic =	30.5238	Anisotropy =	5.5873
11 H	Isotropic =	30.7302	Anisotropy =	5.6185
12 H	Isotropic =	30.5768	Anisotropy =	5.9033
13 H	Isotropic =	29.3688	Anisotropy =	5.9204
14 H	Isotropic =	29.0163	Anisotropy =	6.5502
15 H	Isotropic =	31.5020	Anisotropy =	16.2948
16 H	Isotropic =	30.7297	Anisotropy =	15.8664
17 H	Isotropic =	31.1811	Anisotropy =	12.8757

Conformer_14

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-----
C      0.780807726318  -0.573436208471  1.776140694232
C      0.680806122377   0.125308168137   0.436041800232
C      1.768421381619  -0.289327897446  -0.549331748707
C      1.651043242326   0.430097093779  -1.884776106170
O      0.574282023128  -1.974415702031   1.586847043923
N      2.723694162135   0.019279763013  -2.795659991993
H      1.770210227550  -0.394962205748   2.219724913659
H      0.025203207137  -0.172335153150   2.463511576236
H     -0.310776627375  -0.070949334080   0.008773042467
H      0.739735145320   1.205650951505   0.617920046483
H      2.755667689624  -0.080972358503  -0.116745031218
H      1.717528079619  -1.371689826167  -0.719154578457
H      1.735763294210   1.511216416430  -1.725532042790
H      0.649763915199   0.246269238094  -2.304394300258
H      0.668487301180  -2.407658224143   2.439115645971
H      2.638679043213   0.513417716312  -3.677951281776
H      2.622684066421  -0.967392437531  -3.014929681834
```

SCF Done: E(RwB97X) = -289.040411671

```
Zero-point correction=          0.156109
Thermal correction to Energy=      0.164072
Thermal correction to Enthalpy=     0.165016
Thermal correction to Gibbs Free Energy=  0.123897
Sum of electronic and zero-point Energies= -288.884303
Sum of electronic and thermal Energies=    -288.876340
Sum of electronic and thermal Enthalpies=   -288.875396
Sum of electronic and thermal Free Energies= -288.916515
```

```
1 C  Isotropic = 126.8254  Anisotropy = 52.5214
2 C  Isotropic = 160.4795  Anisotropy = 20.2656
3 C  Isotropic = 158.8571  Anisotropy = 30.3588
4 C  Isotropic = 146.0036  Anisotropy = 37.6541
5 O  Isotropic = 309.8671  Anisotropy = 95.0691
6 N  Isotropic = 234.7837  Anisotropy = 39.4776
7 H  Isotropic = 28.1791  Anisotropy = 6.5184
8 H  Isotropic = 27.9794  Anisotropy = 7.4234
9 H  Isotropic = 30.3285  Anisotropy = 7.0817
10 H  Isotropic = 30.5396  Anisotropy = 7.9512
11 H  Isotropic = 30.5974  Anisotropy = 6.2245
12 H  Isotropic = 30.0368  Anisotropy = 4.5878
13 H  Isotropic = 29.3826  Anisotropy = 5.8635
```

14 H	Isotropic =	29.0362	Anisotropy =	6.6109
15 H	Isotropic =	31.2770	Anisotropy =	20.4729
16 H	Isotropic =	30.7098	Anisotropy =	15.9110
17 H	Isotropic =	31.1412	Anisotropy =	12.6801

Conformer_15

C	0.266653029276	-0.691198921007	1.529659828228
C	1.074933846700	0.215563305068	0.624909244691
C	1.350818608918	-0.384932939621	-0.749529914992
C	2.157971048841	0.546222873724	-1.641838841398
O	1.024247231830	-1.871400415788	1.802430053385
N	2.385173038278	-0.058173057662	-2.957948676590
H	0.032520010501	-0.170701413946	2.466976821382
H	-0.682672882484	-0.956683601163	1.044030826301
H	0.520049884431	1.155343340805	0.512613721344
H	2.019632629045	0.462709848349	1.125683367499
H	1.892903470719	-1.331506170804	-0.635160068427
H	0.400249983843	-0.620324165741	-1.245724189116
H	1.605303848904	1.481386419520	-1.788069332599
H	3.097941659130	0.806922339905	-1.131032060859
H	0.489083871916	-2.448782137369	2.353035549208
H	2.915892141189	0.576974849367	-3.545113246575
H	2.958098578963	-0.890520153638	-2.854223081480

SCF Done: E(RwB97X) = -289.040411669

Zero-point correction=	0.156109
Thermal correction to Energy=	0.164072
Thermal correction to Enthalpy=	0.165016
Thermal correction to Gibbs Free Energy=	0.123897
Sum of electronic and zero-point Energies=	-288.884303
Sum of electronic and thermal Energies=	-288.876340
Sum of electronic and thermal Enthalpies=	-288.875396
Sum of electronic and thermal Free Energies=	-288.916515

1 C	Isotropic =	126.8255	Anisotropy =	52.5215
2 C	Isotropic =	160.4795	Anisotropy =	20.2656
3 C	Isotropic =	158.8572	Anisotropy =	30.3587
4 C	Isotropic =	146.0036	Anisotropy =	37.6541
5 O	Isotropic =	309.8672	Anisotropy =	95.0691
6 N	Isotropic =	234.7837	Anisotropy =	39.4777
7 H	Isotropic =	27.9794	Anisotropy =	7.4234
8 H	Isotropic =	28.1791	Anisotropy =	6.5184
9 H	Isotropic =	30.5396	Anisotropy =	7.9512

10	H	Isotropic =	30.3285	Anisotropy =	7.0817
11	H	Isotropic =	30.0368	Anisotropy =	4.5878
12	H	Isotropic =	30.5974	Anisotropy =	6.2245
13	H	Isotropic =	29.3826	Anisotropy =	5.8635
14	H	Isotropic =	29.0362	Anisotropy =	6.6109
15	H	Isotropic =	31.2770	Anisotropy =	20.4729
16	H	Isotropic =	30.7098	Anisotropy =	15.9110
17	H	Isotropic =	31.1412	Anisotropy =	12.6801

Conformer_16

C	0.734651144173	-0.453691201257	1.879061487991
C	0.586072537186	-0.013003474588	0.432232026622
C	1.835791327372	-0.243426764194	-0.410120957381
C	1.664650827937	0.220714507592	-1.848981584484
O	0.973167192380	-1.853990803821	2.018240304266
N	2.887138937119	-0.014454549884	-2.622875987095
H	1.596120004333	0.039338484981	2.339846076199
H	-0.157415301711	-0.166934315215	2.450626737575
H	-0.270882744216	-0.537088032063	-0.013615476108
H	0.331106871283	1.054659256639	0.432564717798
H	2.092572144011	-1.310060702392	-0.406147602830
H	2.684686419915	0.288581655894	0.038548168576
H	1.455458851899	1.296458974238	-1.862395762959
H	0.787227762296	-0.281025413296	-2.285856610204
H	0.212426446361	-2.317742304401	1.655539418654
H	3.058903067628	-1.013315391125	-2.690117784062
H	2.764524512033	0.314680072893	-3.574947172558

SCF Done: E(RwB97X) = -289.040642105

Zero-point correction=	0.156154
Thermal correction to Energy=	0.164097
Thermal correction to Enthalpy=	0.165041
Thermal correction to Gibbs Free Energy=	0.123870
Sum of electronic and zero-point Energies=	-288.884488
Sum of electronic and thermal Energies=	-288.876545
Sum of electronic and thermal Enthalpies=	-288.875601
Sum of electronic and thermal Free Energies=	-288.916772

1	C	Isotropic =	125.7868	Anisotropy =	53.8432
2	C	Isotropic =	157.5438	Anisotropy =	23.6313
3	C	Isotropic =	159.0549	Anisotropy =	29.9961
4	C	Isotropic =	146.0467	Anisotropy =	37.6606
5	O	Isotropic =	303.0782	Anisotropy =	88.0515

6 N	Isotropic =	234.7948	Anisotropy =	39.2841
7 H	Isotropic =	28.4376	Anisotropy =	6.2972
8 H	Isotropic =	27.9128	Anisotropy =	7.4771
9 H	Isotropic =	30.4809	Anisotropy =	6.6851
10 H	Isotropic =	30.5021	Anisotropy =	7.6647
11 H	Isotropic =	30.0694	Anisotropy =	4.5228
12 H	Isotropic =	30.5583	Anisotropy =	6.3062
13 H	Isotropic =	29.3769	Anisotropy =	5.9061
14 H	Isotropic =	29.0667	Anisotropy =	6.6264
15 H	Isotropic =	31.9500	Anisotropy =	17.0186
16 H	Isotropic =	31.1446	Anisotropy =	12.7004
17 H	Isotropic =	30.7137	Anisotropy =	15.8857

Conformer_17

C	0.991254664609	-0.630503204573	1.573542679193
C	0.533237325345	0.539705245499	0.721730134505
C	1.441207425689	0.982269883122	-0.431936604510
C	1.499340413783	0.082670302948	-1.664022661930
O	0.762317291122	-1.868474549036	0.888186538664
N	2.338486451514	-1.103046833928	-1.466132468271
H	0.426789285337	-0.633697077103	2.513258959694
H	2.057122397438	-0.529293140362	1.819657937511
H	0.427980590625	1.390819828461	1.404444557036
H	-0.474855647329	0.322225427990	0.345424745249
H	1.082394291110	1.963442024264	-0.763897061126
H	2.462241197616	1.136273731894	-0.057864232348
H	1.933159991661	0.658308038218	-2.488505418147
H	0.470365459737	-0.173893349825	-1.964169781465
H	0.982260377130	-2.586663109340	1.488477599655
H	2.391954929341	-1.630451333670	-2.331256528520
H	1.899243555272	-1.708191884558	-0.776438395192

SCF Done: E(RwB97X) = -289.038758297

Zero-point correction=	0.157071
Thermal correction to Energy=	0.164474
Thermal correction to Enthalpy=	0.165418
Thermal correction to Gibbs Free Energy=	0.125998
Sum of electronic and zero-point Energies=	-288.881687
Sum of electronic and thermal Energies=	-288.874284
Sum of electronic and thermal Enthalpies=	-288.873340
Sum of electronic and thermal Free Energies=	-288.912761

1 C	Isotropic =	125.4954	Anisotropy =	50.6253

2	C	Isotropic =	157.6709	Anisotropy =	10.7814
3	C	Isotropic =	156.5073	Anisotropy =	9.8707
4	C	Isotropic =	147.0360	Anisotropy =	20.3956
5	O	Isotropic =	301.0478	Anisotropy =	97.8570
6	N	Isotropic =	235.2236	Anisotropy =	40.4278
7	H	Isotropic =	27.9164	Anisotropy =	7.5160
8	H	Isotropic =	28.1902	Anisotropy =	6.5008
9	H	Isotropic =	30.0992	Anisotropy =	9.5148
10	H	Isotropic =	30.3426	Anisotropy =	7.5139
11	H	Isotropic =	30.0099	Anisotropy =	9.1558
12	H	Isotropic =	30.5138	Anisotropy =	7.4612
13	H	Isotropic =	29.1884	Anisotropy =	8.4672
14	H	Isotropic =	29.1157	Anisotropy =	7.8214
15	H	Isotropic =	30.9372	Anisotropy =	20.5026
16	H	Isotropic =	31.0200	Anisotropy =	16.1831
17	H	Isotropic =	28.6757	Anisotropy =	17.7105

Conformer_18

C	0.411322314034	-0.742101631964	1.326298014410
C	0.931315872933	0.616314881529	0.891484033539
C	1.016845244175	0.900575868616	-0.612876391143
C	2.125731157674	0.203182202233	-1.396909723781
O	1.428501028930	-1.740264702038	1.172299352320
N	1.823916574874	-1.202120449777	-1.685501251563
H	0.116599985251	-0.693366075714	2.381031074988
H	-0.475943344641	-1.016775311224	0.739608615940
H	1.909357450181	0.781070790900	1.362063564581
H	0.252325692962	1.357022813554	1.329545954606
H	1.169223690120	1.980125313627	-0.726881856887
H	0.052118644203	0.672411052093	-1.085529382266
H	3.076210909650	0.327579214827	-0.853019480352
H	2.242789326311	0.717842000760	-2.356468405820
H	1.094323353161	-2.565087893502	1.536320467937
H	1.813960111055	-1.724634483978	-0.812751238391
H	2.561501989127	-1.597873589944	-2.258913348120

SCF Done: E(RwB97X) = -289.038758297

Zero-point correction=	0.157071
Thermal correction to Energy=	0.164474
Thermal correction to Enthalpy=	0.165418
Thermal correction to Gibbs Free Energy=	0.125998
Sum of electronic and zero-point Energies=	-288.881687
Sum of electronic and thermal Energies=	-288.874284

Sum of electronic and thermal Enthalpies= -288.873340
 Sum of electronic and thermal Free Energies= -288.912761

1 C	Isotropic =	125.4954	Anisotropy =	50.6252
2 C	Isotropic =	157.6709	Anisotropy =	10.7814
3 C	Isotropic =	156.5073	Anisotropy =	9.8707
4 C	Isotropic =	147.0360	Anisotropy =	20.3955
5 O	Isotropic =	301.0476	Anisotropy =	97.8568
6 N	Isotropic =	235.2235	Anisotropy =	40.4277
7 H	Isotropic =	27.9164	Anisotropy =	7.5160
8 H	Isotropic =	28.1902	Anisotropy =	6.5009
9 H	Isotropic =	30.3426	Anisotropy =	7.5139
10 H	Isotropic =	30.0992	Anisotropy =	9.5148
11 H	Isotropic =	30.0099	Anisotropy =	9.1558
12 H	Isotropic =	30.5138	Anisotropy =	7.4612
13 H	Isotropic =	29.1157	Anisotropy =	7.8215
14 H	Isotropic =	29.1884	Anisotropy =	8.4672
15 H	Isotropic =	30.9372	Anisotropy =	20.5026
16 H	Isotropic =	28.6757	Anisotropy =	17.7106
17 H	Isotropic =	31.0200	Anisotropy =	16.1830

Conformer_19

C	0.229862586711	-0.546061073330	1.670329326952
C	1.237015827854	0.121096774001	0.748195979704
C	1.174695959062	-0.373874584884	-0.692817815070
C	2.195693104974	0.313893430228	-1.595460556061
O	0.427090683992	-1.954274204715	1.793425207192
N	2.173174495266	-0.114908963193	-2.995320438964
H	0.261240538705	-0.075588286895	2.661567047010
H	-0.784168331635	-0.423869716498	1.277426883170
H	2.247194130923	-0.030994332188	1.153851980690
H	1.051015782606	1.202557289738	0.777260581778
H	1.344748307154	-1.457034282399	-0.722572625083
H	0.167369097597	-0.199440000134	-1.095457224367
H	2.034385673739	1.398064717891	-1.569348928401
H	3.204661325013	0.139486088385	-1.203139429992
H	1.300470957226	-2.095586920106	2.171019601395
H	2.329061172492	-1.117294166275	-3.046952464817
H	1.249688688320	0.045128230375	-3.386807125136

SCF Done: E(RwB97X) = -289.041043907

Zero-point correction= 0.156107
 Thermal correction to Energy= 0.164085

Thermal correction to Enthalpy=	0.165029
Thermal correction to Gibbs Free Energy=	0.123732
Sum of electronic and zero-point Energies=	-288.884937
Sum of electronic and thermal Energies=	-288.876959
Sum of electronic and thermal Enthalpies=	-288.876015
Sum of electronic and thermal Free Energies=	-288.917312

1 C	Isotropic =	125.8661	Anisotropy =	53.9041
2 C	Isotropic =	157.9199	Anisotropy =	23.5886
3 C	Isotropic =	154.9040	Anisotropy =	37.0828
4 C	Isotropic =	145.3279	Anisotropy =	41.8361
5 O	Isotropic =	302.9139	Anisotropy =	87.6307
6 N	Isotropic =	231.6043	Anisotropy =	34.5416
7 H	Isotropic =	27.9366	Anisotropy =	7.4692
8 H	Isotropic =	28.4875	Anisotropy =	6.3006
9 H	Isotropic =	30.5677	Anisotropy =	6.5485
10 H	Isotropic =	30.5474	Anisotropy =	7.5081
11 H	Isotropic =	30.0699	Anisotropy =	4.1013
12 H	Isotropic =	30.6621	Anisotropy =	5.5792
13 H	Isotropic =	29.3549	Anisotropy =	6.0722
14 H	Isotropic =	29.3952	Anisotropy =	6.1320
15 H	Isotropic =	31.9609	Anisotropy =	16.9772
16 H	Isotropic =	30.9722	Anisotropy =	12.7949
17 H	Isotropic =	30.9805	Anisotropy =	12.9870

Conformer_2

C	0.340828502526	-0.762871398561	1.479698086052
C	0.906178286784	0.566142614403	0.989941223838
C	1.017519159462	0.754072979798	-0.527535430861
C	2.093265705829	-0.055926748657	-1.247054039720
O	1.227966707254	-1.861364424422	1.352850680980
N	1.744710931088	-1.481340500995	-1.337344526795
H	-0.606113814738	-0.970199333679	0.954998463947
H	0.104254240866	-0.679206630735	2.545167373101
H	0.247083683367	1.353823766872	1.376209517663
H	1.887818918775	0.724622677718	1.456026905717
H	0.045229388284	0.544438852848	-0.995909014650
H	1.224902712095	1.812373480900	-0.722215248493
H	3.040199769902	0.024262430051	-0.701419859386
H	2.255961438866	0.380082976327	-2.241525238296
H	1.451239032398	-1.920137025700	0.397949433652
H	0.926255598569	-1.595686061906	-1.928957645534
H	2.495099738670	-1.995987654263	-1.787280681216

SCF Done: E(RwB97X) = -289.047323199

Zero-point correction=	0.157768
Thermal correction to Energy=	0.164727
Thermal correction to Enthalpy=	0.165671
Thermal correction to Gibbs Free Energy=	0.127206
Sum of electronic and zero-point Energies=	-288.889555
Sum of electronic and thermal Energies=	-288.882596
Sum of electronic and thermal Enthalpies=	-288.881652
Sum of electronic and thermal Free Energies=	-288.920117

1	C	Isotropic =	127.3500	Anisotropy =	45.6537
2	C	Isotropic =	155.1293	Anisotropy =	10.6847
3	C	Isotropic =	157.7643	Anisotropy =	11.0745
4	C	Isotropic =	147.6685	Anisotropy =	20.8664
5	O	Isotropic =	287.2381	Anisotropy =	39.6568
6	N	Isotropic =	230.4726	Anisotropy =	32.4753
7	H	Isotropic =	28.4429	Anisotropy =	7.3089
8	H	Isotropic =	28.3167	Anisotropy =	7.3222
9	H	Isotropic =	30.2151	Anisotropy =	9.2060
10	H	Isotropic =	30.4643	Anisotropy =	7.6594
11	H	Isotropic =	30.6069	Anisotropy =	7.4839
12	H	Isotropic =	30.1008	Anisotropy =	9.6020
13	H	Isotropic =	29.5289	Anisotropy =	7.3466
14	H	Isotropic =	28.7820	Anisotropy =	9.1626
15	H	Isotropic =	24.9694	Anisotropy =	29.3681
16	H	Isotropic =	30.9567	Anisotropy =	13.3183
17	H	Isotropic =	30.4952	Anisotropy =	16.1609

Conformer_20

C	0.977364661529	-0.794950688709	1.502308852448
C	1.077992066746	-0.751179200954	-0.007744190375
C	1.639705274401	0.579063645429	-0.503381058557
C	1.681174919100	0.691540629764	-2.021896185647
O	0.442459476941	-2.060556762248	1.889802445542
N	2.587083607113	-0.297558043779	-2.614502023848
H	0.327337073019	0.015919269880	1.858599350200
H	1.970432781145	-0.650404499548	1.949294290106
H	0.080474099736	-0.914044441244	-0.435592133725
H	1.712654381368	-1.582542876700	-0.337451467648
H	1.023148568305	1.398917713471	-0.114350785805
H	2.653005978987	0.724698430061	-0.107532198343
H	2.048275966834	1.685303651807	-2.296603933760
H	0.655775508145	0.607862162827	-2.414856532481

H	0.390611757242	-2.081243457496	2.849054372154
H	2.677721631849	-0.127053121081	-3.610504234256
H	2.195382247540	-1.229772411480	-2.525744566005

SCF Done: E(RwB97X) = -289.040485404

Zero-point correction=	0.156530
Thermal correction to Energy=	0.164391
Thermal correction to Enthalpy=	0.165335
Thermal correction to Gibbs Free Energy=	0.124606
Sum of electronic and zero-point Energies=	-288.883955
Sum of electronic and thermal Energies=	-288.876094
Sum of electronic and thermal Enthalpies=	-288.875150
Sum of electronic and thermal Free Energies=	-288.915879

1 C	Isotropic = 125.2269	Anisotropy = 65.7008
2 C	Isotropic = 160.5750	Anisotropy = 26.1194
3 C	Isotropic = 161.6598	Anisotropy = 19.1530
4 C	Isotropic = 148.1508	Anisotropy = 23.5404
5 O	Isotropic = 307.8360	Anisotropy = 108.0020
6 N	Isotropic = 236.6522	Anisotropy = 30.2695
7 H	Isotropic = 28.1922	Anisotropy = 4.9297
8 H	Isotropic = 28.2094	Anisotropy = 4.8177
9 H	Isotropic = 30.5811	Anisotropy = 6.3196
10 H	Isotropic = 30.1162	Anisotropy = 4.5759
11 H	Isotropic = 30.5815	Anisotropy = 8.1370
12 H	Isotropic = 30.6329	Anisotropy = 7.4264
13 H	Isotropic = 29.2047	Anisotropy = 8.4285
14 H	Isotropic = 29.0376	Anisotropy = 8.1371
15 H	Isotropic = 31.2050	Anisotropy = 20.3986
16 H	Isotropic = 30.6820	Anisotropy = 15.9902
17 H	Isotropic = 30.9103	Anisotropy = 11.9727

Conformer_21

C	0.453152959037	-0.894866548503	1.259393667675
C	1.498240969666	-0.671172055363	0.186988022568
C	1.123989501784	0.480777269229	-0.742351728024
C	2.189842870110	0.788405952146	-1.786181283873
O	0.871780821527	-1.978834050460	2.088729980789
N	2.387715906440	-0.335566803139	-2.706887479439
H	-0.516556412300	-1.124218251229	0.796862124901
H	0.331436694357	0.016640554378	1.860499975724
H	2.462015504830	-0.460419171131	0.667969248842
H	1.615707160124	-1.601057009898	-0.382383864496

H	0.955236880630	1.385933271431	-0.145809523438
H	0.179720915828	0.253500661656	-1.253611243940
H	3.120345919049	1.077322191394	-1.272804845836
H	1.870913881494	1.651484720847	-2.378778799447
H	0.198498386435	-2.117904934302	2.760020097436
H	3.019375765930	-0.061992823685	-3.452186545020
H	2.840382275059	-1.106932973371	-2.226867804423

SCF Done: E(RwB97X) = -289.040485404

Zero-point correction=	0.156530
Thermal correction to Energy=	0.164391
Thermal correction to Enthalpy=	0.165335
Thermal correction to Gibbs Free Energy=	0.124606
Sum of electronic and zero-point Energies=	-288.883955
Sum of electronic and thermal Energies=	-288.876094
Sum of electronic and thermal Enthalpies=	-288.875150
Sum of electronic and thermal Free Energies=	-288.915879

1 C	Isotropic = 125.2269	Anisotropy = 65.7008
2 C	Isotropic = 160.5750	Anisotropy = 26.1194
3 C	Isotropic = 161.6599	Anisotropy = 19.1530
4 C	Isotropic = 148.1508	Anisotropy = 23.5404
5 O	Isotropic = 307.8360	Anisotropy = 108.0020
6 N	Isotropic = 236.6522	Anisotropy = 30.2695
7 H	Isotropic = 28.2094	Anisotropy = 4.8177
8 H	Isotropic = 28.1922	Anisotropy = 4.9297
9 H	Isotropic = 30.5811	Anisotropy = 6.3196
10 H	Isotropic = 30.1162	Anisotropy = 4.5759
11 H	Isotropic = 30.5815	Anisotropy = 8.1370
12 H	Isotropic = 30.6329	Anisotropy = 7.4264
13 H	Isotropic = 29.0376	Anisotropy = 8.1371
14 H	Isotropic = 29.2047	Anisotropy = 8.4285
15 H	Isotropic = 31.2050	Anisotropy = 20.3986
16 H	Isotropic = 30.6820	Anisotropy = 15.9902
17 H	Isotropic = 30.9103	Anisotropy = 11.9727

Conformer_22

C	0.379875426053	-0.559982649256	1.675791146186
C	0.484359829538	-0.198185239294	0.203427635097
C	1.878917532312	0.258806528316	-0.213251401749
C	2.012655039766	0.545158302578	-1.704568039965
O	1.181519796435	-1.686588412768	2.032927414351
N	1.891443514497	-0.684113552409	-2.496312669175

H	-0.668076514575	-0.747504941232	1.943073225641
H	0.738167857388	0.265485382645	2.298789861598
H	0.173057559592	-1.060789695831	-0.399133454946
H	-0.238880338467	0.602355046171	-0.000290865646
H	2.138009971498	1.168102316483	0.343500622414
H	2.618436463168	-0.501076048508	0.069893031024
H	2.966446188612	1.062200500750	-1.884267139072
H	1.215124792123	1.228921183018	-2.018387811608
H	0.868625151817	-2.439420738420	1.522318099325
H	2.685211644794	-1.288070503522	-2.303389578361
H	1.939006085450	-0.464797478722	-3.485820075114

SCF Done: E(RwB97X) = -289.040100779

Zero-point correction=	0.156190
Thermal correction to Energy=	0.164114
Thermal correction to Enthalpy=	0.165058
Thermal correction to Gibbs Free Energy=	0.123812
Sum of electronic and zero-point Energies=	-288.883911
Sum of electronic and thermal Energies=	-288.875987
Sum of electronic and thermal Enthalpies=	-288.875043
Sum of electronic and thermal Free Energies=	-288.916289

1 C	Isotropic = 126.0783	Anisotropy = 54.5943
2 C	Isotropic = 157.9691	Anisotropy = 27.8896
3 C	Isotropic = 161.0459	Anisotropy = 26.0102
4 C	Isotropic = 147.9436	Anisotropy = 24.2462
5 O	Isotropic = 302.5383	Anisotropy = 89.0302
6 N	Isotropic = 238.0179	Anisotropy = 35.5926
7 H	Isotropic = 27.8985	Anisotropy = 7.5314
8 H	Isotropic = 28.4652	Anisotropy = 6.4155
9 H	Isotropic = 29.8770	Anisotropy = 4.9767
10 H	Isotropic = 30.5941	Anisotropy = 8.2413
11 H	Isotropic = 30.5266	Anisotropy = 8.5712
12 H	Isotropic = 30.1538	Anisotropy = 5.1996
13 H	Isotropic = 28.7217	Anisotropy = 9.1173
14 H	Isotropic = 29.4806	Anisotropy = 7.0786
15 H	Isotropic = 31.9786	Anisotropy = 16.6436
16 H	Isotropic = 31.5012	Anisotropy = 13.2424
17 H	Isotropic = 30.9008	Anisotropy = 16.0116

Conformer_23

C	0.670484357064	-0.503477728882	1.803591351814
C	1.543098645467	0.008734064938	0.669637070555

C	0.827086935629	0.052995926115	-0.676699592489
C	1.718966423769	0.487874474698	-1.833998043900
O	0.273436674487	-1.864551252244	1.632554906510
N	2.750869531493	-0.515717963619	-2.117967424953
H	1.191820528661	-0.384139552266	2.762118919695
H	-0.260189456777	0.069832483402	1.858911130784
H	2.441689756051	-0.617165365982	0.599930088290
H	1.885126238723	1.017642832419	0.935273722162
H	-0.021082490187	0.745635572856	-0.607563091695
H	0.405268343745	-0.934074489632	-0.905263552831
H	1.089059408160	0.695164284323	-2.711261041009
H	2.222999664509	1.426279234345	-1.574352150834
H	1.072419705445	-2.399872031939	1.611595132766
H	2.310265967459	-1.361158124255	-2.468896018335
H	3.358979766302	-0.186602364276	-2.860511406530

SCF Done: E(RwB97X) = -289.040100781

Zero-point correction=	0.156190
Thermal correction to Energy=	0.164113
Thermal correction to Enthalpy=	0.165058
Thermal correction to Gibbs Free Energy=	0.123812
Sum of electronic and zero-point Energies=	-288.883911
Sum of electronic and thermal Energies=	-288.875987
Sum of electronic and thermal Enthalpies=	-288.875043
Sum of electronic and thermal Free Energies=	-288.916289

1 C	Isotropic =	126.0781	Anisotropy =	54.5943
2 C	Isotropic =	157.9691	Anisotropy =	27.8891
3 C	Isotropic =	161.0459	Anisotropy =	26.0094
4 C	Isotropic =	147.9434	Anisotropy =	24.2461
5 O	Isotropic =	302.5381	Anisotropy =	89.0309
6 N	Isotropic =	238.0180	Anisotropy =	35.5921
7 H	Isotropic =	27.8985	Anisotropy =	7.5314
8 H	Isotropic =	28.4652	Anisotropy =	6.4155
9 H	Isotropic =	29.8769	Anisotropy =	4.9768
10 H	Isotropic =	30.5941	Anisotropy =	8.2412
11 H	Isotropic =	30.5266	Anisotropy =	8.5711
12 H	Isotropic =	30.1537	Anisotropy =	5.1996
13 H	Isotropic =	28.7217	Anisotropy =	9.1173
14 H	Isotropic =	29.4806	Anisotropy =	7.0786
15 H	Isotropic =	31.9786	Anisotropy =	16.6435
16 H	Isotropic =	31.5012	Anisotropy =	13.2424
17 H	Isotropic =	30.9008	Anisotropy =	16.0115

Conformer_24

C	1.003456150322	-0.556007048986	1.866226074921
C	1.030639440155	0.071359803807	0.481554003769
C	1.676884248587	-0.817493449116	-0.578814024368
C	1.687400304362	-0.192747355148	-1.968760341364
O	0.188990115863	-1.725282273548	1.944459501608
N	2.488043679547	1.035345200991	-2.005250868232
H	0.578985078711	0.146240371807	2.587960725492
H	2.026711171476	-0.788901274660	2.193121468367
H	1.583950629837	1.015303381603	0.564256071518
H	0.004932248830	0.323632306152	0.182102246853
H	1.139098334158	-1.771982247924	-0.646924588577
H	2.708382637578	-1.049345118582	-0.281852795323
H	2.131151079387	-0.900717067421	-2.675506207016
H	0.648384432351	-0.024720437695	-2.292864055579
H	0.584889215387	-2.404068245093	1.390551626336
H	2.577497080889	1.357785201882	-2.963061536607
H	2.012704152560	1.779598251931	-1.504597301797

SCF Done: E(RwB97X) = -289.040666854

Zero-point correction=	0.156690
Thermal correction to Energy=	0.164412
Thermal correction to Enthalpy=	0.165356
Thermal correction to Gibbs Free Energy=	0.124823
Sum of electronic and zero-point Energies=	-288.883977
Sum of electronic and thermal Energies=	-288.876255
Sum of electronic and thermal Enthalpies=	-288.875311
Sum of electronic and thermal Free Energies=	-288.915844

1	C	Isotropic =	126.1392	Anisotropy =	54.2784
2	C	Isotropic =	159.4143	Anisotropy =	21.5264
3	C	Isotropic =	161.3931	Anisotropy =	21.2417
4	C	Isotropic =	148.4854	Anisotropy =	24.2080
5	O	Isotropic =	306.6438	Anisotropy =	14.9972
6	N	Isotropic =	236.8598	Anisotropy =	30.1606
7	H	Isotropic =	28.1299	Anisotropy =	7.0156
8	H	Isotropic =	28.2476	Anisotropy =	6.8334
9	H	Isotropic =	30.3089	Anisotropy =	6.5605
10	H	Isotropic =	30.5875	Anisotropy =	7.3555
11	H	Isotropic =	30.2573	Anisotropy =	7.0588
12	H	Isotropic =	30.7160	Anisotropy =	7.6399
13	H	Isotropic =	29.1452	Anisotropy =	8.3390
14	H	Isotropic =	29.0960	Anisotropy =	8.1497
15	H	Isotropic =	30.9977	Anisotropy =	15.6311

16 H Isotropic = 30.6629 Anisotropy = 16.0440
 17 H Isotropic = 30.9477 Anisotropy = 12.1079

Conformer_25

C	0.405500005273	-0.489651096843	1.658052840800
C	1.358638472116	0.034611057639	0.595825898739
C	1.341443098964	-0.780298164476	-0.695579935948
C	2.309410317686	-0.261751230987	-1.752235911607
O	0.749978071643	-1.788137119420	2.139686228219
N	1.960129948940	1.093923207448	-2.188948050393
H	0.424615369927	0.163067306687	2.534307701783
H	-0.623070019327	-0.493839574408	1.270523088929
H	2.376025560028	0.059229039804	1.007774748242
H	1.070551503471	1.072322774362	0.385624511157
H	0.325043406927	-0.784523568367	-1.111329144590
H	1.607256042792	-1.824114706590	-0.484181484236
H	3.335679714645	-0.322866670489	-1.357434172595
H	2.265664206458	-0.915601855007	-2.628701025174
H	0.654555230101	-2.412002813515	1.414436392951
H	2.161240525499	1.762994531885	-1.452463061079
H	2.543438544857	1.361838882277	-2.974658625199

SCF Done: E(RwB97X) = -289.040666865

Zero-point correction=	0.156688
Thermal correction to Energy=	0.164411
Thermal correction to Enthalpy=	0.165355
Thermal correction to Gibbs Free Energy=	0.124819
Sum of electronic and zero-point Energies=	-288.883978
Sum of electronic and thermal Energies=	-288.876256
Sum of electronic and thermal Enthalpies=	-288.875312
Sum of electronic and thermal Free Energies=	-288.915848

1 C	Isotropic = 126.1348	Anisotropy = 54.2728
2 C	Isotropic = 159.4162	Anisotropy = 21.5314
3 C	Isotropic = 161.3915	Anisotropy = 21.2356
4 C	Isotropic = 148.4876	Anisotropy = 24.2103
5 O	Isotropic = 306.6408	Anisotropy = 15.0131
6 N	Isotropic = 236.8573	Anisotropy = 30.1663
7 H	Isotropic = 28.1298	Anisotropy = 7.0153
8 H	Isotropic = 28.2475	Anisotropy = 6.8328
9 H	Isotropic = 30.5873	Anisotropy = 7.3573
10 H	Isotropic = 30.3090	Anisotropy = 6.5613
11 H	Isotropic = 30.7161	Anisotropy = 7.6379

12	H	Isotropic =	30.2566	Anisotropy =	7.0584
13	H	Isotropic =	29.0961	Anisotropy =	8.1495
14	H	Isotropic =	29.1452	Anisotropy =	8.3396
15	H	Isotropic =	30.9980	Anisotropy =	15.6296
16	H	Isotropic =	30.9473	Anisotropy =	12.1065
17	H	Isotropic =	30.6629	Anisotropy =	16.0439

Conformer_26

C	0.718219404219	-0.485965383413	1.723452818093
C	0.729444097639	-0.240965777294	0.223845637483
C	2.076522270259	-0.529740962497	-0.431323470403
C	2.098239455661	-0.277103226206	-1.934197421055
O	0.981471160271	-1.844786360336	2.075510111990
N	1.893519159183	1.142144788352	-2.242916451192
H	-0.243412755706	-0.169672040407	2.148209730799
H	1.503654467265	0.101028506313	2.209766674376
H	-0.051244058099	-0.856275697670	-0.246196284048
H	0.446495300603	0.803830901806	0.052547471506
H	2.354838509660	-1.573777733922	-0.250973450189
H	2.853201637709	0.085661358786	0.044773224701
H	1.291232592630	-0.846376844825	-2.410338922272
H	3.044287539517	-0.659179278591	-2.344702856890
H	0.287780636091	-2.386447744152	1.687308631282
H	2.682580016071	1.680329440037	-1.896742603021
H	1.878170567025	1.279096054019	-3.248022841158

SCF Done: E(RwB97X) = -289.040302765

Zero-point correction=	0.156279
Thermal correction to Energy=	0.164218
Thermal correction to Enthalpy=	0.165162
Thermal correction to Gibbs Free Energy=	0.123603
Sum of electronic and zero-point Energies=	-288.884024
Sum of electronic and thermal Energies=	-288.876085
Sum of electronic and thermal Enthalpies=	-288.875141
Sum of electronic and thermal Free Energies=	-288.916700

1	C	Isotropic =	125.3877	Anisotropy =	54.4415
2	C	Isotropic =	157.8523	Anisotropy =	21.9617
3	C	Isotropic =	161.0441	Anisotropy =	20.5811
4	C	Isotropic =	147.7187	Anisotropy =	24.1854
5	O	Isotropic =	303.2187	Anisotropy =	89.5625
6	N	Isotropic =	238.1695	Anisotropy =	34.9426
7	H	Isotropic =	27.8451	Anisotropy =	7.3314

8 H	Isotropic =	28.4928	Anisotropy =	6.2152
9 H	Isotropic =	30.6384	Anisotropy =	7.0061
10 H	Isotropic =	29.8352	Anisotropy =	6.6245
11 H	Isotropic =	29.9458	Anisotropy =	6.9349
12 H	Isotropic =	30.7101	Anisotropy =	7.0079
13 H	Isotropic =	29.5164	Anisotropy =	7.1111
14 H	Isotropic =	28.6858	Anisotropy =	8.9478
15 H	Isotropic =	31.9810	Anisotropy =	17.0319
16 H	Isotropic =	31.5165	Anisotropy =	13.4918
17 H	Isotropic =	30.8830	Anisotropy =	15.9111

Conformer_27

C	1.015380690750	-0.576171161123	1.801447153110
C	1.812935489591	-0.570668348622	0.508060285989
C	0.984879571581	-0.197332346868	-0.717582741535
C	1.780330336502	-0.180387722826	-2.017543545173
O	-0.046005674644	-1.531721739698	1.806185910861
N	2.811596284957	0.862559247956	-2.002221922097
H	1.683639046609	-0.756008433319	2.653670969341
H	0.536423376391	0.395764397397	1.956083368668
H	2.642299234192	0.135499466910	0.628417208496
H	2.266260033964	-1.561679415696	0.361726669260
H	0.531780161007	0.792496629750	-0.564095923070
H	0.155159263191	-0.904033229712	-0.827750822078
H	2.279528153552	-1.147354613644	-2.151033781269
H	1.082399272218	-0.062027839363	-2.859200851259
H	0.346173141097	-2.403971716071	1.702844323724
H	2.367747670108	1.776111336129	-1.979479613803
H	3.348373948934	0.831325488800	-2.862526689167

SCF Done: E(RwB97X) = -289.040302766

Zero-point correction=	0.156279
Thermal correction to Energy=	0.164218
Thermal correction to Enthalpy=	0.165162
Thermal correction to Gibbs Free Energy=	0.123603
Sum of electronic and zero-point Energies=	-288.884024
Sum of electronic and thermal Energies=	-288.876085
Sum of electronic and thermal Enthalpies=	-288.875141
Sum of electronic and thermal Free Energies=	-288.916700

1 C	Isotropic =	125.3878	Anisotropy =	54.4415
2 C	Isotropic =	157.8521	Anisotropy =	21.9617
3 C	Isotropic =	161.0442	Anisotropy =	20.5814

4	C	Isotropic =	147.7186	Anisotropy =	24.1852
5	O	Isotropic =	303.2187	Anisotropy =	89.5624
6	N	Isotropic =	238.1695	Anisotropy =	34.9424
7	H	Isotropic =	27.8451	Anisotropy =	7.3314
8	H	Isotropic =	28.4928	Anisotropy =	6.2152
9	H	Isotropic =	29.8352	Anisotropy =	6.6245
10	H	Isotropic =	30.6384	Anisotropy =	7.0060
11	H	Isotropic =	30.7101	Anisotropy =	7.0080
12	H	Isotropic =	29.9458	Anisotropy =	6.9348
13	H	Isotropic =	29.5164	Anisotropy =	7.1110
14	H	Isotropic =	28.6858	Anisotropy =	8.9478
15	H	Isotropic =	31.9810	Anisotropy =	17.0319
16	H	Isotropic =	31.5165	Anisotropy =	13.4918
17	H	Isotropic =	30.8830	Anisotropy =	15.9111

Conformer_28

C	0.374268203966	-0.672269333483	1.431059290598
C	1.418816933167	-0.580657680241	0.331921169154
C	1.104911525776	0.537425665388	-0.659447444098
C	2.175239074061	0.721929395553	-1.727489968738
O	0.659791909049	-1.692424414335	2.385781130849
N	2.296628004813	-0.462428884231	-2.583431624180
H	0.337406334707	0.263150213151	1.997197719696
H	-0.620362630994	-0.832655025522	0.992238293569
H	1.466121180827	-1.546432027980	-0.189085296340
H	2.402526226183	-0.409564428929	0.787553287740
H	0.997112803400	1.482500028040	-0.112664202620
H	0.142881437950	0.339195539539	-1.149163212984
H	3.126708845491	0.984432128402	-1.239047387691
H	1.900379299554	1.567019563334	-2.366278969214
H	0.672912612267	-2.534182072435	1.920673954822
H	2.713013825738	-1.229192096060	-2.064726003160
H	2.931444414046	-0.268146570190	-3.350590737402

SCF Done: E(RwB97X) = -289.040825851

Zero-point correction=	0.156711
Thermal correction to Energy=	0.164474
Thermal correction to Enthalpy=	0.165418
Thermal correction to Gibbs Free Energy=	0.124987
Sum of electronic and zero-point Energies=	-288.884115
Sum of electronic and thermal Energies=	-288.876352
Sum of electronic and thermal Enthalpies=	-288.875408
Sum of electronic and thermal Free Energies=	-288.915839

1 C	Isotropic =	124.6100	Anisotropy =	67.1550
2 C	Isotropic =	157.5298	Anisotropy =	31.1400
3 C	Isotropic =	161.7915	Anisotropy =	19.5648
4 C	Isotropic =	148.2844	Anisotropy =	23.7137
5 O	Isotropic =	296.8246	Anisotropy =	46.8626
6 N	Isotropic =	236.7043	Anisotropy =	30.2055
7 H	Isotropic =	28.3944	Anisotropy =	4.6318
8 H	Isotropic =	28.1778	Anisotropy =	4.9257
9 H	Isotropic =	30.2599	Anisotropy =	4.0040
10 H	Isotropic =	30.5451	Anisotropy =	5.9710
11 H	Isotropic =	30.6141	Anisotropy =	8.0876
12 H	Isotropic =	30.6492	Anisotropy =	7.3117
13 H	Isotropic =	29.0561	Anisotropy =	8.1365
14 H	Isotropic =	29.2186	Anisotropy =	8.4454
15 H	Isotropic =	31.4828	Anisotropy =	16.1003
16 H	Isotropic =	30.9583	Anisotropy =	12.0175
17 H	Isotropic =	30.6949	Anisotropy =	15.9820

Conformer_29

C	0.865078054687	-0.588790519901	1.651747769724
C	0.990349373660	-0.653418313040	0.139230338471
C	1.601838389578	0.621991790188	-0.435982340253
C	1.662616842109	0.634919485807	-1.957986840976
O	0.271058523125	-1.758489004877	2.210926102320
N	2.539169879025	-0.421045233071	-2.474387944619
H	1.851136727658	-0.412458675884	2.103603692636
H	0.216173915579	0.242568622356	1.942688238876
H	1.608128266985	-1.522208450906	-0.125266179244
H	-0.004130149740	-0.818599857201	-0.294685768510
H	2.615177120156	0.759549488690	-0.037433340335
H	1.008736384317	1.484558929461	-0.107400690552
H	2.067532322304	1.595582747795	-2.291073271570
H	0.639054239390	0.561677143408	-2.357653855410
H	0.835095022986	-2.506582995436	1.993506667588
H	2.111966681632	-1.331227548084	-2.335016111233
H	2.649418406550	-0.315927609303	-3.477416466915

SCF Done: E(RwB97X) = -289.040825852

Zero-point correction=	0.156711
Thermal correction to Energy=	0.164474
Thermal correction to Enthalpy=	0.165418
Thermal correction to Gibbs Free Energy=	0.124987

Sum of electronic and zero-point Energies=	-288.884115
Sum of electronic and thermal Energies=	-288.876352
Sum of electronic and thermal Enthalpies=	-288.875408
Sum of electronic and thermal Free Energies=	-288.915839

1 C	Isotropic =	124.6100	Anisotropy =	67.1550
2 C	Isotropic =	157.5297	Anisotropy =	31.1401
3 C	Isotropic =	161.7917	Anisotropy =	19.5646
4 C	Isotropic =	148.2842	Anisotropy =	23.7134
5 O	Isotropic =	296.8242	Anisotropy =	46.8643
6 N	Isotropic =	236.7042	Anisotropy =	30.2055
7 H	Isotropic =	28.1778	Anisotropy =	4.9258
8 H	Isotropic =	28.3944	Anisotropy =	4.6318
9 H	Isotropic =	30.2599	Anisotropy =	4.0040
10 H	Isotropic =	30.5451	Anisotropy =	5.9710
11 H	Isotropic =	30.6492	Anisotropy =	7.3117
12 H	Isotropic =	30.6141	Anisotropy =	8.0876
13 H	Isotropic =	29.2186	Anisotropy =	8.4454
14 H	Isotropic =	29.0561	Anisotropy =	8.1364
15 H	Isotropic =	31.4828	Anisotropy =	16.1002
16 H	Isotropic =	30.9583	Anisotropy =	12.0173
17 H	Isotropic =	30.6949	Anisotropy =	15.9820

Conformer_3

C	0.397592381550	-0.669301246861	1.482344531949
C	1.274403081414	0.491507849284	1.023466088569
C	1.174610579649	0.837575254474	-0.469455497494
C	1.224203550553	-0.344385404683	-1.434100502265
O	0.979938442093	-1.945936704182	1.240806862552
N	2.349634617964	-1.241601195917	-1.140757668116
H	0.227471579845	-0.600755804623	2.561759371121
H	-0.588762905738	-0.607070313124	0.995959477473
H	2.311547472701	0.261088153233	1.295399581440
H	0.999714041778	1.384016061788	1.596449797169
H	0.235462093010	1.371861489734	-0.655181771922
H	1.980549041870	1.538785896430	-0.719356005351
H	0.303345258936	-0.932412604145	-1.344829879085
H	1.254809551707	0.041497204403	-2.461511415102
H	1.559309967336	-1.864174244707	0.457880571469
H	3.223870754384	-0.723915016425	-1.156884631987
H	2.424300490949	-1.953879374678	-1.859888910419

SCF Done: E(RwB97X) = -289.044016456

Zero-point correction=	0.157733
Thermal correction to Energy=	0.164770
Thermal correction to Enthalpy=	0.165714
Thermal correction to Gibbs Free Energy=	0.127175
Sum of electronic and zero-point Energies=	-288.886283
Sum of electronic and thermal Energies=	-288.879246
Sum of electronic and thermal Enthalpies=	-288.878302
Sum of electronic and thermal Free Energies=	-288.916842

1 C	Isotropic =	128.0732	Anisotropy =	57.8977
2 C	Isotropic =	162.5288	Anisotropy =	28.5840
3 C	Isotropic =	161.9350	Anisotropy =	12.1311
4 C	Isotropic =	151.5916	Anisotropy =	31.1780
5 O	Isotropic =	293.1663	Anisotropy =	61.1918
6 N	Isotropic =	234.7734	Anisotropy =	30.2027
7 H	Isotropic =	28.2342	Anisotropy =	8.0491
8 H	Isotropic =	28.2079	Anisotropy =	6.4544
9 H	Isotropic =	30.0926	Anisotropy =	6.5274
10 H	Isotropic =	30.2176	Anisotropy =	9.7185
11 H	Isotropic =	30.3725	Anisotropy =	9.6182
12 H	Isotropic =	30.1691	Anisotropy =	9.2699
13 H	Isotropic =	29.1634	Anisotropy =	6.8762
14 H	Isotropic =	28.8371	Anisotropy =	9.4919
15 H	Isotropic =	26.3930	Anisotropy =	26.9636
16 H	Isotropic =	31.0531	Anisotropy =	13.4151
17 H	Isotropic =	30.6509	Anisotropy =	16.2217

Conformer_30

C	0.000269794898	-0.712895542574	1.277404676025
C	0.843589629729	0.481116646773	0.853973226897
C	1.915274575630	0.168870881566	-0.190968969407
C	1.358634547891	-0.295385756949	-1.531057937229
O	0.763051150728	-1.745143197897	1.901562309818
N	2.442534095769	-0.475595576759	-2.500387955505
H	-0.734851496161	-0.398485292935	2.022494225499
H	-0.555810018133	-1.122354983406	0.423460353697
H	0.163367535814	1.248828318694	0.463243976377
H	1.320250468452	0.903430461406	1.746014783079
H	2.513811361838	1.073196920542	-0.357630234931
H	2.615751189437	-0.587194300950	0.188169382099
H	0.601560641792	0.428032303954	-1.872111670557
H	0.848942765595	-1.258615255246	-1.418928559066
H	1.371241134051	-2.104230010000	1.248914813521
H	2.869100780514	0.423083571481	-2.705537487496

H 2.070781842157 -0.819459187700 -3.379614932824

SCF Done: E(RwB97X) = -289.040235079

Zero-point correction= 0.156451
Thermal correction to Energy= 0.164321
Thermal correction to Enthalpy= 0.165265
Thermal correction to Gibbs Free Energy= 0.124265
Sum of electronic and zero-point Energies= -288.883784
Sum of electronic and thermal Energies= -288.875914
Sum of electronic and thermal Enthalpies= -288.874970
Sum of electronic and thermal Free Energies= -288.915970

1 C	Isotropic =	130.0766	Anisotropy =	63.8263
2 C	Isotropic =	159.8276	Anisotropy =	15.1763
3 C	Isotropic =	163.5619	Anisotropy =	33.9568
4 C	Isotropic =	148.7078	Anisotropy =	35.5441
5 O	Isotropic =	311.4548	Anisotropy =	18.6682
6 N	Isotropic =	234.9776	Anisotropy =	38.2225
7 H	Isotropic =	28.3781	Anisotropy =	7.4730
8 H	Isotropic =	28.1706	Anisotropy =	5.7248
9 H	Isotropic =	30.4940	Anisotropy =	8.4145
10 H	Isotropic =	30.1322	Anisotropy =	9.1802
11 H	Isotropic =	30.5320	Anisotropy =	7.6007
12 H	Isotropic =	30.2600	Anisotropy =	5.1859
13 H	Isotropic =	29.2491	Anisotropy =	6.8470
14 H	Isotropic =	29.1206	Anisotropy =	5.9345
15 H	Isotropic =	30.9901	Anisotropy =	15.5818
16 H	Isotropic =	31.1631	Anisotropy =	13.1839
17 H	Isotropic =	30.6857	Anisotropy =	15.8795

Conformer_4

C	0.889584594794	-0.587318220284	1.688524418978
C	0.307305940132	0.330322808443	0.618135999124
C	1.317358967747	0.861356309414	-0.409643897664
C	2.283800682437	-0.167803085382	-0.990033009290
O	1.025945620129	-1.938280518216	1.260072001151
N	1.583037455187	-1.369369952295	-1.462060123468
H	1.864018683750	-0.198305691092	2.023915900815
H	0.231371470717	-0.600117297484	2.563377436308
H	-0.157166199326	1.191201486218	1.111582140661
H	-0.504793394115	-0.208288229968	0.115043084831
H	1.920382718861	1.652659463524	0.050961875429
H	0.763731642269	1.335983037232	-1.229344904057

H	2.994027584904	-0.483996381227	-0.217164991665
H	2.872277027598	0.311054171483	-1.783636608347
H	1.165125633748	-1.929880536555	0.292658624879
H	2.231787196319	-1.985969205454	-1.940593483506
H	0.872204374850	-1.115848158357	-2.142494464179

SCF Done: E(RwB97X) = -289.044016457

Zero-point correction=	0.157733
Thermal correction to Energy=	0.164770
Thermal correction to Enthalpy=	0.165714
Thermal correction to Gibbs Free Energy=	0.127175
Sum of electronic and zero-point Energies=	-288.886283
Sum of electronic and thermal Energies=	-288.879246
Sum of electronic and thermal Enthalpies=	-288.878302
Sum of electronic and thermal Free Energies=	-288.916842

1 C	Isotropic = 128.0732	Anisotropy = 57.8977
2 C	Isotropic = 162.5288	Anisotropy = 28.5840
3 C	Isotropic = 161.9351	Anisotropy = 12.1310
4 C	Isotropic = 151.5916	Anisotropy = 31.1780
5 O	Isotropic = 293.1663	Anisotropy = 61.1917
6 N	Isotropic = 234.7734	Anisotropy = 30.2029
7 H	Isotropic = 28.2079	Anisotropy = 6.4544
8 H	Isotropic = 28.2342	Anisotropy = 8.0491
9 H	Isotropic = 30.2176	Anisotropy = 9.7185
10 H	Isotropic = 30.0926	Anisotropy = 6.5274
11 H	Isotropic = 30.3725	Anisotropy = 9.6182
12 H	Isotropic = 30.1691	Anisotropy = 9.2698
13 H	Isotropic = 29.1634	Anisotropy = 6.8762
14 H	Isotropic = 28.8371	Anisotropy = 9.4919
15 H	Isotropic = 26.3930	Anisotropy = 26.9636
16 H	Isotropic = 30.6509	Anisotropy = 16.2217
17 H	Isotropic = 31.0531	Anisotropy = 13.4151

Conformer_5

C	1.231597910595	-0.622605055531	1.645135403847
C	0.645858757211	0.580170963172	0.911355874289
C	0.714412694771	0.516368938706	-0.621274741185
C	2.056896437161	0.068355420315	-1.199731860137
O	0.726585719892	-1.866947484949	1.185585439187
N	2.168963480690	-1.401750396511	-1.202801933522
H	0.994015770934	-0.549622114594	2.711108516250
H	2.327679797276	-0.612794240277	1.559197117295

H	1.186531349275	1.469400678054	1.261510488064
H	-0.400622593916	0.711315173002	1.211725418991
H	0.469397109034	1.508397945380	-1.015766006684
H	-0.061122997636	-0.159518216965	-1.002758994181
H	2.878918748171	0.471464296461	-0.598232058033
H	2.172945069393	0.477505694308	-2.211333937424
H	1.163021073619	-1.990347298406	0.319939385758
H	1.642284268659	-1.775007955568	-1.987403326093
H	3.132937404873	-1.680486346598	-1.354354786421

SCF Done: E(RwB97X) = -289.044572756

Zero-point correction=	0.157991
Thermal correction to Energy=	0.164969
Thermal correction to Enthalpy=	0.165913
Thermal correction to Gibbs Free Energy=	0.127586
Sum of electronic and zero-point Energies=	-288.886582
Sum of electronic and thermal Energies=	-288.879604
Sum of electronic and thermal Enthalpies=	-288.878660
Sum of electronic and thermal Free Energies=	-288.916987

1 C	Isotropic = 132.1014	Anisotropy = 59.8453
2 C	Isotropic = 159.0511	Anisotropy = 11.4570
3 C	Isotropic = 163.9245	Anisotropy = 28.1884
4 C	Isotropic = 150.7546	Anisotropy = 29.1886
5 O	Isotropic = 296.3514	Anisotropy = 63.8075
6 N	Isotropic = 230.4268	Anisotropy = 30.9082
7 H	Isotropic = 28.3484	Anisotropy = 7.6982
8 H	Isotropic = 28.0954	Anisotropy = 6.3478
9 H	Isotropic = 30.6344	Anisotropy = 9.2390
10 H	Isotropic = 30.1456	Anisotropy = 9.3328
11 H	Isotropic = 30.3038	Anisotropy = 9.8519
12 H	Isotropic = 30.4397	Anisotropy = 6.5555
13 H	Isotropic = 29.3810	Anisotropy = 6.6261
14 H	Isotropic = 28.8981	Anisotropy = 9.7935
15 H	Isotropic = 26.5436	Anisotropy = 25.8774
16 H	Isotropic = 30.8923	Anisotropy = 13.9459
17 H	Isotropic = 30.4820	Anisotropy = 15.7847

Conformer_6

C	0.205840480593	-0.853558528490	1.202801502597
C	0.641200679887	0.579103500467	0.909316830955
C	1.690890495434	0.736207000444	-0.200276052263
C	1.428622349939	-0.073060752057	-1.470666832114

O	1.291160707632	-1.739873178490	1.428938954618
N	1.896870136107	-1.462982018332	-1.320193373184
H	-0.417421612816	-0.867421040227	2.102480679324
H	-0.414467450990	-1.230143522571	0.376799656982
H	-0.260546477451	1.143606273107	0.637557093361
H	1.030032786147	1.033361649930	1.828557236611
H	1.756036836801	1.798068007258	-0.461014722747
H	2.681797657102	0.457993096059	0.179867886377
H	1.913440080220	0.419129926433	-2.323257117499
H	0.354911297229	-0.096737892766	-1.686545314186
H	1.670323133443	-1.876147831693	0.538595819897
H	2.905067542989	-1.490686177898	-1.443002577510
H	1.508941357736	-2.046058511175	-2.054659671219

SCF Done: E(RwB97X) = -289.044572756

Zero-point correction=	0.157991
Thermal correction to Energy=	0.164969
Thermal correction to Enthalpy=	0.165913
Thermal correction to Gibbs Free Energy=	0.127586
Sum of electronic and zero-point Energies=	-288.886582
Sum of electronic and thermal Energies=	-288.879604
Sum of electronic and thermal Enthalpies=	-288.878660
Sum of electronic and thermal Free Energies=	-288.916987

1 C	Isotropic = 132.1014	Anisotropy = 59.8454
2 C	Isotropic = 159.0511	Anisotropy = 11.4570
3 C	Isotropic = 163.9245	Anisotropy = 28.1885
4 C	Isotropic = 150.7547	Anisotropy = 29.1887
5 O	Isotropic = 296.3515	Anisotropy = 63.8071
6 N	Isotropic = 230.4268	Anisotropy = 30.9083
7 H	Isotropic = 28.3484	Anisotropy = 7.6982
8 H	Isotropic = 28.0954	Anisotropy = 6.3478
9 H	Isotropic = 30.6344	Anisotropy = 9.2390
10 H	Isotropic = 30.1456	Anisotropy = 9.3328
11 H	Isotropic = 30.3038	Anisotropy = 9.8519
12 H	Isotropic = 30.4397	Anisotropy = 6.5555
13 H	Isotropic = 28.8981	Anisotropy = 9.7935
14 H	Isotropic = 29.3810	Anisotropy = 6.6261
15 H	Isotropic = 26.5436	Anisotropy = 25.8773
16 H	Isotropic = 30.8923	Anisotropy = 13.9459
17 H	Isotropic = 30.4820	Anisotropy = 15.7847

Conformer_7

C	0.179294402764	-0.542157691633	1.706051065733
C	1.017121277327	0.270492594358	0.731980979415
C	1.301243005171	-0.451544276342	-0.581915335484
C	2.100975710357	0.400409966256	-1.556735145603
O	0.832868479282	-1.725344251787	2.164816098724
N	2.342446666592	-0.324575141748	-2.807281757481
H	-0.027471396483	0.046181861048	2.603473281532
H	-0.785977946903	-0.800369358953	1.248364440034
H	0.474493155435	1.201949988057	0.525235051356
H	1.959267039423	0.550186698224	1.219716820120
H	0.355226767207	-0.745179087923	-1.055137348023
H	1.863429696858	-1.376942996336	-0.393203935331
H	1.535459594989	1.308652952765	-1.793651934317
H	3.034053797007	0.721991148944	-1.069001135494
H	0.940215649777	-2.317476334971	1.415071015794
H	2.856726199280	0.263000662115	-3.455395763035
H	2.936027901917	-1.128476732072	-2.624586397941

SCF Done: E(RwB97X) = -289.040842375

Zero-point correction=	0.156420
Thermal correction to Energy=	0.164265
Thermal correction to Enthalpy=	0.165209
Thermal correction to Gibbs Free Energy=	0.124515
Sum of electronic and zero-point Energies=	-288.884423
Sum of electronic and thermal Energies=	-288.876578
Sum of electronic and thermal Enthalpies=	-288.875633
Sum of electronic and thermal Free Energies=	-288.916327

1 C	Isotropic = 126.0847	Anisotropy = 53.7720
2 C	Isotropic = 158.5281	Anisotropy = 22.1795
3 C	Isotropic = 159.9572	Anisotropy = 28.7245
4 C	Isotropic = 146.0339	Anisotropy = 37.6843
5 O	Isotropic = 306.1537	Anisotropy = 17.1140
6 N	Isotropic = 234.7853	Anisotropy = 39.0749
7 H	Isotropic = 28.1883	Anisotropy = 7.1551
8 H	Isotropic = 28.1835	Anisotropy = 6.8918
9 H	Isotropic = 30.5903	Anisotropy = 7.7628
10 H	Isotropic = 30.3527	Anisotropy = 7.0983
11 H	Isotropic = 30.6372	Anisotropy = 6.3525
12 H	Isotropic = 30.3534	Anisotropy = 4.4764
13 H	Isotropic = 29.3550	Anisotropy = 5.9972
14 H	Isotropic = 29.0275	Anisotropy = 6.6556
15 H	Isotropic = 31.0140	Anisotropy = 15.7016
16 H	Isotropic = 30.6987	Anisotropy = 15.9258
17 H	Isotropic = 31.1349	Anisotropy = 12.7463

Conformer_8

C	0.682416395075	-0.429744982879	1.940761853198
C	0.628714916867	0.183636613578	0.550781244106
C	1.686323734792	-0.365487869597	-0.402272704798
C	1.641320776197	0.297656264585	-1.771172534237
O	0.384409184120	-1.825641536324	1.955575458432
N	2.677982459272	-0.249565655886	-2.650751552763
H	1.668078444035	-0.251864050232	2.393232522196
H	-0.066180326879	0.037469495128	2.585413511083
H	-0.373279746679	0.028755594720	0.131529269935
H	0.765897905260	1.267053131656	0.661196479191
H	2.684788250521	-0.224470681107	0.031651165582
H	1.548978916612	-1.447253916881	-0.539921882433
H	0.629793558974	0.184556952914	-2.190642242217
H	1.822121769746	1.372725237534	-1.659902143319
H	1.083085379216	-2.285586596896	1.481694021598
H	2.484077085849	-1.229495174431	-2.835448429144
H	2.650671297021	0.216957174117	-3.551524036409

SCF Done: E(RwB97X) = -289.040842374

Zero-point correction=	0.156420
Thermal correction to Energy=	0.164265
Thermal correction to Enthalpy=	0.165209
Thermal correction to Gibbs Free Energy=	0.124515
Sum of electronic and zero-point Energies=	-288.884423
Sum of electronic and thermal Energies=	-288.876578
Sum of electronic and thermal Enthalpies=	-288.875633
Sum of electronic and thermal Free Energies=	-288.916327

1	C	Isotropic =	126.0847	Anisotropy =	53.7720
2	C	Isotropic =	158.5281	Anisotropy =	22.1795
3	C	Isotropic =	159.9572	Anisotropy =	28.7245
4	C	Isotropic =	146.0339	Anisotropy =	37.6843
5	O	Isotropic =	306.1537	Anisotropy =	17.1140
6	N	Isotropic =	234.7853	Anisotropy =	39.0749
7	H	Isotropic =	28.1835	Anisotropy =	6.8918
8	H	Isotropic =	28.1883	Anisotropy =	7.1551
9	H	Isotropic =	30.3527	Anisotropy =	7.0983
10	H	Isotropic =	30.5903	Anisotropy =	7.7628
11	H	Isotropic =	30.6372	Anisotropy =	6.3525
12	H	Isotropic =	30.3534	Anisotropy =	4.4764
13	H	Isotropic =	29.0275	Anisotropy =	6.6556

14 H	Isotropic =	29.3550	Anisotropy =	5.9972
15 H	Isotropic =	31.0140	Anisotropy =	15.7016
16 H	Isotropic =	31.1349	Anisotropy =	12.7463
17 H	Isotropic =	30.6987	Anisotropy =	15.9258

Conformer_9

C	1.204422704196	-1.234921836279	1.439900078029
C	0.804901590934	-0.661570205647	0.096741404247
C	2.012857035671	-0.226264839391	-0.725980552102
C	1.620792004427	0.358876266749	-2.074817342525
O	0.021969950974	-1.622759286084	2.139570972597
N	2.809671183731	0.732666575538	-2.845853594455
H	1.863757444492	-2.102068200844	1.298426737075
H	1.757030659800	-0.483294183905	2.019965387329
H	0.232058192409	-1.418009220396	-0.453517261645
H	0.136805535388	0.192981154041	0.260739684131
H	2.595689056285	0.519641739358	-0.170994578497
H	2.675742450167	-1.086731811357	-0.890027426923
H	0.984302481976	-0.363910627624	-2.608199216872
H	1.017847038235	1.260631740122	-1.919913595328
H	0.282657037682	-1.984126492793	2.990801196378
H	3.333815679416	-0.103178659779	-3.087696051995
H	2.533879954217	1.155637888292	-3.725945839443

SCF Done: E(RwB97X) = -289.040619691

Zero-point correction=	0.156063
Thermal correction to Energy=	0.164159
Thermal correction to Enthalpy=	0.165103
Thermal correction to Gibbs Free Energy=	0.123833
Sum of electronic and zero-point Energies=	-288.884556
Sum of electronic and thermal Energies=	-288.876461
Sum of electronic and thermal Enthalpies=	-288.875517
Sum of electronic and thermal Free Energies=	-288.916787

1 C	Isotropic =	125.5898	Anisotropy =	65.7755
2 C	Isotropic =	159.8741	Anisotropy =	29.3336
3 C	Isotropic =	160.3991	Anisotropy =	29.8321
4 C	Isotropic =	146.1243	Anisotropy =	37.8650
5 O	Isotropic =	307.9655	Anisotropy =	107.9899
6 N	Isotropic =	234.8273	Anisotropy =	38.7196
7 H	Isotropic =	28.1944	Anisotropy =	4.8779
8 H	Isotropic =	28.1626	Anisotropy =	4.8751
9 H	Isotropic =	30.3627	Anisotropy =	5.8988

10	H	Isotropic =	30.3892	Anisotropy =	5.9525
11	H	Isotropic =	30.5626	Anisotropy =	6.0235
12	H	Isotropic =	30.6913	Anisotropy =	5.6531
13	H	Isotropic =	28.9963	Anisotropy =	6.5369
14	H	Isotropic =	29.3320	Anisotropy =	5.8853
15	H	Isotropic =	31.2334	Anisotropy =	20.3230
16	H	Isotropic =	31.1722	Anisotropy =	12.8867
17	H	Isotropic =	30.7152	Anisotropy =	15.8630

4-amino-butan-1-ol_protonated

Conformer_1

O	0.946539653008	1.707588952860	-0.446203940929
C	0.071418941547	0.810129325304	-1.156126818159
C	0.726905246353	-0.548516168108	-1.301791752396
C	0.884474692723	-1.386821998282	-0.027762468655
C	2.025558297682	-1.005139556637	0.904291787094
N	1.707515471943	0.207520376810	1.712979072044
H	0.560488216919	2.589358802686	-0.456005198761
H	-0.130589639590	1.225545449151	-2.147964435179
H	-0.880417645299	0.723261365096	-0.617185567500
H	1.700829140147	-0.426423651547	-1.791271599904
H	0.098683925591	-1.114195367545	-1.997818114526
H	-0.056662221386	-1.401710474813	0.537002785542
H	1.076467789252	-2.420989030064	-0.327566168022
H	2.232608752076	-1.806884713765	1.613108097792
H	2.939322299908	-0.783813577238	0.349428195456
H	0.915456744256	0.035733810780	2.335253289168
H	2.499583804214	0.486963926167	2.292990588687
H	1.459416530654	0.992092529146	1.080542248247

SCF Done: E(RwB97X) = -289.515630980

Zero-point correction=	0.172080
Thermal correction to Energy=	0.179524
Thermal correction to Enthalpy=	0.180468
Thermal correction to Gibbs Free Energy=	0.140726
Sum of electronic and zero-point Energies=	-289.343551
Sum of electronic and thermal Energies=	-289.336107
Sum of electronic and thermal Enthalpies=	-289.335163
Sum of electronic and thermal Free Energies=	-289.374905

1	O	Isotropic =	296.9564	Anisotropy =	83.2018
2	C	Isotropic =	125.0997	Anisotropy =	51.8762
3	C	Isotropic =	159.2826	Anisotropy =	10.3438

4	C	Isotropic =	161.9526	Anisotropy =	9.5819
5	C	Isotropic =	146.9070	Anisotropy =	23.6046
6	N	Isotropic =	218.1461	Anisotropy =	19.5798
7	H	Isotropic =	30.2210	Anisotropy =	20.8156
8	H	Isotropic =	27.7805	Anisotropy =	7.6684
9	H	Isotropic =	28.0925	Anisotropy =	7.3520
10	H	Isotropic =	30.1016	Anisotropy =	7.9983
11	H	Isotropic =	29.9709	Anisotropy =	9.9502
12	H	Isotropic =	30.2259	Anisotropy =	7.9375
13	H	Isotropic =	29.7530	Anisotropy =	10.0865
14	H	Isotropic =	28.5067	Anisotropy =	9.2203
15	H	Isotropic =	28.8994	Anisotropy =	7.8881
16	H	Isotropic =	27.7016	Anisotropy =	14.6283
17	H	Isotropic =	27.3803	Anisotropy =	17.2704
18	H	Isotropic =	22.9607	Anisotropy =	24.9008

Conformer_10

O	-0.170334508514	1.781473829443	-0.738392420361
C	0.682348496415	0.940225387577	-1.514451693150
C	0.440513401436	-0.502702422985	-1.113857233294
C	0.680127355609	-0.800282456920	0.365476339107
C	2.127973032914	-0.602141482173	0.775700826645
N	2.308913088365	-0.976361172809	2.209396321569
H	-0.005820535873	2.692569275620	-0.995280068770
H	1.732679145834	1.219738577674	-1.357851064053
H	0.464654095372	1.059382471210	-2.583055316127
H	1.084788874995	-1.138768810959	-1.732221651242
H	-0.593815126369	-0.765884737352	-1.359028982986
H	0.038460650742	-0.159666012185	0.980097888458
H	0.394137065590	-1.838515006147	0.568507141792
H	2.803438263078	-1.234429793217	0.197150992309
H	2.449568737029	0.435928093137	0.684333510867
H	2.056930754199	-1.954430206951	2.370007150839
H	3.277234099132	-0.853252389203	2.510799888623
H	1.720103110045	-0.403383143759	2.818268369773

SCF Done: E(RwB97X) = -289.511266076

Zero-point correction=	0.172290
Thermal correction to Energy=	0.180104
Thermal correction to Enthalpy=	0.181048
Thermal correction to Gibbs Free Energy=	0.140246
Sum of electronic and zero-point Energies=	-289.338976
Sum of electronic and thermal Energies=	-289.331162

Sum of electronic and thermal Enthalpies= -289.330218
 Sum of electronic and thermal Free Energies= -289.371020

1 O	Isotropic =	314.5274	Anisotropy =	96.4953
2 C	Isotropic =	131.3370	Anisotropy =	62.6329
3 C	Isotropic =	162.7192	Anisotropy =	13.0797
4 C	Isotropic =	167.2626	Anisotropy =	25.8648
5 C	Isotropic =	147.9148	Anisotropy =	40.6561
6 N	Isotropic =	219.8151	Anisotropy =	24.9923
7 H	Isotropic =	31.2306	Anisotropy =	20.6814
8 H	Isotropic =	28.1619	Anisotropy =	5.4986
9 H	Isotropic =	28.1264	Anisotropy =	7.8633
10 H	Isotropic =	30.3795	Anisotropy =	8.8044
11 H	Isotropic =	29.9210	Anisotropy =	9.4899
12 H	Isotropic =	29.6918	Anisotropy =	5.7862
13 H	Isotropic =	30.2174	Anisotropy =	8.5543
14 H	Isotropic =	28.8307	Anisotropy =	7.0141
15 H	Isotropic =	28.4112	Anisotropy =	6.4019
16 H	Isotropic =	27.2463	Anisotropy =	14.6224
17 H	Isotropic =	26.9834	Anisotropy =	17.2348
18 H	Isotropic =	27.3083	Anisotropy =	14.2460

Conformer_11

O	0.444126433583	2.149772819495	-0.941705819142
C	-0.054704521941	0.883281689304	-1.372404412607
C	0.930561590449	-0.193247678563	-0.968491023130
C	1.099398212731	-0.308401819267	0.543290509693
C	2.091392108279	-1.398782697074	0.898436524564
N	2.264263214578	-1.490913594134	2.377959477942
H	-0.198919967972	2.821880653690	-1.182436496215
H	-0.181546318870	0.877561904198	-2.461974704291
H	-1.034194518421	0.687123770654	-0.915391936038
H	1.899237353439	0.015802777581	-1.438237553003
H	0.574881612471	-1.146638486998	-1.376220421754
H	1.447259281745	0.646374025811	0.951888254972
H	0.130980104552	-0.531739317804	1.007970135912
H	1.755550511961	-2.379982297685	0.559506543708
H	3.079003588996	-1.198682038907	0.479964121090
H	2.938209449216	-2.216667622130	2.629986945041
H	2.601550897130	-0.607763108501	2.767202502766
H	1.381250968073	-1.714378979670	2.842657350493

SCF Done: E(RwB97X) = -289.511981825

Zero-point correction=	0.171835
Thermal correction to Energy=	0.179794
Thermal correction to Enthalpy=	0.180738
Thermal correction to Gibbs Free Energy=	0.139673
Sum of electronic and zero-point Energies=	-289.340147
Sum of electronic and thermal Energies=	-289.332188
Sum of electronic and thermal Enthalpies=	-289.331244
Sum of electronic and thermal Free Energies=	-289.372309

1	O	Isotropic =	310.4474	Anisotropy =	94.5802
2	C	Isotropic =	127.4711	Anisotropy =	52.8171
3	C	Isotropic =	161.6317	Anisotropy =	19.6256
4	C	Isotropic =	163.6503	Anisotropy =	24.6368
5	C	Isotropic =	145.7944	Anisotropy =	41.2626
6	N	Isotropic =	219.4716	Anisotropy =	25.4579
7	H	Isotropic =	31.2041	Anisotropy =	20.5872
8	H	Isotropic =	27.9385	Anisotropy =	7.5206
9	H	Isotropic =	28.1600	Anisotropy =	6.6829
10	H	Isotropic =	30.2405	Anisotropy =	7.4289
11	H	Isotropic =	30.4185	Anisotropy =	8.2065
12	H	Isotropic =	29.7200	Anisotropy =	5.5302
13	H	Isotropic =	30.3175	Anisotropy =	6.8822
14	H	Isotropic =	28.6506	Anisotropy =	6.7732
15	H	Isotropic =	28.6932	Anisotropy =	6.7618
16	H	Isotropic =	26.9831	Anisotropy =	17.2304
17	H	Isotropic =	27.2332	Anisotropy =	14.1743
18	H	Isotropic =	27.2214	Anisotropy =	14.3890

Conformer_12

O	0.038576584131	2.074767356526	-0.740430436299
C	0.350745671906	0.958257154292	-1.573670404418
C	0.421322417568	-0.287429826175	-0.715711354290
C	1.531704399195	-0.228430114560	0.328712262095
C	1.564699160289	-1.496165598015	1.159897635263
N	2.641157632853	-1.421163440384	2.190903299653
H	0.019067951388	2.862189512435	-1.290679864602
H	1.311948586679	1.121020356188	-2.079966913754
H	-0.421005893234	0.833250406911	-2.343123342262
H	-0.547401073929	-0.436691746417	-0.223784226568
H	0.580440431276	-1.145619472306	-1.378959118939
H	1.377250639853	0.633452413097	0.986632400069
H	2.500481758267	-0.093490696064	-0.168180379631
H	0.627672806774	-1.652018855801	1.696765594344
H	1.774040771660	-2.376542558326	0.550366434297

H	2.498328855017	-0.626802048697	2.818452255358
H	2.667562794948	-2.266672441671	2.764364410713
H	3.562006505361	-1.311010401032	1.760211748969

SCF Done: E(RwB97X) = -289.511981827

Zero-point correction=	0.171835
Thermal correction to Energy=	0.179794
Thermal correction to Enthalpy=	0.180738
Thermal correction to Gibbs Free Energy=	0.139673
Sum of electronic and zero-point Energies=	-289.340147
Sum of electronic and thermal Energies=	-289.332188
Sum of electronic and thermal Enthalpies=	-289.331244
Sum of electronic and thermal Free Energies=	-289.372309

1 O	Isotropic = 310.4474	Anisotropy = 94.5801
2 C	Isotropic = 127.4711	Anisotropy = 52.8171
3 C	Isotropic = 161.6317	Anisotropy = 19.6256
4 C	Isotropic = 163.6503	Anisotropy = 24.6368
5 C	Isotropic = 145.7944	Anisotropy = 41.2626
6 N	Isotropic = 219.4716	Anisotropy = 25.4579
7 H	Isotropic = 31.2041	Anisotropy = 20.5872
8 H	Isotropic = 28.1600	Anisotropy = 6.6829
9 H	Isotropic = 27.9385	Anisotropy = 7.5206
10 H	Isotropic = 30.2405	Anisotropy = 7.4289
11 H	Isotropic = 30.4185	Anisotropy = 8.2065
12 H	Isotropic = 29.7200	Anisotropy = 5.5302
13 H	Isotropic = 30.3175	Anisotropy = 6.8822
14 H	Isotropic = 28.6932	Anisotropy = 6.7618
15 H	Isotropic = 28.6506	Anisotropy = 6.7732
16 H	Isotropic = 27.2332	Anisotropy = 14.1743
17 H	Isotropic = 26.9831	Anisotropy = 17.2304
18 H	Isotropic = 27.2214	Anisotropy = 14.3890

Conformer_13

O	0.423273226108	2.204904173593	-0.903787232303
C	0.016843685298	0.874522334399	-1.223960751208
C	0.316455789222	-0.021664718802	-0.039604130770
C	1.809706181069	-0.107890330043	0.266649773964
C	2.141558701522	-0.912975636889	1.508489455212
N	1.760669456115	-2.350627958582	1.348359189456
H	0.265823436132	2.760217267057	-1.671820505649
H	-1.056816984466	0.849890319872	-1.447131748146
H	0.555863684122	0.516709017618	-2.111927661253

H	-0.092004976026	-1.013988221199	-0.267042488869
H	-0.222205631780	0.354893668594	0.838697364194
H	2.208618763855	0.897870596126	0.425459621586
H	2.346233877147	-0.529576500198	-0.592692740125
H	1.607950075352	-0.546042076041	2.386991380644
H	3.211714665356	-0.900757997644	1.714554887538
H	2.193768939482	-2.758476564506	0.516171860071
H	2.060272076446	-2.903995221189	2.153351633795
H	0.749375035044	-2.470412152167	1.259742091863

SCF Done: E(RwB97X) = -289.511695802

Zero-point correction=	0.172146
Thermal correction to Energy=	0.180070
Thermal correction to Enthalpy=	0.181015
Thermal correction to Gibbs Free Energy=	0.139550
Sum of electronic and zero-point Energies=	-289.339550
Sum of electronic and thermal Energies=	-289.331625
Sum of electronic and thermal Enthalpies=	-289.330681
Sum of electronic and thermal Free Energies=	-289.372146

1 O	Isotropic = 311.1687	Anisotropy = 95.2114
2 C	Isotropic = 127.8431	Anisotropy = 53.5321
3 C	Isotropic = 162.2704	Anisotropy = 18.3043
4 C	Isotropic = 164.9140	Anisotropy = 16.9851
5 C	Isotropic = 145.7896	Anisotropy = 30.6371
6 N	Isotropic = 222.8044	Anisotropy = 17.7585
7 H	Isotropic = 31.1997	Anisotropy = 20.6715
8 H	Isotropic = 27.9057	Anisotropy = 7.4345
9 H	Isotropic = 28.2178	Anisotropy = 6.6192
10 H	Isotropic = 30.2143	Anisotropy = 7.0286
11 H	Isotropic = 30.3271	Anisotropy = 7.5597
12 H	Isotropic = 29.6247	Anisotropy = 7.5074
13 H	Isotropic = 30.3223	Anisotropy = 7.8024
14 H	Isotropic = 28.6939	Anisotropy = 7.7865
15 H	Isotropic = 28.4126	Anisotropy = 8.9794
16 H	Isotropic = 27.5103	Anisotropy = 14.6192
17 H	Isotropic = 27.0183	Anisotropy = 17.3805
18 H	Isotropic = 26.9826	Anisotropy = 13.2332

Conformer_14

O	0.269087109760	2.200929877913	-0.793265896808
C	0.141905712835	0.877780714161	-1.313566847826
C	1.197477769490	0.001164944173	-0.670969216009

C	1.011294867080	-0.128551956900	0.838842863092
C	2.107819134924	-0.913840200228	1.532680828911
N	2.127600299448	-2.341116172482	1.085406283688
H	-0.426366260239	2.742314219343	-1.175739135167
H	0.275922950609	0.884423394948	-2.402214869179
H	-0.859258204143	0.480086822533	-1.097769396593
H	2.188736927981	0.417338119894	-0.889077066782
H	1.147163667626	-0.981883203848	-1.155075790117
H	0.040208977643	-0.589275644307	1.059923452353
H	0.999252811506	0.866566398002	1.292165380576
H	1.959159781467	-0.933185694473	2.612204876966
H	3.097976149168	-0.507450780173	1.319184308275
H	2.812370298031	-2.884512330302	1.614368058771
H	1.214922709715	-2.783811659531	1.217662580255
H	2.372225297099	-2.428376848722	0.096739585593

SCF Done: E(RwB97X) = -289.511695802

Zero-point correction=	0.172146
Thermal correction to Energy=	0.180070
Thermal correction to Enthalpy=	0.181015
Thermal correction to Gibbs Free Energy=	0.139550
Sum of electronic and zero-point Energies=	-289.339550
Sum of electronic and thermal Energies=	-289.331625
Sum of electronic and thermal Enthalpies=	-289.330681
Sum of electronic and thermal Free Energies=	-289.372146

1 O	Isotropic = 311.1687	Anisotropy = 95.2114
2 C	Isotropic = 127.8431	Anisotropy = 53.5321
3 C	Isotropic = 162.2704	Anisotropy = 18.3043
4 C	Isotropic = 164.9140	Anisotropy = 16.9851
5 C	Isotropic = 145.7896	Anisotropy = 30.6371
6 N	Isotropic = 222.8044	Anisotropy = 17.7585
7 H	Isotropic = 31.1997	Anisotropy = 20.6715
8 H	Isotropic = 27.9057	Anisotropy = 7.4345
9 H	Isotropic = 28.2178	Anisotropy = 6.6192
10 H	Isotropic = 30.3270	Anisotropy = 7.5597
11 H	Isotropic = 30.2143	Anisotropy = 7.0286
12 H	Isotropic = 30.3223	Anisotropy = 7.8024
13 H	Isotropic = 29.6247	Anisotropy = 7.5074
14 H	Isotropic = 28.4126	Anisotropy = 8.9794
15 H	Isotropic = 28.6939	Anisotropy = 7.7865
16 H	Isotropic = 27.0183	Anisotropy = 17.3805
17 H	Isotropic = 27.5103	Anisotropy = 14.6192
18 H	Isotropic = 26.9826	Anisotropy = 13.2332

Conformer_15

O	0.379418094863	2.386513591866	-1.166748778658
C	0.075149865495	1.009520186916	-0.956001036959
C	1.183851795144	0.396469939076	-0.125994276295
C	0.929952140438	-1.085796351249	0.135523551744
C	2.073503427047	-1.796165019192	0.835076896361
N	2.278211715521	-1.274629352627	2.221416418500
H	-0.326497347656	2.771284473854	-1.693172653747
H	-0.886659678696	0.906363921098	-0.435714432888
H	-0.003201852036	0.484997720303	-1.917700167440
H	1.257819804617	0.952990250574	0.816289126368
H	2.136041269046	0.520670936067	-0.655292675418
H	0.010605446194	-1.220328799442	0.718426166621
H	0.776029320720	-1.605748581136	-0.816010083780
H	3.019216551716	-1.659892714258	0.308249410968
H	1.873351312450	-2.862593008309	0.936122926172
H	1.423131794799	-1.355641067186	2.776380663072
H	3.009336307449	-1.799056918756	2.705965981780
H	2.557940032889	-0.291559207598	2.224582963598

SCF Done: E(RwB97X) = -289.511448660

Zero-point correction=	0.171924
Thermal correction to Energy=	0.179933
Thermal correction to Enthalpy=	0.180877
Thermal correction to Gibbs Free Energy=	0.139609
Sum of electronic and zero-point Energies=	-289.339524
Sum of electronic and thermal Energies=	-289.331516
Sum of electronic and thermal Enthalpies=	-289.330572
Sum of electronic and thermal Free Energies=	-289.371839

1 O	Isotropic =	308.5808	Anisotropy =	107.7287
2 C	Isotropic =	126.0573	Anisotropy =	65.7175
3 C	Isotropic =	161.6230	Anisotropy =	25.7418
4 C	Isotropic =	166.1549	Anisotropy =	14.8972
5 C	Isotropic =	145.7708	Anisotropy =	29.5978
6 N	Isotropic =	222.6459	Anisotropy =	17.7186
7 H	Isotropic =	31.1488	Anisotropy =	20.4848
8 H	Isotropic =	28.1743	Anisotropy =	4.8975
9 H	Isotropic =	28.1503	Anisotropy =	4.9799
10 H	Isotropic =	30.0556	Anisotropy =	4.9562
11 H	Isotropic =	30.3590	Anisotropy =	6.4928
12 H	Isotropic =	30.2797	Anisotropy =	7.6667
13 H	Isotropic =	30.2885	Anisotropy =	8.6490

14 H	Isotropic =	28.6692	Anisotropy =	7.7678
15 H	Isotropic =	28.4635	Anisotropy =	9.0358
16 H	Isotropic =	27.4974	Anisotropy =	14.6803
17 H	Isotropic =	27.0196	Anisotropy =	17.3458
18 H	Isotropic =	26.9508	Anisotropy =	13.2418

Conformer_16

O	-0.053366947686	2.347234939691	-0.894052172735
C	0.442306881890	1.042862238312	-1.187350651301
C	0.796619626055	0.361325249648	0.117996782332
C	1.330108872334	-1.049459582335	-0.116620508950
C	1.565258745991	-1.842296528042	1.155315908473
N	2.654465063080	-1.240465156054	1.984333917643
H	-0.276409689607	2.775842431883	-1.724735527369
H	-0.319186653598	0.456323814763	-1.718602266431
H	1.329264544497	1.107541576525	-1.831974279672
H	1.538421905783	0.978472740441	0.639477836070
H	-0.097067387432	0.317952193514	0.751786791052
H	0.609125389583	-1.620890594741	-0.710849598233
H	2.259302463096	-1.016176228628	-0.698483258265
H	0.674968059887	-1.872701697564	1.785354539219
H	1.878366962127	-2.862129236271	0.932955146942
H	3.524490127992	-1.164866046266	1.452308482733
H	2.411903277192	-0.304810739122	2.316598066143
H	2.847328758815	-1.813759375755	2.808040792351

SCF Done: E(RwB97X) = -289.511448660

Zero-point correction=	0.171924
Thermal correction to Energy=	0.179933
Thermal correction to Enthalpy=	0.180877
Thermal correction to Gibbs Free Energy=	0.139609
Sum of electronic and zero-point Energies=	-289.339524
Sum of electronic and thermal Energies=	-289.331516
Sum of electronic and thermal Enthalpies=	-289.330572
Sum of electronic and thermal Free Energies=	-289.371839

1 O	Isotropic =	308.5808	Anisotropy =	107.7287
2 C	Isotropic =	126.0573	Anisotropy =	65.7175
3 C	Isotropic =	161.6230	Anisotropy =	25.7418
4 C	Isotropic =	166.1549	Anisotropy =	14.8972
5 C	Isotropic =	145.7708	Anisotropy =	29.5978
6 N	Isotropic =	222.6459	Anisotropy =	17.7187
7 H	Isotropic =	31.1488	Anisotropy =	20.4848

8 H	Isotropic =	28.1503	Anisotropy =	4.9799
9 H	Isotropic =	28.1743	Anisotropy =	4.8975
10 H	Isotropic =	30.0556	Anisotropy =	4.9562
11 H	Isotropic =	30.3590	Anisotropy =	6.4928
12 H	Isotropic =	30.2885	Anisotropy =	8.6490
13 H	Isotropic =	30.2797	Anisotropy =	7.6667
14 H	Isotropic =	28.6692	Anisotropy =	7.7678
15 H	Isotropic =	28.4635	Anisotropy =	9.0358
16 H	Isotropic =	27.4974	Anisotropy =	14.6803
17 H	Isotropic =	26.9508	Anisotropy =	13.2418
18 H	Isotropic =	27.0196	Anisotropy =	17.3458

Conformer_17

O	0.680146115988	1.787616002583	-1.371137546167
C	-0.147503886081	0.935202351644	-0.580580110728
C	0.323643311945	-0.495049028321	-0.754771382586
C	1.773988405905	-0.741419881323	-0.333501018096
C	2.095379208991	-0.425512225085	1.116711592091
N	1.311025335372	-1.289465155000	2.051278661069
H	0.386998951001	2.693353600264	-1.241299287039
H	-1.193591432073	1.014572636842	-0.901078971270
H	-0.101137331110	1.236021265973	0.475228513919
H	0.216872290801	-0.775852971863	-1.807676204708
H	-0.360035212186	-1.147213665841	-0.197583782561
H	2.036590086279	-1.786352416587	-0.533442691735
H	2.442318984037	-0.128502198706	-0.944537145049
H	1.869678682100	0.607463837221	1.384195264880
H	3.146791223095	-0.616737509348	1.330631027537
H	0.306561221137	-1.108766100290	1.989097111860
H	1.457719018118	-2.281291201688	1.848546225586
H	1.587255026681	-1.128567340476	3.021419742997

SCF Done: E(RwB97X) = -289.511111839

Zero-point correction=	0.172296
Thermal correction to Energy=	0.180052
Thermal correction to Enthalpy=	0.180996
Thermal correction to Gibbs Free Energy=	0.140461
Sum of electronic and zero-point Energies=	-289.338816
Sum of electronic and thermal Energies=	-289.331060
Sum of electronic and thermal Enthalpies=	-289.330116
Sum of electronic and thermal Free Energies=	-289.370651

1 O	Isotropic =	314.3874	Anisotropy =	96.8419

2 C	Isotropic =	132.5237	Anisotropy =	66.7101
3 C	Isotropic =	166.0966	Anisotropy =	22.2976
4 C	Isotropic =	168.4909	Anisotropy =	18.7327
5 C	Isotropic =	150.7859	Anisotropy =	44.0559
6 N	Isotropic =	223.9770	Anisotropy =	17.4847
7 H	Isotropic =	31.2465	Anisotropy =	20.7353
8 H	Isotropic =	28.0940	Anisotropy =	7.8020
9 H	Isotropic =	27.9632	Anisotropy =	5.2539
10 H	Isotropic =	30.0371	Anisotropy =	9.6250
11 H	Isotropic =	30.3153	Anisotropy =	7.8715
12 H	Isotropic =	30.1407	Anisotropy =	9.6903
13 H	Isotropic =	29.7122	Anisotropy =	8.2824
14 H	Isotropic =	28.3981	Anisotropy =	6.7641
15 H	Isotropic =	28.5897	Anisotropy =	9.3659
16 H	Isotropic =	27.0651	Anisotropy =	12.9654
17 H	Isotropic =	27.5624	Anisotropy =	15.2631
18 H	Isotropic =	27.0691	Anisotropy =	17.4560

Conformer_18

O	-0.264970131498	1.659508130830	-0.782550710968
C	0.983754029267	1.096194191067	-1.181867561895
C	0.891983582010	-0.413892199521	-1.080112939599
C	0.528931870663	-0.936787819110	0.311480214561
C	1.469918966779	-0.528989224413	1.431557508519
N	2.846322286243	-1.072563420878	1.217347647447
H	-0.193535459991	2.616082699132	-0.837612589644
H	1.793413286586	1.482760468844	-0.547598473980
H	1.214649973808	1.376148099825	-2.217098702400
H	1.847178461903	-0.833307179777	-1.419442210219
H	0.136333923887	-0.770932064667	-1.787700432236
H	-0.463847566813	-0.573165150997	0.590149600832
H	0.465401475228	-2.030294304751	0.281777596842
H	1.573345004469	0.553106377594	1.521384957485
H	1.128454019536	-0.924741034384	2.387905315357
H	3.457634417648	-0.850521921500	2.005293687799
H	2.829944920038	-2.090399486780	1.116506489450
H	3.283086940237	-0.686706160515	0.377180602649

SCF Done: E(RwB97X) = -289.511119100

Zero-point correction=	0.172156
Thermal correction to Energy=	0.179971
Thermal correction to Enthalpy=	0.180916
Thermal correction to Gibbs Free Energy=	0.140083

Sum of electronic and zero-point Energies=	-289.338963
Sum of electronic and thermal Energies=	-289.331148
Sum of electronic and thermal Enthalpies=	-289.330204
Sum of electronic and thermal Free Energies=	-289.371036

1 O	Isotropic =	314.8059	Anisotropy =	96.5285
2 C	Isotropic =	132.5332	Anisotropy =	66.9090
3 C	Isotropic =	166.2174	Anisotropy =	22.1705
4 C	Isotropic =	168.5262	Anisotropy =	19.1267
5 C	Isotropic =	150.6080	Anisotropy =	44.0326
6 N	Isotropic =	223.8371	Anisotropy =	17.4631
7 H	Isotropic =	31.2506	Anisotropy =	20.7434
8 H	Isotropic =	27.9732	Anisotropy =	5.2984
9 H	Isotropic =	28.0819	Anisotropy =	7.8048
10 H	Isotropic =	30.3081	Anisotropy =	7.9444
11 H	Isotropic =	30.0202	Anisotropy =	9.6949
12 H	Isotropic =	29.7179	Anisotropy =	8.2952
13 H	Isotropic =	30.1391	Anisotropy =	9.6570
14 H	Isotropic =	28.4031	Anisotropy =	6.6617
15 H	Isotropic =	28.5842	Anisotropy =	9.3512
16 H	Isotropic =	27.0559	Anisotropy =	17.4402
17 H	Isotropic =	27.5429	Anisotropy =	15.2982
18 H	Isotropic =	27.0669	Anisotropy =	12.9311

Conformer_19

O	0.341423560574	2.289428249356	-1.579703646411
C	0.025286003370	1.277982875406	-0.625662506440
C	1.291277201146	0.508739850019	-0.309803031855
C	1.038747836822	-0.597657767340	0.708432978395
C	2.312854799822	-1.359770692619	1.015958231485
N	2.047477189001	-2.437461002088	2.013065564208
H	-0.463030732295	2.775940708133	-1.778444561318
H	-0.377879027667	1.730824719318	0.290200217055
H	-0.736867606675	0.598055746662	-1.029683904713
H	1.688179643233	0.078721156127	-1.236759964459
H	2.045129671540	1.205053231766	0.075619780416
H	0.641554365049	-0.167699736268	1.635784872404
H	0.284518120088	-1.294277339640	0.323119041572
H	2.718984426966	-1.844982175324	0.127311262335
H	3.077912984585	-0.712442550386	1.446907443557
H	2.896389849757	-2.962112167151	2.232446123834
H	1.688022826503	-2.051364840582	2.889139848426
H	1.354618888183	-3.103378265391	1.663372251509

SCF Done: E(RwB97X) = -289.511638437

Zero-point correction=	0.171188
Thermal correction to Energy=	0.179517
Thermal correction to Enthalpy=	0.180462
Thermal correction to Gibbs Free Energy=	0.137740
Sum of electronic and zero-point Energies=	-289.340450
Sum of electronic and thermal Energies=	-289.332121
Sum of electronic and thermal Enthalpies=	-289.331177
Sum of electronic and thermal Free Energies=	-289.373898

1	O	Isotropic =	308.6801	Anisotropy =	108.0484
2	C	Isotropic =	126.1306	Anisotropy =	65.4062
3	C	Isotropic =	161.2112	Anisotropy =	27.9664
4	C	Isotropic =	164.9845	Anisotropy =	24.6857
5	C	Isotropic =	146.0306	Anisotropy =	41.3259
6	N	Isotropic =	219.5107	Anisotropy =	25.5366
7	H	Isotropic =	31.1824	Anisotropy =	20.4113
8	H	Isotropic =	28.1432	Anisotropy =	4.9211
9	H	Isotropic =	28.1432	Anisotropy =	4.9212
10	H	Isotropic =	30.2744	Anisotropy =	6.2228
11	H	Isotropic =	30.2744	Anisotropy =	6.2228
12	H	Isotropic =	30.3192	Anisotropy =	6.6459
13	H	Isotropic =	30.3192	Anisotropy =	6.6459
14	H	Isotropic =	28.6371	Anisotropy =	6.7154
15	H	Isotropic =	28.6371	Anisotropy =	6.7153
16	H	Isotropic =	26.9889	Anisotropy =	17.2173
17	H	Isotropic =	27.2608	Anisotropy =	14.3441
18	H	Isotropic =	27.2608	Anisotropy =	14.3442

Conformer_2

O	0.343220518859	1.620551610722	-0.109566308855
C	0.381760987608	0.854948172797	-1.329251822313
C	0.225491758630	-0.620843849934	-1.021988408059
C	1.395421909240	-1.313077053675	-0.312898437653
C	1.521603429511	-1.077883047785	1.185512090594
N	2.095609400232	0.263604021762	1.496342222077
H	0.337756131651	2.557210312180	-0.331583339973
H	1.329250769143	1.042202170699	-1.850016041920
H	-0.437800265419	1.181227007986	-1.976542152673
H	0.079853001869	-1.116867566234	-1.987315224236
H	-0.699205452105	-0.772729192784	-0.451996830345
H	1.272067279441	-2.392748839692	-0.436744595643
H	2.343521475873	-1.055336289248	-0.802382758326

H	2.185444811269	-1.813645349209	1.639443905046
H	0.550825141754	-1.128663013626	1.682336329855
H	2.123959565897	0.432799547564	2.502546374907
H	3.051133341332	0.344155952329	1.143384385548
H	1.520086195215	1.000895406147	1.046620611969

SCF Done: E(RwB97X) = -289.515630974

Zero-point correction=	0.172080
Thermal correction to Energy=	0.179524
Thermal correction to Enthalpy=	0.180468
Thermal correction to Gibbs Free Energy=	0.140727
Sum of electronic and zero-point Energies=	-289.343551
Sum of electronic and thermal Energies=	-289.336107
Sum of electronic and thermal Enthalpies=	-289.335162
Sum of electronic and thermal Free Energies=	-289.374904

1 O	Isotropic = 296.9517	Anisotropy = 83.2063
2 C	Isotropic = 125.0996	Anisotropy = 51.8749
3 C	Isotropic = 159.2840	Anisotropy = 10.3441
4 C	Isotropic = 161.9520	Anisotropy = 9.5834
5 C	Isotropic = 146.9072	Anisotropy = 23.6049
6 N	Isotropic = 218.1466	Anisotropy = 19.5795
7 H	Isotropic = 30.2212	Anisotropy = 20.8152
8 H	Isotropic = 28.0926	Anisotropy = 7.3516
9 H	Isotropic = 27.7805	Anisotropy = 7.6685
10 H	Isotropic = 29.9708	Anisotropy = 9.9503
11 H	Isotropic = 30.1017	Anisotropy = 7.9982
12 H	Isotropic = 29.7531	Anisotropy = 10.0865
13 H	Isotropic = 30.2259	Anisotropy = 7.9378
14 H	Isotropic = 28.5067	Anisotropy = 9.2204
15 H	Isotropic = 28.8994	Anisotropy = 7.8888
16 H	Isotropic = 27.3803	Anisotropy = 17.2703
17 H	Isotropic = 27.7017	Anisotropy = 14.6280
18 H	Isotropic = 22.9602	Anisotropy = 24.9029

Conformer_20

O	-0.326553018428	2.266584769518	-1.378270775317
C	0.022164181330	0.900336570928	-1.177715046129
C	0.878302838546	0.692060571738	0.060676406255
C	1.235335737330	-0.777551433894	0.257081131225
C	2.054342477956	-0.980357406032	1.516665855643
N	2.413935022810	-2.419576118969	1.679346614182
H	0.485829277183	2.758520085578	-1.530695341304

H	0.537793591226	0.505135719434	-2.063645808412
H	-0.924353389978	0.361178200156	-1.078943984449
H	0.336521355181	1.066929754242	0.936747809954
H	1.797535511429	1.284861636934	-0.031706250944
H	0.319501052585	-1.377557463764	0.319691604100
H	1.804428660219	-1.140886868691	-0.607057550611
H	2.992029026591	-0.423510982604	1.484930123538
H	1.500146658222	-0.690891457924	2.410508368109
H	2.973802126746	-2.752591047374	0.890864709235
H	2.957487100058	-2.575010421761	2.530529148377
H	1.579151790995	-3.007574107516	1.734692986548

SCF Done: E(RwB97X) = -289.511889141

Zero-point correction=	0.171572
Thermal correction to Energy=	0.179757
Thermal correction to Enthalpy=	0.180701
Thermal correction to Gibbs Free Energy=	0.138726
Sum of electronic and zero-point Energies=	-289.340317
Sum of electronic and thermal Energies=	-289.332132
Sum of electronic and thermal Enthalpies=	-289.331188
Sum of electronic and thermal Free Energies=	-289.373163

1 O	Isotropic = 297.7263	Anisotropy = 45.5084
2 C	Isotropic = 125.5884	Anisotropy = 66.7788
3 C	Isotropic = 158.3681	Anisotropy = 32.5767
4 C	Isotropic = 165.2328	Anisotropy = 24.4190
5 C	Isotropic = 146.0430	Anisotropy = 41.3585
6 N	Isotropic = 219.5173	Anisotropy = 25.4939
7 H	Isotropic = 31.4114	Anisotropy = 16.4546
8 H	Isotropic = 28.1275	Anisotropy = 4.9811
9 H	Isotropic = 28.3399	Anisotropy = 4.5970
10 H	Isotropic = 30.2527	Anisotropy = 5.8552
11 H	Isotropic = 30.4295	Anisotropy = 5.8891
12 H	Isotropic = 30.3687	Anisotropy = 6.5980
13 H	Isotropic = 30.3396	Anisotropy = 6.5345
14 H	Isotropic = 28.6750	Anisotropy = 6.6872
15 H	Isotropic = 28.6546	Anisotropy = 6.7381
16 H	Isotropic = 27.2657	Anisotropy = 14.3599
17 H	Isotropic = 27.0039	Anisotropy = 17.1934
18 H	Isotropic = 27.2735	Anisotropy = 14.3470

Conformer_21

O	-0.014908579214	2.156711422792	-1.750317277422

C	-0.129724442781	0.953838351319	-0.996410795182
C	1.156950733371	0.593836863519	-0.271957769758
C	1.011466828494	-0.698674729819	0.524317998794
C	2.311494123934	-1.070984914927	1.209716025239
N	2.143385731705	-2.324240771184	2.002313704592
H	0.153377919953	2.875656490423	-1.133878941616
H	-0.957633001930	1.032156586817	-0.278522032828
H	-0.390218355730	0.172891669033	-1.716555447314
H	1.964374357793	0.493214286858	-1.006462503023
H	1.432369241376	1.413535005752	0.404190198812
H	0.706929387435	-1.514113179063	-0.142763362010
H	0.224274255286	-0.584040103328	1.279170227095
H	2.637710897989	-0.298656354473	1.907879465320
H	3.109296595609	-1.257958443068	0.489695122381
H	1.433425257569	-2.209785407750	2.729575565052
H	3.014674781620	-2.595156620661	2.462292332525
H	1.852854267522	-3.104030152241	1.408017489344

SCF Done: E(RwB97X) = -289.511889138

Zero-point correction=	0.171572
Thermal correction to Energy=	0.179757
Thermal correction to Enthalpy=	0.180701
Thermal correction to Gibbs Free Energy=	0.138725
Sum of electronic and zero-point Energies=	-289.340317
Sum of electronic and thermal Energies=	-289.332133
Sum of electronic and thermal Enthalpies=	-289.331188
Sum of electronic and thermal Free Energies=	-289.373164

1 O	Isotropic = 297.7265	Anisotropy = 45.5074
2 C	Isotropic = 125.5883	Anisotropy = 66.7788
3 C	Isotropic = 158.3681	Anisotropy = 32.5766
4 C	Isotropic = 165.2328	Anisotropy = 24.4190
5 C	Isotropic = 146.0430	Anisotropy = 41.3584
6 N	Isotropic = 219.5173	Anisotropy = 25.4940
7 H	Isotropic = 31.4114	Anisotropy = 16.4546
8 H	Isotropic = 28.1275	Anisotropy = 4.9811
9 H	Isotropic = 28.3400	Anisotropy = 4.5970
10 H	Isotropic = 30.2527	Anisotropy = 5.8553
11 H	Isotropic = 30.4295	Anisotropy = 5.8890
12 H	Isotropic = 30.3687	Anisotropy = 6.5980
13 H	Isotropic = 30.3396	Anisotropy = 6.5345
14 H	Isotropic = 28.6750	Anisotropy = 6.6872
15 H	Isotropic = 28.6546	Anisotropy = 6.7381
16 H	Isotropic = 27.2657	Anisotropy = 14.3599
17 H	Isotropic = 27.0039	Anisotropy = 17.1934

18 H Isotropic = 27.2735 Anisotropy = 14.3470

Conformer_22

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O      0.136628372836    2.065377300263   -1.577287115902  
C      0.376099595453    1.241668000906   -0.437787547794  
C      0.881168870195   -0.101062109835   -0.929411405549  
C      1.008188944353   -1.147915599181    0.175050060875  
C      1.995890094283   -0.745957701379    1.256963909189  
N      2.192371965316   -1.872117099635    2.216843830068  
H     -0.143763353191    2.930727764783   -1.267484445203  
H      1.113392134783    1.719347210667    0.220092107228  
H     -0.550848725233    1.104966341218    0.136663099765  
H      1.848571424634    0.037040491019   -1.426318699447  
H      0.182288574768   -0.474848533480   -1.684648956383  
H      0.028652755492   -1.331655875590    0.632845359850  
H      1.338033234860   -2.092656197750   -0.270742676835  
H      1.646476344232    0.103591544174    1.844495828719  
H      2.976996966674   -0.510229261390    0.840990504818  
H      2.569568544764   -2.698396866438    1.746327538706  
H      2.841595985779   -1.619222709371    2.964130238387  
H      1.308988270000   -2.144756698983    2.654078369506
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SCF Done: E(RwB97X) = -289.510715186

```
Zero-point correction=          0.172234  
Thermal correction to Energy=      0.180132  
Thermal correction to Enthalpy=     0.181077  
Thermal correction to Gibbs Free Energy= 0.140308  
Sum of electronic and zero-point Energies= -289.338481  
Sum of electronic and thermal Energies= -289.330583  
Sum of electronic and thermal Enthalpies= -289.329639  
Sum of electronic and thermal Free Energies= -289.370407
```

```
1 O Isotropic = 309.2325 Anisotropy = 105.2489  
2 C Isotropic = 127.1161 Anisotropy = 64.4803  
3 C Isotropic = 161.6982 Anisotropy = 22.5603  
4 C Isotropic = 164.5832 Anisotropy = 21.5748  
5 C Isotropic = 146.7745 Anisotropy = 40.2001  
6 N Isotropic = 219.4177 Anisotropy = 25.7619  
7 H Isotropic = 31.1642 Anisotropy = 20.2684  
8 H Isotropic = 28.1131 Anisotropy = 6.1320  
9 H Isotropic = 28.3052 Anisotropy = 4.8667  
10 H Isotropic = 30.1299 Anisotropy = 6.6629  
11 H Isotropic = 30.1109 Anisotropy = 7.8316
```

12	H	Isotropic =	30.1191	Anisotropy =	7.1202
13	H	Isotropic =	30.0737	Anisotropy =	8.0245
14	H	Isotropic =	28.7458	Anisotropy =	6.3489
15	H	Isotropic =	28.8166	Anisotropy =	6.4295
16	H	Isotropic =	27.3161	Anisotropy =	14.5595
17	H	Isotropic =	27.0390	Anisotropy =	17.1377
18	H	Isotropic =	27.3615	Anisotropy =	14.3607

Conformer_23

O	-0.193212112254	2.025885236458	-1.396940795619
C	0.781677630372	1.290439090140	-0.660041504176
C	0.353473785611	-0.164197232913	-0.640441827730
C	1.398488804955	-1.100877117752	-0.038381423088
C	1.710104986502	-0.780504576667	1.413484680768
N	2.613392316107	-1.821623740699	1.986520369051
H	0.053408008987	2.954410691763	-1.375879373509
H	1.769013613645	1.383197698236	-1.133825716387
H	0.857999005782	1.689009225399	0.359712183842
H	-0.590711086913	-0.255224175372	-0.090814375816
H	0.157191357322	-0.477882530381	-1.670785303049
H	1.027733842439	-2.129795111848	-0.101077804994
H	2.325056556876	-1.055471226223	-0.623395005122
H	2.226174101992	0.173255337542	1.527652141568
H	0.808076712078	-0.771679697301	2.027848784288
H	3.488825533472	-1.882490890683	1.461368636097
H	2.850489341914	-1.618390402914	2.959334787694
H	2.175917601113	-2.745960576786	1.961761546183

SCF Done: E(RwB97X) = -289.510715076

Zero-point correction=	0.172231
Thermal correction to Energy=	0.180130
Thermal correction to Enthalpy=	0.181075
Thermal correction to Gibbs Free Energy=	0.140300
Sum of electronic and zero-point Energies=	-289.338485
Sum of electronic and thermal Energies=	-289.330585
Sum of electronic and thermal Enthalpies=	-289.329641
Sum of electronic and thermal Free Energies=	-289.370415

1	O	Isotropic =	309.2350	Anisotropy =	105.2561
2	C	Isotropic =	127.1142	Anisotropy =	64.4791
3	C	Isotropic =	161.6986	Anisotropy =	22.5630
4	C	Isotropic =	164.5825	Anisotropy =	21.5771
5	C	Isotropic =	146.7731	Anisotropy =	40.1993

6	N	Isotropic =	219.4188	Anisotropy =	25.7591
7	H	Isotropic =	31.1644	Anisotropy =	20.2687
8	H	Isotropic =	28.3051	Anisotropy =	4.8668
9	H	Isotropic =	28.1126	Anisotropy =	6.1309
10	H	Isotropic =	30.1303	Anisotropy =	6.6611
11	H	Isotropic =	30.1107	Anisotropy =	7.8316
12	H	Isotropic =	30.0734	Anisotropy =	8.0247
13	H	Isotropic =	30.1198	Anisotropy =	7.1181
14	H	Isotropic =	28.7453	Anisotropy =	6.3494
15	H	Isotropic =	28.8162	Anisotropy =	6.4309
16	H	Isotropic =	27.3617	Anisotropy =	14.3603
17	H	Isotropic =	27.0390	Anisotropy =	17.1377
18	H	Isotropic =	27.3158	Anisotropy =	14.5600

Conformer_24

O	0.063868968233	2.433600937419	-1.074519989091
C	0.950995014333	1.447974533455	-0.553839258131
C	0.304037022181	0.072774063819	-0.481050224193
C	1.257307267630	-1.026051942498	-0.014633507118
C	1.776911261171	-0.790582300290	1.393369402913
N	2.571974238188	-1.967677818959	1.851450458429
H	-0.192522872029	2.161322189254	-1.960887093324
H	1.230406276460	1.805161628242	0.440792143993
H	1.866939157774	1.399065839154	-1.159594187974
H	-0.064441410478	-0.193613040643	-1.478787585013
H	-0.567874571649	0.118636504077	0.181944797877
H	0.731271471447	-1.986589957920	-0.040825287281
H	2.107064651044	-1.104249159254	-0.703676620979
H	2.440765830484	0.072386500706	1.453683757906
H	0.962096994653	-0.661893461213	2.107948215814
H	3.366433695393	-2.141973995521	1.231518071739
H	2.940944445614	-1.827058468864	2.793788678990
H	2.002422559551	-2.817232050964	1.866118225442

SCF Done: E(RwB97X) = -289.511059316

Zero-point correction=	0.172331
Thermal correction to Energy=	0.180207
Thermal correction to Enthalpy=	0.181152
Thermal correction to Gibbs Free Energy=	0.140337
Sum of electronic and zero-point Energies=	-289.338728
Sum of electronic and thermal Energies=	-289.330852
Sum of electronic and thermal Enthalpies=	-289.329908
Sum of electronic and thermal Free Energies=	-289.370722

1 O	Isotropic =	297.5474	Anisotropy =	46.9175
2 C	Isotropic =	126.3943	Anisotropy =	65.8073
3 C	Isotropic =	158.7304	Anisotropy =	26.7439
4 C	Isotropic =	164.9827	Anisotropy =	21.8697
5 C	Isotropic =	146.8905	Anisotropy =	40.2390
6 N	Isotropic =	219.4832	Anisotropy =	25.6792
7 H	Isotropic =	31.5463	Anisotropy =	16.4390
8 H	Isotropic =	28.3193	Anisotropy =	5.5578
9 H	Isotropic =	28.2459	Anisotropy =	4.9181
10 H	Isotropic =	30.2434	Anisotropy =	7.5135
11 H	Isotropic =	30.0965	Anisotropy =	6.2313
12 H	Isotropic =	30.1200	Anisotropy =	8.0381
13 H	Isotropic =	30.1343	Anisotropy =	6.9729
14 H	Isotropic =	28.6852	Anisotropy =	6.2925
15 H	Isotropic =	28.8062	Anisotropy =	6.4228
16 H	Isotropic =	27.3558	Anisotropy =	14.3868
17 H	Isotropic =	27.0272	Anisotropy =	17.1667
18 H	Isotropic =	27.3272	Anisotropy =	14.5262

Conformer_25

O	0.218110992595	2.449379227093	-1.162035470458
C	0.372247029073	1.390077723043	-0.221991883239
C	0.960501637321	0.138741730960	-0.856910176633
C	1.052886361001	-1.046451707064	0.102506150358
C	1.966548707748	-0.771843533533	1.284753506836
N	2.141452562049	-2.011024857927	2.097986496578
H	-0.372741943261	2.143740568589	-1.857014183734
H	-0.592235114440	1.152791638379	0.248908581271
H	1.031932517326	1.785037085264	0.555039147776
H	1.952492159424	0.371435966482	-1.261515956591
H	0.328481855309	-0.153931437848	-1.703733453407
H	0.054458445726	-1.309584391089	0.472488287471
H	1.434060834147	-1.916125468180	-0.443758704555
H	2.962106722650	-0.462318021744	0.961999292683
H	1.561209066616	-0.015760655810	1.957881214467
H	2.562558041451	-2.761486429416	1.544973639814
H	2.744888783265	-1.847074061436	2.906008668246
H	1.243841342002	-2.354503375763	2.447514843117

SCF Done: E(RwB97X) = -289.511059316

Zero-point correction=	0.172331
Thermal correction to Energy=	0.180208

Thermal correction to Enthalpy=	0.181152
Thermal correction to Gibbs Free Energy=	0.140335
Sum of electronic and zero-point Energies=	-289.338728
Sum of electronic and thermal Energies=	-289.330851
Sum of electronic and thermal Enthalpies=	-289.329907
Sum of electronic and thermal Free Energies=	-289.370725

1 O	Isotropic =	297.5485	Anisotropy =	46.9048
2 C	Isotropic =	126.3946	Anisotropy =	65.8088
3 C	Isotropic =	158.7311	Anisotropy =	26.7432
4 C	Isotropic =	164.9850	Anisotropy =	21.8684
5 C	Isotropic =	146.8900	Anisotropy =	40.2381
6 N	Isotropic =	219.4854	Anisotropy =	25.6769
7 H	Isotropic =	31.5463	Anisotropy =	16.4384
8 H	Isotropic =	28.2458	Anisotropy =	4.9182
9 H	Isotropic =	28.3190	Anisotropy =	5.5588
10 H	Isotropic =	30.0970	Anisotropy =	6.2303
11 H	Isotropic =	30.2430	Anisotropy =	7.5137
12 H	Isotropic =	30.1347	Anisotropy =	6.9722
13 H	Isotropic =	30.1198	Anisotropy =	8.0388
14 H	Isotropic =	28.8060	Anisotropy =	6.4233
15 H	Isotropic =	28.6847	Anisotropy =	6.2930
16 H	Isotropic =	27.3269	Anisotropy =	14.5267
17 H	Isotropic =	27.0272	Anisotropy =	17.1666
18 H	Isotropic =	27.3561	Anisotropy =	14.3868

Conformer_26

O	0.227421025980	2.234595893388	-1.564169834917
C	1.048968857594	1.295338192233	-0.875566509560
C	0.294210633451	0.021025357332	-0.526975231995
C	1.179683250452	-1.074632308190	0.064552021193
C	1.792788265085	-0.683649615502	1.398555856354
N	2.523039727848	-1.844778471219	1.987332776196
H	-0.486941356719	2.490119705593	-0.972829916750
H	1.472304500522	1.761054387884	0.023713172430
H	1.878066191309	1.067680918694	-1.552436509869
H	-0.172864150991	-0.361834466870	-1.440019670858
H	-0.516639926610	0.258665529254	0.174101452194
H	0.577405920211	-1.978683941585	0.206180043070
H	1.981084311083	-1.328203349805	-0.640107720917
H	2.520807288552	0.122385544469	1.304189939575
H	1.030234704570	-0.390039602610	2.122001937395
H	3.265598197215	-2.170014310053	1.363873111389
H	2.954706119407	-1.602123670102	2.881025756015

H 1.893526441043 -2.634005792912 2.152379329055

SCF Done: E(RwB97X) = -289.510798471

Zero-point correction= 0.172121
Thermal correction to Energy= 0.180151
Thermal correction to Enthalpy= 0.181095
Thermal correction to Gibbs Free Energy= 0.139283
Sum of electronic and zero-point Energies= -289.338678
Sum of electronic and thermal Energies= -289.330647
Sum of electronic and thermal Enthalpies= -289.329703
Sum of electronic and thermal Free Energies= -289.371516

1	O	Isotropic =	300.2906	Anisotropy =	49.2444
2	C	Isotropic =	126.6604	Anisotropy =	65.9471
3	C	Isotropic =	158.8416	Anisotropy =	26.4523
4	C	Isotropic =	164.6483	Anisotropy =	21.8193
5	C	Isotropic =	146.8431	Anisotropy =	40.1046
6	N	Isotropic =	219.4139	Anisotropy =	25.8040
7	H	Isotropic =	31.5578	Anisotropy =	16.7034
8	H	Isotropic =	28.0599	Anisotropy =	6.3414
9	H	Isotropic =	28.4921	Anisotropy =	4.4171
10	H	Isotropic =	30.0577	Anisotropy =	7.5526
11	H	Isotropic =	30.2789	Anisotropy =	6.0382
12	H	Isotropic =	30.1027	Anisotropy =	8.0062
13	H	Isotropic =	30.1382	Anisotropy =	6.9436
14	H	Isotropic =	28.6580	Anisotropy =	6.3495
15	H	Isotropic =	28.8251	Anisotropy =	6.4791
16	H	Isotropic =	27.3593	Anisotropy =	14.3927
17	H	Isotropic =	27.0366	Anisotropy =	17.1375
18	H	Isotropic =	27.3348	Anisotropy =	14.5104

Conformer_27

O	-0.243905440299	2.190020357551	-1.292373255542
C	0.077010035830	1.203360613831	-0.315216327219
C	0.927021863659	0.080844345750	-0.891836073518
C	1.155332426227	-1.076937837678	0.078653447210
C	1.946298967444	-0.669183864265	1.310092758621
N	2.257541484058	-1.869895274236	2.140493355593
H	0.579210242550	2.590964468933	-1.587353777238
H	-0.879905186678	0.806777372252	0.037511598338
H	0.576462919329	1.676223759884	0.540210948360
H	1.894316076694	0.486695221083	-1.216008055844
H	0.425446821381	-0.305318731821	-1.784971171216

H	0.191837928008	-1.497279144398	0.391830918509
H	1.700069284683	-1.872597134754	-0.441243480934
H	2.901282739135	-0.213386795105	1.043028128497
H	1.394339968082	0.015973004761	1.953917275630
H	2.819560649687	-2.546592988295	1.618360886558
H	2.779882550371	-1.618692614622	2.981897752330
H	1.402796669839	-2.345974758870	2.438205071866

SCF Done: E(RwB97X) = -289.510798494

Zero-point correction=	0.172122
Thermal correction to Energy=	0.180151
Thermal correction to Enthalpy=	0.181096
Thermal correction to Gibbs Free Energy=	0.139290
Sum of electronic and zero-point Energies=	-289.338677
Sum of electronic and thermal Energies=	-289.330647
Sum of electronic and thermal Enthalpies=	-289.329703
Sum of electronic and thermal Free Energies=	-289.371509

1 O	Isotropic = 300.2907	Anisotropy = 49.2537
2 C	Isotropic = 126.6603	Anisotropy = 65.9488
3 C	Isotropic = 158.8416	Anisotropy = 26.4532
4 C	Isotropic = 164.6491	Anisotropy = 21.8197
5 C	Isotropic = 146.8428	Anisotropy = 40.1049
6 N	Isotropic = 219.4143	Anisotropy = 25.8034
7 H	Isotropic = 31.5578	Anisotropy = 16.7033
8 H	Isotropic = 28.4920	Anisotropy = 4.4174
9 H	Isotropic = 28.0598	Anisotropy = 6.3413
10 H	Isotropic = 30.2792	Anisotropy = 6.0376
11 H	Isotropic = 30.0576	Anisotropy = 7.5526
12 H	Isotropic = 30.1384	Anisotropy = 6.9431
13 H	Isotropic = 30.1027	Anisotropy = 8.0064
14 H	Isotropic = 28.8250	Anisotropy = 6.4794
15 H	Isotropic = 28.6579	Anisotropy = 6.3496
16 H	Isotropic = 27.3348	Anisotropy = 14.5103
17 H	Isotropic = 27.0366	Anisotropy = 17.1376
18 H	Isotropic = 27.3593	Anisotropy = 14.3927

Conformer_3

O	0.692960697217	1.690531574691	-0.288428440132
C	0.063154563777	0.745782608323	-1.169612828987
C	0.971492739790	-0.460982109344	-1.304465922273
C	0.983820476126	-1.419321489336	-0.107794937521
C	1.206514784520	-0.789936617622	1.259469998584

N	2.401601707998	0.103553093174	1.269396183318
H	0.117651039811	2.452199066070	-0.173554185614
H	-0.088639661333	1.210887111469	-2.149267371002
H	-0.916576006263	0.457027209078	-0.768654330354
H	1.984805910246	-0.102479484150	-1.525410923506
H	0.655363389431	-1.028625086118	-2.184608783713
H	1.749845776065	-2.183530546447	-0.277971654628
H	0.025082901757	-1.944813162374	-0.051004415712
H	1.370772983903	-1.556817036250	2.016474486534
H	0.363381495100	-0.170178040938	1.565771026584
H	3.233810935427	-0.367827150002	0.908009287795
H	2.204743589887	0.932535499678	0.692377518436
H	2.613612676540	0.424194560096	2.215575292190

SCF Done: E(RwB97X) = -289.514332761

Zero-point correction=	0.172464
Thermal correction to Energy=	0.179930
Thermal correction to Enthalpy=	0.180874
Thermal correction to Gibbs Free Energy=	0.141541
Sum of electronic and zero-point Energies=	-289.341869
Sum of electronic and thermal Energies=	-289.334403
Sum of electronic and thermal Enthalpies=	-289.333459
Sum of electronic and thermal Free Energies=	-289.372791

1 O	Isotropic = 304.0344	Anisotropy = 103.2136
2 C	Isotropic = 125.9581	Anisotropy = 58.3588
3 C	Isotropic = 165.2370	Anisotropy = 23.5389
4 C	Isotropic = 164.3773	Anisotropy = 8.6068
5 C	Isotropic = 148.9010	Anisotropy = 34.6408
6 N	Isotropic = 220.8580	Anisotropy = 15.2712
7 H	Isotropic = 30.6788	Anisotropy = 21.2965
8 H	Isotropic = 27.8275	Anisotropy = 8.3701
9 H	Isotropic = 27.9198	Anisotropy = 6.7848
10 H	Isotropic = 30.0742	Anisotropy = 7.0374
11 H	Isotropic = 30.0702	Anisotropy = 10.3181
12 H	Isotropic = 29.9248	Anisotropy = 9.8198
13 H	Isotropic = 30.0748	Anisotropy = 9.8626
14 H	Isotropic = 28.5264	Anisotropy = 9.5281
15 H	Isotropic = 28.4773	Anisotropy = 6.8634
16 H	Isotropic = 27.5194	Anisotropy = 14.8598
17 H	Isotropic = 24.9597	Anisotropy = 17.6573
18 H	Isotropic = 27.2021	Anisotropy = 17.3456

Conformer_4

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-----
O    0.634104441672    1.682959852062   -0.254855934646
C    0.377795441843    0.786441533245   -1.348589537282
C    0.048637384619   -0.580009017485   -0.779371970491
C    1.243025008421   -1.385858715906   -0.255321319406
C    2.173071652720   -0.665233707918    0.709480117880
N    1.421397987349   -0.022960045040    1.827124026377
H    0.868163341303    2.549043684393   -0.600441282952
H    1.255914749691    0.737420980575   -2.004731325805
H   -0.468762219566    1.161925209480   -1.932916633167
H   -0.706597966970   -0.449718304031    0.005986593785
H   -0.433758541766   -1.169069652408   -1.564934979976
H    0.868713606049   -2.297210022749    0.223322462953
H    1.864184144731   -1.707484824649   -1.097498377861
H    2.882574379102   -1.361774362991    1.156223156736
H    2.728695246837    0.135015970963    0.219911646612
H    0.868787700916    0.760133685410    1.452555421023
H    0.795814351892   -0.682447436547    2.295197731788
H    2.058639291158    0.352525173594    2.531360204432

```

SCF Done: E(RwB97X) = -289.514332764

```

Zero-point correction=          0.172464
Thermal correction to Energy=      0.179930
Thermal correction to Enthalpy=     0.180874
Thermal correction to Gibbs Free Energy= 0.141542
Sum of electronic and zero-point Energies= -289.341869
Sum of electronic and thermal Energies= -289.334403
Sum of electronic and thermal Enthalpies= -289.333459
Sum of electronic and thermal Free Energies= -289.372791

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1 O  Isotropic = 304.0344  Anisotropy = 103.2138
2 C  Isotropic = 125.9583  Anisotropy = 58.3592
3 C  Isotropic = 165.2373  Anisotropy = 23.5388
4 C  Isotropic = 164.3774  Anisotropy = 8.6065
5 C  Isotropic = 148.9011  Anisotropy = 34.6412
6 N  Isotropic = 220.8578  Anisotropy = 15.2719
7 H  Isotropic = 30.6788  Anisotropy = 21.2964
8 H  Isotropic = 27.9198  Anisotropy = 6.7848
9 H  Isotropic = 27.8275  Anisotropy = 8.3702
10 H Isotropic = 30.0742  Anisotropy = 7.0374
11 H Isotropic = 30.0702  Anisotropy = 10.3181
12 H Isotropic = 29.9248  Anisotropy = 9.8198
13 H Isotropic = 30.0748  Anisotropy = 9.8626
14 H Isotropic = 28.5264  Anisotropy = 9.5282
15 H Isotropic = 28.4773  Anisotropy = 6.8634

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16 H	Isotropic =	24.9596	Anisotropy =	17.6576
17 H	Isotropic =	27.5195	Anisotropy =	14.8598
18 H	Isotropic =	27.2021	Anisotropy =	17.3456

Conformer_5

O	0.554983230304	1.786722558934	-0.214457146606
C	-0.289395327284	0.702503861809	-0.630402287197
C	0.476002026659	-0.457714854370	-1.248892196408
C	1.694409959788	-0.952624456640	-0.456452162024
C	1.475226943419	-1.118030404998	1.042578178496
N	1.747589764538	0.165211161419	1.766069438364
H	1.033392294501	2.124854591619	-0.979108994588
H	-0.812327937041	0.386266295824	0.277088467157
H	-1.046627325950	1.069685614856	-1.330361915805
H	0.805362898548	-0.182570486943	-2.257179111059
H	-0.240661995967	-1.278456342335	-1.368585310251
H	1.993899338765	-1.922991675635	-0.860277324949
H	2.551906697647	-0.288042163712	-0.613417128868
H	0.450829079639	-1.410334671742	1.279708394363
H	2.152253154003	-1.858134632956	1.467440170527
H	1.337673071739	0.969437682877	1.261140314372
H	1.382110943557	0.146997913363	2.719318311299
H	2.753273183134	0.335420008629	1.826290303176

SCF Done: E(RwB97X) = -289.512529086

Zero-point correction=	0.172656
Thermal correction to Energy=	0.179976
Thermal correction to Enthalpy=	0.180920
Thermal correction to Gibbs Free Energy=	0.141888
Sum of electronic and zero-point Energies=	-289.339874
Sum of electronic and thermal Energies=	-289.332553
Sum of electronic and thermal Enthalpies=	-289.331609
Sum of electronic and thermal Free Energies=	-289.370641

1 O	Isotropic =	298.9648	Anisotropy =	61.2690
2 C	Isotropic =	129.3602	Anisotropy =	66.2470
3 C	Isotropic =	161.3226	Anisotropy =	11.8839
4 C	Isotropic =	168.7913	Anisotropy =	23.9263
5 C	Isotropic =	149.4245	Anisotropy =	35.6371
6 N	Isotropic =	218.8090	Anisotropy =	22.3647
7 H	Isotropic =	30.8276	Anisotropy =	17.8964
8 H	Isotropic =	28.0548	Anisotropy =	6.0649
9 H	Isotropic =	27.7556	Anisotropy =	8.1613

10	H	Isotropic =	29.9415	Anisotropy =	9.5124
11	H	Isotropic =	30.2778	Anisotropy =	9.7722
12	H	Isotropic =	29.8877	Anisotropy =	10.3642
13	H	Isotropic =	30.0613	Anisotropy =	7.2743
14	H	Isotropic =	28.5998	Anisotropy =	7.2169
15	H	Isotropic =	28.5299	Anisotropy =	9.5517
16	H	Isotropic =	24.2803	Anisotropy =	21.5002
17	H	Isotropic =	27.2778	Anisotropy =	17.2517
18	H	Isotropic =	27.4745	Anisotropy =	15.3686

Conformer_6

O	0.698123997315	1.809226125167	-0.290146309866
C	1.072968596490	0.916522395217	-1.350375907898
C	0.442622486138	-0.462951569019	-1.231272258836
C	0.553766159973	-1.131783838561	0.146307038864
C	1.925654972447	-1.047244600934	0.804537018483
N	2.057491885973	0.213928434500	1.602279015711
H	-0.258514794957	1.921935859515	-0.296458781574
H	2.163877833656	0.853802727852	-1.295714678175
H	0.821375792107	1.363123029553	-2.317544553986
H	0.925930494861	-1.095198998170	-1.985080539838
H	-0.616752684039	-0.405966184643	-1.505684909256
H	-0.191336766721	-0.718942288813	0.836228580901
H	0.300378300218	-2.189002276035	0.034660619330
H	2.735132135250	-1.051471809903	0.072558710075
H	2.086941177481	-1.868360444606	1.501947896185
H	1.673270142683	1.022187363695	1.083765208440
H	1.528439910097	0.143053448737	2.473529411377
H	3.029630361029	0.405842626447	1.848664440062

SCF Done: E(RwB97X) = -289.512529086

Zero-point correction=	0.172655
Thermal correction to Energy=	0.179976
Thermal correction to Enthalpy=	0.180920
Thermal correction to Gibbs Free Energy=	0.141888
Sum of electronic and zero-point Energies=	-289.339874
Sum of electronic and thermal Energies=	-289.332553
Sum of electronic and thermal Enthalpies=	-289.331609
Sum of electronic and thermal Free Energies=	-289.370641

1	O	Isotropic =	298.9652	Anisotropy =	61.2693
2	C	Isotropic =	129.3602	Anisotropy =	66.2470
3	C	Isotropic =	161.3225	Anisotropy =	11.8839

4	C	Isotropic =	168.7913	Anisotropy =	23.9264
5	C	Isotropic =	149.4245	Anisotropy =	35.6372
6	N	Isotropic =	218.8089	Anisotropy =	22.3648
7	H	Isotropic =	30.8276	Anisotropy =	17.8964
8	H	Isotropic =	28.0548	Anisotropy =	6.0649
9	H	Isotropic =	27.7556	Anisotropy =	8.1613
10	H	Isotropic =	30.2778	Anisotropy =	9.7722
11	H	Isotropic =	29.9415	Anisotropy =	9.5124
12	H	Isotropic =	30.0613	Anisotropy =	7.2742
13	H	Isotropic =	29.8877	Anisotropy =	10.3642
14	H	Isotropic =	28.5998	Anisotropy =	7.2168
15	H	Isotropic =	28.5299	Anisotropy =	9.5516
16	H	Isotropic =	24.2803	Anisotropy =	21.5000
17	H	Isotropic =	27.4745	Anisotropy =	15.3686
18	H	Isotropic =	27.2778	Anisotropy =	17.2517

Conformer_7

O	0.447731063258	1.834076455693	-0.464098630555
C	0.376495573628	0.882583592254	-1.528391020601
C	0.184113703217	-0.509142774392	-0.959749275812
C	1.351845857712	-1.029581847383	-0.119395771074
C	1.390858628034	-0.433003773581	1.277200941922
N	2.522606928862	-1.020285468330	2.055729279449
H	0.562432460856	2.706520212617	-0.850608729173
H	1.298653918894	0.915337413047	-2.124488896072
H	-0.463422521621	1.124889191991	-2.191220040388
H	0.038892123273	-1.183732260733	-1.809682668681
H	-0.742934741899	-0.538430138032	-0.374175667797
H	1.269654291751	-2.118682751993	-0.027247962157
H	2.298747562700	-0.820937510056	-0.633205244538
H	0.479006089071	-0.658492301915	1.832675064176
H	1.539352003052	0.645195615679	1.258512929744
H	2.557025513466	-0.642827824719	3.004431484363
H	2.437130848995	-2.036528523952	2.130124590683
H	3.421210696753	-0.818457306195	1.611789616510

SCF Done: E(RwB97X) = -289.510927511

Zero-point correction=	0.171878
Thermal correction to Energy=	0.179772
Thermal correction to Enthalpy=	0.180716
Thermal correction to Gibbs Free Energy=	0.139796
Sum of electronic and zero-point Energies=	-289.339049
Sum of electronic and thermal Energies=	-289.331156

Sum of electronic and thermal Enthalpies= -289.330212
Sum of electronic and thermal Free Energies= -289.371132

1 O	Isotropic =	305.4164	Anisotropy =	100.5118
2 C	Isotropic =	124.0870	Anisotropy =	49.6595
3 C	Isotropic =	162.5398	Anisotropy =	12.5055
4 C	Isotropic =	160.5163	Anisotropy =	25.2906
5 C	Isotropic =	145.1567	Anisotropy =	44.3734
6 N	Isotropic =	218.8369	Anisotropy =	26.6717
7 H	Isotropic =	31.1552	Anisotropy =	20.6340
8 H	Isotropic =	28.0637	Anisotropy =	6.7982
9 H	Isotropic =	27.8977	Anisotropy =	7.7332
10 H	Isotropic =	30.1903	Anisotropy =	9.8677
11 H	Isotropic =	30.1875	Anisotropy =	7.6460
12 H	Isotropic =	29.9033	Anisotropy =	7.9715
13 H	Isotropic =	30.1094	Anisotropy =	6.5415
14 H	Isotropic =	28.7379	Anisotropy =	6.2856
15 H	Isotropic =	27.8009	Anisotropy =	8.5914
16 H	Isotropic =	27.0303	Anisotropy =	17.0411
17 H	Isotropic =	27.3680	Anisotropy =	14.5422
18 H	Isotropic =	27.2918	Anisotropy =	14.2024

Conformer_8

O	0.614877328677	1.853571172676	-0.556973187427
C	-0.075667473622	0.829812873831	-1.276838337103
C	0.746515203132	-0.443475150904	-1.272592350162
C	0.947457774715	-1.076797976276	0.105513129978
C	1.996724079850	-0.362460255305	0.940178089258
N	2.175627570612	-1.060766053241	2.248703889523
H	0.077154515735	2.649816745645	-0.580461615133
H	-0.245996604957	1.150344059111	-2.312099159405
H	-1.054533468387	0.640617229003	-0.815529518910
H	1.718421158647	-0.251068198650	-1.743286250795
H	0.225193450655	-1.161948274945	-1.913347396884
H	-0.005883557711	-1.089807271472	0.648770812711
H	1.259001102677	-2.119969589944	-0.021445937744
H	1.715029866591	0.665606592270	1.160728296954
H	2.970194230478	-0.368235161027	0.447030458896
H	2.889215462434	-0.604136273366	2.819647509085
H	1.306875811001	-1.064913768055	2.787742804815
H	2.460993549475	-2.033790699352	2.116858762344

SCF Done: E(RwB97X) = -289.510927561

Zero-point correction=	0.171879
Thermal correction to Energy=	0.179772
Thermal correction to Enthalpy=	0.180716
Thermal correction to Gibbs Free Energy=	0.139799
Sum of electronic and zero-point Energies=	-289.339048
Sum of electronic and thermal Energies=	-289.331156
Sum of electronic and thermal Enthalpies=	-289.330211
Sum of electronic and thermal Free Energies=	-289.371128

1 O	Isotropic = 305.4172	Anisotropy = 100.5098
2 C	Isotropic = 124.0856	Anisotropy = 49.6570
3 C	Isotropic = 162.5424	Anisotropy = 12.5062
4 C	Isotropic = 160.5162	Anisotropy = 25.2919
5 C	Isotropic = 145.1567	Anisotropy = 44.3754
6 N	Isotropic = 218.8367	Anisotropy = 26.6713
7 H	Isotropic = 31.1551	Anisotropy = 20.6338
8 H	Isotropic = 27.8976	Anisotropy = 7.7333
9 H	Isotropic = 28.0637	Anisotropy = 6.7982
10 H	Isotropic = 30.1876	Anisotropy = 7.6459
11 H	Isotropic = 30.1903	Anisotropy = 9.8679
12 H	Isotropic = 30.1096	Anisotropy = 6.5407
13 H	Isotropic = 29.9031	Anisotropy = 7.9717
14 H	Isotropic = 27.8008	Anisotropy = 8.5921
15 H	Isotropic = 28.7378	Anisotropy = 6.2865
16 H	Isotropic = 27.0303	Anisotropy = 17.0412
17 H	Isotropic = 27.2918	Anisotropy = 14.2019
18 H	Isotropic = 27.3679	Anisotropy = 14.5423

Conformer_9

O	0.692890077084	1.907872956104	-1.190841012235
C	-0.207635856216	0.810112135972	-1.046059770487
C	0.572914288523	-0.483251245750	-1.183447936848
C	1.708744155228	-0.650259190472	-0.175293510691
C	1.212936141408	-0.735989884490	1.256705362851
N	2.360876895565	-0.968885562580	2.182032679883
H	0.189989181446	2.721340300766	-1.098595118649
H	-0.982245492556	0.848114069224	-1.821970799201
H	-0.712460597925	0.861654380416	-0.072221502712
H	0.993355919574	-0.533425105255	-2.193356466522
H	-0.133487409140	-1.316747656549	-1.092139094552
H	2.261529244616	-1.566060482938	-0.413369505307
H	2.409987731658	0.186306190279	-0.266468975445
H	0.520986961101	-1.568004063586	1.397122916968
H	0.731138241418	0.184726694893	1.587621539418

H	3.044093218454	-0.210361588666	2.121971588361
H	2.053437749340	-1.031748567645	3.154235909822
H	2.847249550421	-1.839293379723	1.954573695345

SCF Done: E(RwB97X) = -289.511266201

Zero-point correction=	0.172298
Thermal correction to Energy=	0.180109
Thermal correction to Enthalpy=	0.181054
Thermal correction to Gibbs Free Energy=	0.140259
Sum of electronic and zero-point Energies=	-289.338968
Sum of electronic and thermal Energies=	-289.331157
Sum of electronic and thermal Enthalpies=	-289.330213
Sum of electronic and thermal Free Energies=	-289.371007

1 O	Isotropic = 314.5310	Anisotropy = 96.4867
2 C	Isotropic = 131.3400	Anisotropy = 62.6425
3 C	Isotropic = 162.7209	Anisotropy = 13.0820
4 C	Isotropic = 167.2606	Anisotropy = 25.8685
5 C	Isotropic = 147.9187	Anisotropy = 40.6514
6 N	Isotropic = 219.8149	Anisotropy = 24.9911
7 H	Isotropic = 31.2303	Anisotropy = 20.6828
8 H	Isotropic = 28.1264	Anisotropy = 7.8621
9 H	Isotropic = 28.1619	Anisotropy = 5.4985
10 H	Isotropic = 29.9208	Anisotropy = 9.4903
11 H	Isotropic = 30.3793	Anisotropy = 8.8055
12 H	Isotropic = 30.2169	Anisotropy = 8.5539
13 H	Isotropic = 29.6927	Anisotropy = 5.7870
14 H	Isotropic = 28.8306	Anisotropy = 7.0151
15 H	Isotropic = 28.4111	Anisotropy = 6.4023
16 H	Isotropic = 27.3082	Anisotropy = 14.2448
17 H	Isotropic = 26.9833	Anisotropy = 17.2349
18 H	Isotropic = 27.2459	Anisotropy = 14.6237

Cyclohexanamine_neutral
Conformer_1

C	-2.079552433019	-0.605957222163	-1.118267756156
C	-0.624112661206	-0.999316129631	-1.384653455703
C	0.320930485802	-0.547541381683	-0.266429252028
C	-0.180819251120	-1.067663774373	1.090923263194
C	-1.633865001517	-0.675072610022	1.366006600497
C	-2.556558339055	-1.134007627234	0.235621019154
N	0.497142541249	0.912134281086	-0.314263773316
H	-2.183781845720	0.487495054469	-1.140014838710
H	-2.716878555478	-0.989807052071	-1.922104876248

H	-0.563051787357	-2.092016728198	-1.467008495190
H	-0.282752909082	-0.585571780202	-2.339929506974
H	1.309226805837	-0.981557479430	-0.455965323404
H	-0.097880774262	-2.162904842636	1.096745053817
H	0.475192100143	-0.695526691640	1.886851382147
H	-1.959357707251	-1.102449229601	2.320717513133
H	-1.709941138544	0.415346123556	1.475310536967
H	-3.584774821791	-0.809126819089	0.429321516949
H	-2.571495524013	-2.232445004547	0.207282078923
H	1.131110436699	1.201176477756	0.424876052073
H	-0.382479620312	1.382912435654	-0.124217739126

SCF Done: E(RwB97X) = -291.243850673

Zero-point correction=	0.188828
Thermal correction to Energy=	0.195729
Thermal correction to Enthalpy=	0.196673
Thermal correction to Gibbs Free Energy=	0.158518
Sum of electronic and zero-point Energies=	-291.055023
Sum of electronic and thermal Energies=	-291.048122
Sum of electronic and thermal Enthalpies=	-291.047178
Sum of electronic and thermal Free Energies=	-291.085333

1 C	Isotropic = 169.9975	Anisotropy = 15.6625
2 C	Isotropic = 158.0069	Anisotropy = 13.9898
3 C	Isotropic = 143.7782	Anisotropy = 28.9430
4 C	Isotropic = 155.3106	Anisotropy = 18.1552
5 C	Isotropic = 170.6608	Anisotropy = 17.9495
6 C	Isotropic = 164.1631	Anisotropy = 2.8661
7 N	Isotropic = 226.9232	Anisotropy = 54.7801
8 H	Isotropic = 30.4726	Anisotropy = 7.3000
9 H	Isotropic = 30.5102	Anisotropy = 10.9964
10 H	Isotropic = 30.3681	Anisotropy = 8.6694
11 H	Isotropic = 30.3216	Anisotropy = 9.3176
12 H	Isotropic = 29.0494	Anisotropy = 8.6349
13 H	Isotropic = 30.3734	Anisotropy = 8.5589
14 H	Isotropic = 30.4784	Anisotropy = 9.0648
15 H	Isotropic = 30.5301	Anisotropy = 11.0060
16 H	Isotropic = 30.2910	Anisotropy = 7.2515
17 H	Isotropic = 30.3070	Anisotropy = 10.3759
18 H	Isotropic = 30.6812	Anisotropy = 8.9852
19 H	Isotropic = 31.1757	Anisotropy = 15.4991
20 H	Isotropic = 30.2241	Anisotropy = 9.7957

Conformer_10

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C      -1.573654499576   -0.758298692365    1.395495710969
C      -0.161406580795   -1.192264134979    0.967346270775
C       0.306890125277   -0.508456321283   -0.316729110106
C      -0.643919009737   -0.839705523653   -1.487950178932
C      -2.043154054453   -1.280590467765   -1.033777159959
C      -2.500078586060   -0.494844213870    0.193213409627
N       0.359544568517    0.947593818924   -0.102906102988
H      -2.000336512555   -1.543447322684    2.029836267029
H      -1.516941682415    0.140450802766    2.017480956680
H       0.555519861968   -0.997305556922    1.773351203119
H      -0.141184124937   -2.274619476943    0.794086074066
H       1.305472117588   -0.897463304158   -0.562566077874
H      -0.727026018215    0.047877184794   -2.126959186254
H      -0.199034145120   -1.625004408478   -2.108120002432
H      -2.754188140924   -1.159072296218   -1.857535907590
H      -2.034013549301   -2.350697460498   -0.789845656071
H      -2.492454697808    0.572991045901   -0.052906922669
H      -3.533352986540   -0.751212981155    0.449132563942
H       1.021224861896    1.157045062596    0.639539932189
H       0.720693053192    1.400024245989   -0.937386083520

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SCF Done: E(RwB97X) = -291.234094615

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Zero-point correction=          0.188762
Thermal correction to Energy=      0.195862
Thermal correction to Enthalpy=    0.196806
Thermal correction to Gibbs Free Energy=  0.158063
Sum of electronic and zero-point Energies= -291.045332
Sum of electronic and thermal Energies=    -291.038232
Sum of electronic and thermal Enthalpies=   -291.037288
Sum of electronic and thermal Free Energies= -291.076031

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1 C  Isotropic = 173.5253  Anisotropy = 16.5980
2 C  Isotropic = 165.4933  Anisotropy = 14.7487
3 C  Isotropic = 145.6432  Anisotropy = 26.9595
4 C  Isotropic = 159.6990  Anisotropy = 20.6388
5 C  Isotropic = 170.7989  Anisotropy = 3.9558
6 C  Isotropic = 171.2493  Anisotropy = 7.0688
7 N  Isotropic = 216.1389  Anisotropy = 52.6976
8 H  Isotropic = 30.4489  Anisotropy = 10.4923
9 H  Isotropic = 30.1952  Anisotropy = 9.4109
10 H  Isotropic = 30.4771  Anisotropy = 9.6380
11 H  Isotropic = 30.4007  Anisotropy = 9.3578
12 H  Isotropic = 28.6498  Anisotropy = 9.3375
13 H  Isotropic = 30.8026  Anisotropy = 7.9659

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14	H	Isotropic =	30.1003	Anisotropy =	9.7685
15	H	Isotropic =	30.4952	Anisotropy =	10.7601
16	H	Isotropic =	30.5132	Anisotropy =	9.3280
17	H	Isotropic =	30.2847	Anisotropy =	7.8980
18	H	Isotropic =	30.4847	Anisotropy =	10.8944
19	H	Isotropic =	31.1144	Anisotropy =	15.0843
20	H	Isotropic =	31.0462	Anisotropy =	14.3630

Conformer_11

C	-1.626786429389	-1.325655400988	1.238891588872
C	-0.154361528183	-0.892646522080	1.184303156132
C	0.321998690600	-0.510040859164	-0.234223112956
C	-0.575711798689	-1.147403000454	-1.294237308742
C	-2.044964262376	-0.707317010981	-1.177173300344
C	-2.483355068860	-0.496689802452	0.284538703628
N	0.305649233208	0.953471546103	-0.396823793954
H	-1.998899380763	-1.240826495153	2.265171584018
H	-1.712164666205	-2.385532773959	0.966704962765
H	0.000577245721	-0.030822344715	1.844829717877
H	0.475915861966	-1.697985754711	1.575974665909
H	1.340148493466	-0.901133570582	-0.373311931919
H	-0.189584748416	-0.916633973119	-2.293881202019
H	-0.502974843475	-2.235435505652	-1.181030687821
H	-2.674226019770	-1.470561103667	-1.648757755179
H	-2.206058916716	0.214993855041	-1.743939355925
H	-2.381539602492	0.560951931765	0.552741917696
H	-3.542032396389	-0.750340575235	0.401752692316
H	0.942228498942	1.376113013145	0.272219826019
H	0.662741637821	1.195894346856	-1.316950366373

SCF Done: E(RwB97X) = -291.234094615

Zero-point correction=	0.188762
Thermal correction to Energy=	0.195862
Thermal correction to Enthalpy=	0.196806
Thermal correction to Gibbs Free Energy=	0.158063
Sum of electronic and zero-point Energies=	-291.045332
Sum of electronic and thermal Energies=	-291.038232
Sum of electronic and thermal Enthalpies=	-291.037288
Sum of electronic and thermal Free Energies=	-291.076031

1	C	Isotropic =	170.7989	Anisotropy =	3.9557
2	C	Isotropic =	159.6990	Anisotropy =	20.6388
3	C	Isotropic =	145.6431	Anisotropy =	26.9595

4	C	Isotropic =	165.4933	Anisotropy =	14.7488
5	C	Isotropic =	173.5253	Anisotropy =	16.5979
6	C	Isotropic =	171.2493	Anisotropy =	7.0688
7	N	Isotropic =	216.1388	Anisotropy =	52.6976
8	H	Isotropic =	30.4952	Anisotropy =	10.7601
9	H	Isotropic =	30.5132	Anisotropy =	9.3280
10	H	Isotropic =	30.8026	Anisotropy =	7.9659
11	H	Isotropic =	30.1003	Anisotropy =	9.7685
12	H	Isotropic =	28.6498	Anisotropy =	9.3375
13	H	Isotropic =	30.4771	Anisotropy =	9.6380
14	H	Isotropic =	30.4007	Anisotropy =	9.3578
15	H	Isotropic =	30.4489	Anisotropy =	10.4923
16	H	Isotropic =	30.1952	Anisotropy =	9.4109
17	H	Isotropic =	30.2847	Anisotropy =	7.8980
18	H	Isotropic =	30.4847	Anisotropy =	10.8944
19	H	Isotropic =	31.0462	Anisotropy =	14.3630
20	H	Isotropic =	31.1144	Anisotropy =	15.0843

Conformer_12

C	-2.194396097845	-1.032238038436	-1.141819911356
C	-0.996209435842	-0.069511458641	-1.223354254744
C	0.127259132268	-0.519042197444	-0.296048410053
C	-0.328601208330	-0.425891615033	1.168645690568
C	-1.835184871376	-0.693829871301	1.335695855715
C	-2.347393024108	-1.651499249034	0.260667788484
N	1.322714161294	0.307836857090	-0.497976834768
H	-3.107971523873	-0.490457212379	-1.409610507778
H	-2.080251498926	-1.830866354224	-1.883024671018
H	-0.629830913239	-0.004465839214	-2.254149608274
H	-1.296141415905	0.945525311327	-0.932167055172
H	0.340757260415	-1.575567656955	-0.524662920415
H	0.252019301604	-1.134026428341	1.771523998376
H	-0.087430365363	0.577434763929	1.540052958743
H	-2.038288961744	-1.089749941889	2.335628778873
H	-2.390476221375	0.249079535612	1.258596794271
H	-3.394687248859	-1.911531820693	0.444739054238
H	-1.779973691728	-2.588461061143	0.321124772446
H	1.709545688252	0.129572618299	-1.420392545023
H	2.042840934681	0.035889658470	0.165631026886

SCF Done: E(RwB97X) = -291.235586089

Zero-point correction=	0.188917
Thermal correction to Energy=	0.196025

Thermal correction to Enthalpy=	0.196969
Thermal correction to Gibbs Free Energy=	0.158155
Sum of electronic and zero-point Energies=	-291.046669
Sum of electronic and thermal Energies=	-291.039561
Sum of electronic and thermal Enthalpies=	-291.038617
Sum of electronic and thermal Free Energies=	-291.077431

1 C	Isotropic =	170.0252	Anisotropy =	10.0404
2 C	Isotropic =	161.2793	Anisotropy =	24.2508
3 C	Isotropic =	144.9119	Anisotropy =	32.6562
4 C	Isotropic =	159.4893	Anisotropy =	25.2264
5 C	Isotropic =	170.7608	Anisotropy =	7.7607
6 C	Isotropic =	171.0997	Anisotropy =	5.5920
7 N	Isotropic =	219.0311	Anisotropy =	50.6011
8 H	Isotropic =	30.3266	Anisotropy =	10.3284
9 H	Isotropic =	30.3198	Anisotropy =	10.1711
10 H	Isotropic =	30.5168	Anisotropy =	8.2581
11 H	Isotropic =	30.7016	Anisotropy =	6.9356
12 H	Isotropic =	28.8326	Anisotropy =	5.8147
13 H	Isotropic =	30.0635	Anisotropy =	8.8045
14 H	Isotropic =	30.8556	Anisotropy =	7.3192
15 H	Isotropic =	30.4377	Anisotropy =	10.8818
16 H	Isotropic =	30.4270	Anisotropy =	8.8801
17 H	Isotropic =	30.5327	Anisotropy =	10.9202
18 H	Isotropic =	30.5980	Anisotropy =	8.9396
19 H	Isotropic =	30.9156	Anisotropy =	15.3183
20 H	Isotropic =	30.8772	Anisotropy =	14.2212

Conformer_13

C	-2.018651727358	-1.253013327734	-1.076705608412
C	-0.596417775563	-0.837760182864	-1.480827917936
C	0.322182693980	-0.536836170848	-0.276220028801
C	-0.201702215605	-1.222230553771	0.985294375123
C	-1.617892876317	-0.762532855703	1.371561251488
C	-2.499060605811	-0.469094846151	0.142476597124
N	0.397734836416	0.915781421446	-0.046653033958
H	-2.699684696650	-1.108932727799	-1.921898847663
H	-2.039777196975	-2.325265334950	-0.843160257361
H	-0.147867017359	-1.626803860081	-2.093565392186
H	-0.640040129623	0.056920494024	-2.113830303221
H	1.320070021089	-0.944355042253	-0.493217513745
H	-0.198101783608	-2.303179652015	0.802368369723
H	0.492433756330	-1.049527915806	1.815956943484
H	-2.081223960825	-1.544097282432	1.984247770226

H	-1.562887922287	0.129301033369	2.003570173481
H	-2.461663651895	0.600546599315	-0.092860096562
H	-3.545135083248	-0.706324629674	0.362317113932
H	0.795547268888	1.368111742272	-0.864342021537
H	1.038638066421	1.104593091655	0.719188426801

SCF Done: E(RwB97X) = -291.234094542

Zero-point correction=	0.188762
Thermal correction to Energy=	0.195863
Thermal correction to Enthalpy=	0.196807
Thermal correction to Gibbs Free Energy=	0.158063
Sum of electronic and zero-point Energies=	-291.045332
Sum of electronic and thermal Energies=	-291.038232
Sum of electronic and thermal Enthalpies=	-291.037288
Sum of electronic and thermal Free Energies=	-291.076032

1 C	Isotropic = 170.8036	Anisotropy = 3.9597
2 C	Isotropic = 159.7079	Anisotropy = 20.6399
3 C	Isotropic = 145.6473	Anisotropy = 26.9666
4 C	Isotropic = 165.4899	Anisotropy = 14.7480
5 C	Isotropic = 173.5297	Anisotropy = 16.6034
6 C	Isotropic = 171.2525	Anisotropy = 7.0683
7 N	Isotropic = 216.1427	Anisotropy = 52.6921
8 H	Isotropic = 30.4950	Anisotropy = 10.7595
9 H	Isotropic = 30.5131	Anisotropy = 9.3293
10 H	Isotropic = 30.1008	Anisotropy = 9.7689
11 H	Isotropic = 30.8021	Anisotropy = 7.9673
12 H	Isotropic = 28.6499	Anisotropy = 9.3381
13 H	Isotropic = 30.4007	Anisotropy = 9.3582
14 H	Isotropic = 30.4769	Anisotropy = 9.6380
15 H	Isotropic = 30.4488	Anisotropy = 10.4926
16 H	Isotropic = 30.1951	Anisotropy = 9.4101
17 H	Isotropic = 30.2843	Anisotropy = 7.8998
18 H	Isotropic = 30.4847	Anisotropy = 10.8942
19 H	Isotropic = 31.0458	Anisotropy = 14.3648
20 H	Isotropic = 31.1145	Anisotropy = 15.0817

Conformer_2

C	-1.613009045847	-1.265406553354	1.346388146385
C	-0.431314529109	-0.316806828145	1.140820819758
C	0.178542756267	-0.472103901608	-0.250104369310
C	-0.884110806520	-0.267025241293	-1.326871850095
C	-2.068600505932	-1.215316706197	-1.136535743723

C	-2.673515800440	-1.074700241475	0.261062268303
N	1.262937666869	0.498800533699	-0.429494041115
H	-1.254447411318	-2.303452601803	1.323167167911
H	-2.050739309916	-1.107688122965	2.337906743759
H	-0.765867361414	0.723522067329	1.257268353157
H	0.338345378443	-0.493017787523	1.902267662169
H	0.549860662669	-1.507556407142	-0.339126414831
H	-1.230754774617	0.774633517142	-1.276325946195
H	-0.436057927324	-0.407877925376	-2.318152343308
H	-2.828574170851	-1.022169050635	-1.901209534986
H	-1.732579307132	-2.250884863406	-1.282596230606
H	-3.487762368391	-1.795230466122	0.395932438044
H	-3.116289560507	-0.074337710410	0.362487882181
H	1.990931761881	0.333346782774	0.259567494066
H	1.697804653189	0.365571506508	-1.337952501565

SCF Done: E(RwB97X) = -291.246045274

Zero-point correction=	0.188616
Thermal correction to Energy=	0.195556
Thermal correction to Enthalpy=	0.196500
Thermal correction to Gibbs Free Energy=	0.158240
Sum of electronic and zero-point Energies=	-291.057429
Sum of electronic and thermal Energies=	-291.050490
Sum of electronic and thermal Enthalpies=	-291.049545
Sum of electronic and thermal Free Energies=	-291.087806

1 C	Isotropic = 165.5275	Anisotropy = 8.5360
2 C	Isotropic = 154.9127	Anisotropy = 19.9120
3 C	Isotropic = 139.6072	Anisotropy = 28.9357
4 C	Isotropic = 154.9127	Anisotropy = 19.9122
5 C	Isotropic = 165.5275	Anisotropy = 8.5360
6 C	Isotropic = 164.4771	Anisotropy = 3.4008
7 N	Isotropic = 217.6301	Anisotropy = 56.0446
8 H	Isotropic = 30.6145	Anisotropy = 8.8558
9 H	Isotropic = 30.2681	Anisotropy = 10.6396
10 H	Isotropic = 30.9459	Anisotropy = 6.5862
11 H	Isotropic = 30.2163	Anisotropy = 8.2471
12 H	Isotropic = 29.1646	Anisotropy = 5.8155
13 H	Isotropic = 30.9459	Anisotropy = 6.5862
14 H	Isotropic = 30.2163	Anisotropy = 8.2471
15 H	Isotropic = 30.2681	Anisotropy = 10.6396
16 H	Isotropic = 30.6145	Anisotropy = 8.8558
17 H	Isotropic = 30.3367	Anisotropy = 10.4297
18 H	Isotropic = 30.7265	Anisotropy = 8.9179
19 H	Isotropic = 30.8377	Anisotropy = 14.4896

20 H Isotropic = 30.8377 Anisotropy = 14.4896

Conformer_3

```
-----  
C      -1.675712705836  -0.644827265123  1.324595634225  
C      -0.211300485251  -1.011363121920  1.074963451581  
C       0.291172997237  -0.522442487038  -0.293607001003  
C      -0.632246697116  -1.031360090617  -1.405302068328  
C      -2.099106158867  -0.664834738291  -1.164461877602  
C      -2.576480356991  -1.161106166388  0.201268683420  
N       0.433657129608  0.938763109863  -0.385923071805  
H      -2.000217713091  -1.049464923377  2.289481160847  
H      -1.778397327914  0.446371338880  1.398484094763  
H       0.428098189255  -0.599094615490  1.864601568736  
H      -0.102855957583  -2.103594275544  1.116172333656  
H       1.291054581752  -0.938855222377  -0.460571398262  
H      -0.291577018369  -0.639742648438  -2.370096666182  
H      -0.544589784020  -2.124319227366  -1.452707586048  
H      -2.229214047827  0.424502432896  -1.222161936139  
H      -2.719337329988  -1.089275266377  -1.961228923525  
H      -2.565272023490  -2.259916363850  0.207732073430  
H      -3.613869175518  -0.854915595082  0.375451693761  
H       1.053018674364  1.265811722626  0.349723249765  
H      -0.458624790357  1.394263403012  -0.219113415291
```

SCF Done: E(RwB97X) = -291.243850747

```
Zero-point correction=          0.188829  
Thermal correction to Energy=      0.195731  
Thermal correction to Enthalpy=     0.196675  
Thermal correction to Gibbs Free Energy= 0.158517  
Sum of electronic and zero-point Energies= -291.055022  
Sum of electronic and thermal Energies= -291.048120  
Sum of electronic and thermal Enthalpies= -291.047176  
Sum of electronic and thermal Free Energies= -291.085334
```

```
1 C Isotropic = 170.6645 Anisotropy = 17.9413  
2 C Isotropic = 155.3109 Anisotropy = 18.1609  
3 C Isotropic = 143.7841 Anisotropy = 28.9466  
4 C Isotropic = 158.0169 Anisotropy = 13.9907  
5 C Isotropic = 170.0026 Anisotropy = 15.6623  
6 C Isotropic = 164.1660 Anisotropy = 2.8674  
7 N Isotropic = 226.9254 Anisotropy = 54.7951  
8 H Isotropic = 30.5307 Anisotropy = 11.0061  
9 H Isotropic = 30.2914 Anisotropy = 7.2512
```

10	H	Isotropic =	30.4786	Anisotropy =	9.0651
11	H	Isotropic =	30.3740	Anisotropy =	8.5588
12	H	Isotropic =	29.0493	Anisotropy =	8.6358
13	H	Isotropic =	30.3219	Anisotropy =	9.3170
14	H	Isotropic =	30.3681	Anisotropy =	8.6712
15	H	Isotropic =	30.4732	Anisotropy =	7.3046
16	H	Isotropic =	30.5104	Anisotropy =	10.9959
17	H	Isotropic =	30.6816	Anisotropy =	8.9855
18	H	Isotropic =	30.3073	Anisotropy =	10.3758
19	H	Isotropic =	31.1777	Anisotropy =	15.4979
20	H	Isotropic =	30.2246	Anisotropy =	9.7952

Conformer_4

C	-1.619179827758	-1.324079160162	1.349249455434
C	-0.451854170085	-0.348611718094	1.192001959894
C	0.162853057020	-0.410302669945	-0.204915831407
C	-0.913329835393	-0.192051975926	-1.273763020287
C	-2.076772024667	-1.173850659179	-1.125482116616
C	-2.684557010568	-1.103203315226	0.275364386689
N	1.277111829835	0.539654913853	-0.293853808941
H	-1.241094678506	-2.352883192948	1.275301458171
H	-2.057760008184	-1.222882319570	2.347865138538
H	-0.805210160211	0.678030764950	1.370032794635
H	0.322779402824	-0.552765707520	1.939458209779
H	0.585873551630	-1.414829682658	-0.347062040609
H	-1.287280410242	0.838249802088	-1.180828272623
H	-0.461595098799	-0.279246975548	-2.269351033846
H	-2.840364814256	-0.969548054121	-1.883882804875
H	-1.715069957412	-2.194515930055	-1.311166094951
H	-3.143779244802	-0.115519737487	0.419829826146
H	-3.486591306774	-1.842243630691	0.379792889543
H	0.918612547658	1.485610321154	-0.187166470418
H	1.688908158690	0.500388927086	-1.221824624257

SCF Done: E(RwB97X) = -291.245974907

Zero-point correction=	0.188661
Thermal correction to Energy=	0.195622
Thermal correction to Enthalpy=	0.196566
Thermal correction to Gibbs Free Energy=	0.158244
Sum of electronic and zero-point Energies=	-291.057313
Sum of electronic and thermal Energies=	-291.050353
Sum of electronic and thermal Enthalpies=	-291.049409
Sum of electronic and thermal Free Energies=	-291.087731

1 C	Isotropic =	164.1730	Anisotropy =	7.8304
2 C	Isotropic =	154.9770	Anisotropy =	19.8759
3 C	Isotropic =	139.0405	Anisotropy =	30.0402
4 C	Isotropic =	150.0696	Anisotropy =	27.2721
5 C	Isotropic =	164.7122	Anisotropy =	9.2127
6 C	Isotropic =	164.5936	Anisotropy =	4.1864
7 N	Isotropic =	214.8233	Anisotropy =	57.9261
8 H	Isotropic =	30.5988	Anisotropy =	8.8142
9 H	Isotropic =	30.2142	Anisotropy =	10.5481
10 H	Isotropic =	30.9741	Anisotropy =	6.4625
11 H	Isotropic =	30.1252	Anisotropy =	8.3981
12 H	Isotropic =	29.5908	Anisotropy =	5.8006
13 H	Isotropic =	30.9591	Anisotropy =	6.1207
14 H	Isotropic =	30.1379	Anisotropy =	7.6803
15 H	Isotropic =	30.2888	Anisotropy =	10.6070
16 H	Isotropic =	30.6404	Anisotropy =	8.7053
17 H	Isotropic =	30.7861	Anisotropy =	8.8818
18 H	Isotropic =	30.3669	Anisotropy =	10.3939
19 H	Isotropic =	31.3231	Anisotropy =	11.7244
20 H	Isotropic =	30.7291	Anisotropy =	14.4555

Conformer_5

C	-1.693631710909	-0.519441472879	1.279681314933
C	-0.264753930873	-0.993278230037	1.019026630652
C	0.254305150270	-0.508032084879	-0.349075423541
C	-0.910065166549	-0.330503423484	-1.343833616185
C	-2.006573140083	-1.366709185506	-1.105619894869
C	-2.668765791383	-1.150049050885	0.268994739361
N	1.053455420603	0.715122291216	-0.179345069151
H	-1.998302164105	-0.763466997316	2.302196450676
H	-1.729217355615	0.574341425335	1.201305970236
H	0.417533456809	-0.642650926133	1.800320183916
H	-0.244430353597	-2.088872265794	1.053276743804
H	0.933928781201	-1.270066090178	-0.748351997119
H	-1.331542891676	0.675872757879	-1.215491102673
H	-0.529472237691	-0.382225426702	-2.369666323620
H	-2.757805807011	-1.324823697648	-1.900398539839
H	-1.562174894123	-2.368712319252	-1.155472736910
H	-3.547648877446	-0.504492471457	0.161579105423
H	-3.032389333111	-2.108798473352	0.655099326353
H	1.332275528409	1.066055240696	-1.091745497267
H	0.466575316881	1.441430400376	0.225219735818

SCF Done: E(RwB97X) = -291.234781267

Zero-point correction=	0.188491
Thermal correction to Energy=	0.195664
Thermal correction to Enthalpy=	0.196608
Thermal correction to Gibbs Free Energy=	0.157459
Sum of electronic and zero-point Energies=	-291.046290
Sum of electronic and thermal Energies=	-291.039117
Sum of electronic and thermal Enthalpies=	-291.038173
Sum of electronic and thermal Free Energies=	-291.077322

1 C	Isotropic =	173.8794	Anisotropy =	13.3352
2 C	Isotropic =	161.3787	Anisotropy =	19.0625
3 C	Isotropic =	143.3544	Anisotropy =	31.2159
4 C	Isotropic =	156.2781	Anisotropy =	30.1072
5 C	Isotropic =	171.8116	Anisotropy =	7.9114
6 C	Isotropic =	169.2464	Anisotropy =	8.2371
7 N	Isotropic =	214.6540	Anisotropy =	53.1808
8 H	Isotropic =	30.5576	Anisotropy =	10.9862
9 H	Isotropic =	30.4268	Anisotropy =	7.9968
10 H	Isotropic =	30.6220	Anisotropy =	8.6486
11 H	Isotropic =	30.1900	Anisotropy =	8.7059
12 H	Isotropic =	29.1029	Anisotropy =	7.6619
13 H	Isotropic =	30.8836	Anisotropy =	6.1055
14 H	Isotropic =	30.1418	Anisotropy =	8.4540
15 H	Isotropic =	30.5191	Anisotropy =	10.9730
16 H	Isotropic =	30.6921	Anisotropy =	9.3482
17 H	Isotropic =	30.3762	Anisotropy =	10.2920
18 H	Isotropic =	30.4385	Anisotropy =	10.4245
19 H	Isotropic =	30.8500	Anisotropy =	14.3901
20 H	Isotropic =	30.9161	Anisotropy =	10.2418

Conformer_6

C	-1.567322924400	-1.414599963713	1.289725248979
C	-0.450353159643	-0.380567158123	1.163421646532
C	0.284266830900	-0.511244608728	-0.185680040010
C	-0.689643463958	-0.946998009492	-1.298427596779
C	-2.114717328306	-0.473657552332	-1.016883385957
C	-2.672436404370	-1.149758493374	0.248769279624
N	0.979852902370	0.723221317831	-0.580407876809
H	-1.987545391248	-1.408792549941	2.300248558348
H	-1.141183412441	-2.414584566868	1.139987816286
H	-0.882867991961	0.626981101305	1.231873954866
H	0.268936458092	-0.469140497870	1.984783987239

H	1.055944113115	-1.283258146883	-0.083136602803
H	-0.326342268511	-0.561607665854	-2.256739511828
H	-0.690487355681	-2.040279841629	-1.379953873253
H	-2.763923257592	-0.680189719625	-1.873496408406
H	-2.112506950175	0.616001984839	-0.888792531514
H	-3.156083037295	-2.095455781543	-0.020009176913
H	-3.451538009242	-0.515117772414	0.685746095244
H	1.566588788438	1.040645583457	0.186633166875
H	0.292761861907	1.460402340957	-0.722162749722

SCF Done: E(RwB97X) = -291.234781267

Zero-point correction=	0.188491
Thermal correction to Energy=	0.195664
Thermal correction to Enthalpy=	0.196608
Thermal correction to Gibbs Free Energy=	0.157459
Sum of electronic and zero-point Energies=	-291.046290
Sum of electronic and thermal Energies=	-291.039117
Sum of electronic and thermal Enthalpies=	-291.038173
Sum of electronic and thermal Free Energies=	-291.077322

1 C	Isotropic =	171.8116	Anisotropy =	7.9114
2 C	Isotropic =	156.2781	Anisotropy =	30.1072
3 C	Isotropic =	143.3544	Anisotropy =	31.2159
4 C	Isotropic =	161.3787	Anisotropy =	19.0625
5 C	Isotropic =	173.8794	Anisotropy =	13.3352
6 C	Isotropic =	169.2464	Anisotropy =	8.2371
7 N	Isotropic =	214.6540	Anisotropy =	53.1808
8 H	Isotropic =	30.5191	Anisotropy =	10.9730
9 H	Isotropic =	30.6921	Anisotropy =	9.3482
10 H	Isotropic =	30.8836	Anisotropy =	6.1055
11 H	Isotropic =	30.1418	Anisotropy =	8.4540
12 H	Isotropic =	29.1029	Anisotropy =	7.6619
13 H	Isotropic =	30.6220	Anisotropy =	8.6486
14 H	Isotropic =	30.1900	Anisotropy =	8.7059
15 H	Isotropic =	30.5576	Anisotropy =	10.9862
16 H	Isotropic =	30.4268	Anisotropy =	7.9968
17 H	Isotropic =	30.4385	Anisotropy =	10.4245
18 H	Isotropic =	30.3762	Anisotropy =	10.2920
19 H	Isotropic =	30.8500	Anisotropy =	14.3901
20 H	Isotropic =	30.9161	Anisotropy =	10.2418

Conformer_7

C -1.590644096931 -0.758984623761 1.401267274430

C	-0.184217908431	-1.210871766659	0.975610367839
C	0.300737845869	-0.503407450334	-0.295753050742
C	-0.647528044836	-0.816252139537	-1.476830943917
C	-2.038863732388	-1.290453396751	-1.032938285639
C	-2.517483427721	-0.514107209245	0.192142271283
N	0.448075360854	0.953501281345	-0.132589616711
H	-2.021281395904	-1.525907791939	2.053815598013
H	-1.525680589710	0.151833520016	2.006121309937
H	0.531043874078	-1.040995359241	1.788439813807
H	-0.184891081980	-2.290971532357	0.783959448836
H	1.299291170586	-0.882167704388	-0.536733609800
H	-0.745749536174	0.091586466429	-2.083497642224
H	-0.194678593474	-1.573745134895	-2.124832797300
H	-2.747097686405	-1.180323974102	-1.860514067005
H	-2.010368569165	-2.360265273959	-0.790461741519
H	-2.538624266967	0.554745799797	-0.057824823632
H	-3.547175221690	-0.787725849570	0.442833286106
H	1.025456338776	1.146769215410	0.681264173312
H	-0.455120438388	1.378342923743	0.058423034926

SCF Done: E(RwB97X) = -291.233771703

Zero-point correction=	0.188731
Thermal correction to Energy=	0.195897
Thermal correction to Enthalpy=	0.196841
Thermal correction to Gibbs Free Energy=	0.157802
Sum of electronic and zero-point Energies=	-291.045040
Sum of electronic and thermal Energies=	-291.037874
Sum of electronic and thermal Enthalpies=	-291.036930
Sum of electronic and thermal Free Energies=	-291.075970

1 C	Isotropic =	174.6168	Anisotropy =	18.8810
2 C	Isotropic =	162.8040	Anisotropy =	18.3298
3 C	Isotropic =	144.7072	Anisotropy =	29.2343
4 C	Isotropic =	159.5357	Anisotropy =	20.2845
5 C	Isotropic =	170.5202	Anisotropy =	3.9623
6 C	Isotropic =	170.8962	Anisotropy =	7.9614
7 N	Isotropic =	216.9734	Anisotropy =	66.8907
8 H	Isotropic =	30.3773	Anisotropy =	10.5893
9 H	Isotropic =	30.1910	Anisotropy =	9.2831
10 H	Isotropic =	30.5795	Anisotropy =	9.5686
11 H	Isotropic =	30.3224	Anisotropy =	9.2337
12 H	Isotropic =	29.0022	Anisotropy =	8.8356
13 H	Isotropic =	30.7299	Anisotropy =	7.7464
14 H	Isotropic =	29.8765	Anisotropy =	9.6525
15 H	Isotropic =	30.5175	Anisotropy =	10.9039

16 H	Isotropic =	30.5356	Anisotropy =	9.2792
17 H	Isotropic =	30.5896	Anisotropy =	7.9857
18 H	Isotropic =	30.3803	Anisotropy =	10.8661
19 H	Isotropic =	31.1638	Anisotropy =	15.5005
20 H	Isotropic =	30.7033	Anisotropy =	9.1056

Conformer_8

C	-1.623180783578	-1.335428828882	1.236211975870
C	-0.161526687634	-0.868870689945	1.176091119417
C	0.308849350054	-0.504321017138	-0.251450002480
C	-0.600124779279	-1.165897582150	-1.294587216010
C	-2.062905618566	-0.707893872069	-1.176577573719
C	-2.499379685406	-0.516048156581	0.290958965514
N	0.399051062901	0.958770504111	-0.400246151610
H	-1.991399756683	-1.262073158054	2.264627848657
H	-1.690000632014	-2.394930621157	0.958551438819
H	-0.031989095819	0.014319505419	1.812532646412
H	0.486213855722	-1.647472444634	1.592007111911
H	1.325308371873	-0.885029518184	-0.394669731679
H	-0.218136819636	-0.959967669912	-2.300980337273
H	-0.540440614863	-2.252529941636	-1.156695736083
H	-2.702223018237	-1.452238529695	-1.663058081843
H	-2.210091338858	0.225873717199	-1.729816030594
H	-2.423032439738	0.542260480389	0.572971896145
H	-3.552990002386	-0.787050809548	0.411130402047
H	0.651908202195	1.187150342951	-1.357839579069
H	-0.510209570047	1.384278289514	-0.242362964433

SCF Done: E(RwB97X) = -291.233771703

Zero-point correction=	0.188731
Thermal correction to Energy=	0.195897
Thermal correction to Enthalpy=	0.196841
Thermal correction to Gibbs Free Energy=	0.157802
Sum of electronic and zero-point Energies=	-291.045040
Sum of electronic and thermal Energies=	-291.037874
Sum of electronic and thermal Enthalpies=	-291.036930
Sum of electronic and thermal Free Energies=	-291.075970

1 C	Isotropic =	170.5202	Anisotropy =	3.9622
2 C	Isotropic =	159.5358	Anisotropy =	20.2845
3 C	Isotropic =	144.7071	Anisotropy =	29.2345
4 C	Isotropic =	162.8040	Anisotropy =	18.3298
5 C	Isotropic =	174.6166	Anisotropy =	18.8807

6 C	Isotropic =	170.8962	Anisotropy =	7.9612
7 N	Isotropic =	216.9733	Anisotropy =	66.8900
8 H	Isotropic =	30.5175	Anisotropy =	10.9039
9 H	Isotropic =	30.5356	Anisotropy =	9.2793
10 H	Isotropic =	30.7299	Anisotropy =	7.7464
11 H	Isotropic =	29.8765	Anisotropy =	9.6525
12 H	Isotropic =	29.0022	Anisotropy =	8.8356
13 H	Isotropic =	30.5795	Anisotropy =	9.5686
14 H	Isotropic =	30.3224	Anisotropy =	9.2338
15 H	Isotropic =	30.3773	Anisotropy =	10.5893
16 H	Isotropic =	30.1910	Anisotropy =	9.2832
17 H	Isotropic =	30.5896	Anisotropy =	7.9857
18 H	Isotropic =	30.3803	Anisotropy =	10.8661
19 H	Isotropic =	31.1638	Anisotropy =	15.5004
20 H	Isotropic =	30.7033	Anisotropy =	9.1056

Conformer_9

C	-1.842750876163	-0.726544306980	1.319154645166
C	-0.332418914546	-0.469099702461	1.170340350775
C	0.133371670744	-0.526128204093	-0.293104966845
C	-0.978896247680	-0.040418130279	-1.215634384188
C	-2.186765818843	-0.993315558735	-1.169243416078
C	-2.356196760713	-1.649271809681	0.214547636025
N	1.337996796479	0.294506140411	-0.463497108098
H	-2.057060668199	-1.147725489368	2.306345246322
H	-2.388319274165	0.223552663462	1.264057696400
H	-0.084230538218	0.521069495802	1.571255123708
H	0.236742759705	-1.199461688871	1.757412168152
H	0.338597886509	-1.577952159549	-0.549306805134
H	-1.271352717173	0.969063781379	-0.898688086781
H	-0.604355106490	0.049433013824	-2.241619819683
H	-3.093049603590	-0.435422708002	-1.428602076999
H	-2.074794572637	-1.772408432920	-1.931274755482
H	-1.798284909356	-2.593064052760	0.253305811586
H	-3.407288541107	-1.903963782860	0.383838715159
H	2.050425208703	-0.002316888630	0.197753670342
H	1.730230226742	0.137767820310	-1.387539644348

SCF Done: E(RwB97X) = -291.235586091

Zero-point correction=	0.188916
Thermal correction to Energy=	0.196025
Thermal correction to Enthalpy=	0.196969
Thermal correction to Gibbs Free Energy=	0.158154

Sum of electronic and zero-point Energies=	-291.046670
Sum of electronic and thermal Energies=	-291.039561
Sum of electronic and thermal Enthalpies=	-291.038617
Sum of electronic and thermal Free Energies=	-291.077432

1 C	Isotropic =	170.7597	Anisotropy =	7.7602
2 C	Isotropic =	159.4891	Anisotropy =	25.2267
3 C	Isotropic =	144.9142	Anisotropy =	32.6538
4 C	Isotropic =	161.2797	Anisotropy =	24.2543
5 C	Isotropic =	170.0260	Anisotropy =	10.0404
6 C	Isotropic =	171.0979	Anisotropy =	5.5949
7 N	Isotropic =	219.0329	Anisotropy =	50.5992
8 H	Isotropic =	30.4379	Anisotropy =	10.8818
9 H	Isotropic =	30.4271	Anisotropy =	8.8800
10 H	Isotropic =	30.8557	Anisotropy =	7.3194
11 H	Isotropic =	30.0636	Anisotropy =	8.8047
12 H	Isotropic =	28.8328	Anisotropy =	5.8161
13 H	Isotropic =	30.7017	Anisotropy =	6.9352
14 H	Isotropic =	30.5167	Anisotropy =	8.2580
15 H	Isotropic =	30.3266	Anisotropy =	10.3281
16 H	Isotropic =	30.3200	Anisotropy =	10.1713
17 H	Isotropic =	30.5983	Anisotropy =	8.9398
18 H	Isotropic =	30.5325	Anisotropy =	10.9200
19 H	Isotropic =	30.8776	Anisotropy =	14.2200
20 H	Isotropic =	30.9155	Anisotropy =	15.3202

Cyclohexanamine_protonated

Conformer_1

C	-2.067393498523	-0.779285608897	-1.261757217126
C	-0.540022833143	-0.700143351099	-1.264572567136
C	-0.046837155627	-0.010902420140	0.000002904528
C	-0.540018768310	-0.700140936758	1.264581276406
C	-2.067389443284	-0.779283204746	1.261770976516
C	-2.587598191821	-1.467979188737	0.000008366849
N	1.451579658837	0.010298709796	0.000000481461
H	-2.481511167336	0.235583991303	-1.320640380538
H	-2.405156273769	-1.311016187847	-2.156307170384
H	-0.116866197714	-1.712943644892	-1.302568626030
H	-0.181792593851	-0.159360024253	-2.146992680117
H	-0.353401546223	1.039167746829	0.000002395893
H	-0.116862015074	-1.712941159522	1.302577914563
H	-0.181785703510	-0.159355923789	2.146999208602
H	-2.405149344831	-1.311012088960	2.156322976405
H	-2.481506930402	0.235586503815	1.320653541134

H	-3.682353366090	-1.475096294582	0.000010129185
H	-2.262474725519	-2.516903000594	0.000008844630
H	1.833894406002	-0.939126049126	0.000000772752
H	1.817321515002	0.490925268817	-0.825344761358
H	1.817324175186	0.490926863384	0.825343595885

SCF Done: E(RwB97X) = -291.717604251

Zero-point correction=	0.204158
Thermal correction to Energy=	0.211220
Thermal correction to Enthalpy=	0.212165
Thermal correction to Gibbs Free Energy=	0.173584
Sum of electronic and zero-point Energies=	-291.513446
Sum of electronic and thermal Energies=	-291.506384
Sum of electronic and thermal Enthalpies=	-291.505440
Sum of electronic and thermal Free Energies=	-291.544021

1 C	Isotropic = 165.8513	Anisotropy = 9.4527
2 C	Isotropic = 159.1100	Anisotropy = 13.9351
3 C	Isotropic = 136.2114	Anisotropy = 37.0175
4 C	Isotropic = 159.1100	Anisotropy = 13.9351
5 C	Isotropic = 165.8513	Anisotropy = 9.4527
6 C	Isotropic = 165.3858	Anisotropy = 3.9571
7 N	Isotropic = 206.0118	Anisotropy = 43.0288
8 H	Isotropic = 30.5053	Anisotropy = 9.0961
9 H	Isotropic = 30.1056	Anisotropy = 10.8000
10 H	Isotropic = 30.5445	Anisotropy = 7.2980
11 H	Isotropic = 29.8861	Anisotropy = 9.1231
12 H	Isotropic = 28.6265	Anisotropy = 5.9928
13 H	Isotropic = 30.5445	Anisotropy = 7.2980
14 H	Isotropic = 29.8861	Anisotropy = 9.1231
15 H	Isotropic = 30.1056	Anisotropy = 10.8000
16 H	Isotropic = 30.5053	Anisotropy = 9.0961
17 H	Isotropic = 30.2770	Anisotropy = 10.6101
18 H	Isotropic = 30.6684	Anisotropy = 9.0325
19 H	Isotropic = 27.5673	Anisotropy = 13.0102
20 H	Isotropic = 27.1569	Anisotropy = 15.6765
21 H	Isotropic = 27.1569	Anisotropy = 15.6765

Conformer_2

C	-1.678828039991	-1.259497941912	-1.259399028090
C	-0.830596734300	0.014505898583	-1.270117863934
C	-0.003186717554	0.194245640686	0.000002819153
C	-0.830607160225	0.014507018555	1.270116952201

C	-1.678837203922	-1.259497941067	1.259391994999
C	-2.540985292769	-1.343186840578	-0.000006691375
N	1.145074524501	-0.781183464246	0.000009028941
H	-2.304221322057	-1.278501179339	-2.156983747223
H	-1.032851340990	-2.146428625028	-1.316169206378
H	-0.173576034343	0.043041174524	-2.146151286551
H	-1.488750920708	0.887448904168	-1.340190652418
H	0.475060325411	1.175135648236	0.000003945419
H	-0.173594297165	0.043044053096	2.146156222314
H	-1.488763180415	0.887449178358	1.340182988943
H	-1.032860561063	-2.146428525931	1.316167782132
H	-2.304237223039	-1.278501289211	2.156971937899
H	-3.119409817114	-2.272498934929	-0.000008948272
H	-3.264027572620	-0.516585415812	-0.000009194246
H	1.734358712194	-0.650815843219	-0.825343284965
H	1.734365142522	-0.650796008499	0.825353513221
H	0.834374713645	-1.755455506433	0.000022718227

SCF Done: E(RwB97X) = -291.715976706

Zero-point correction=	0.204761
Thermal correction to Energy=	0.211609
Thermal correction to Enthalpy=	0.212553
Thermal correction to Gibbs Free Energy=	0.174483
Sum of electronic and zero-point Energies=	-291.511216
Sum of electronic and thermal Energies=	-291.504367
Sum of electronic and thermal Enthalpies=	-291.503423
Sum of electronic and thermal Free Energies=	-291.541493

1 C	Isotropic = 170.3075	Anisotropy = 15.7194
2 C	Isotropic = 161.8490	Anisotropy = 8.7629
3 C	Isotropic = 138.9685	Anisotropy = 38.6037
4 C	Isotropic = 161.8491	Anisotropy = 8.7628
5 C	Isotropic = 170.3075	Anisotropy = 15.7196
6 C	Isotropic = 165.1318	Anisotropy = 3.5668
7 N	Isotropic = 214.1764	Anisotropy = 31.7909
8 H	Isotropic = 30.3093	Anisotropy = 11.0408
9 H	Isotropic = 30.4014	Anisotropy = 7.8666
10 H	Isotropic = 30.0281	Anisotropy = 9.6739
11 H	Isotropic = 30.0937	Anisotropy = 9.3375
12 H	Isotropic = 28.2575	Anisotropy = 8.5301
13 H	Isotropic = 30.0281	Anisotropy = 9.6739
14 H	Isotropic = 30.0937	Anisotropy = 9.3375
15 H	Isotropic = 30.4014	Anisotropy = 7.8666
16 H	Isotropic = 30.3093	Anisotropy = 11.0408
17 H	Isotropic = 30.2139	Anisotropy = 10.5678

18 H	Isotropic =	30.5453	Anisotropy =	9.0814
19 H	Isotropic =	27.3522	Anisotropy =	16.2244
20 H	Isotropic =	27.3522	Anisotropy =	16.2245
21 H	Isotropic =	26.6274	Anisotropy =	11.1109

Conformer_3

C	-2.024726438211	-0.970518190231	1.313796363377
C	-0.490870259901	-0.930538480342	1.182888657498
C	-0.097929792450	-0.015430890989	0.034456122199
C	-0.559377972387	-0.571375157716	-1.317115767262
C	-1.885162102861	-1.341005558315	-1.180635944719
C	-2.731601947236	-0.777674660567	-0.040378396141
N	1.388055140665	0.166654290348	0.011119214714
H	-2.311673277849	-1.931851362788	1.750690313995
H	-2.354475848206	-0.196731281934	2.014079114814
H	-0.034498118363	-0.589815119789	2.117455492867
H	-0.095299358206	-1.932518642627	0.975984918648
H	-0.504947080171	0.984739562459	0.201605062000
H	0.215108722101	-1.238575129343	-1.712918020951
H	-0.663958636312	0.255337066620	-2.026567052487
H	-2.430629385992	-1.301531084491	-2.127387196000
H	-1.680508638499	-2.399253222809	-0.981229393945
H	-2.908123043979	0.289584790673	-0.222548105181
H	-3.714915138934	-1.256238857108	-0.019662257661
H	1.721837633960	0.623463649929	0.862955056413
H	1.868570233618	-0.733679805538	-0.068255888695
H	1.679225309211	0.741558084558	-0.783332293482

SCF Done: E(RwB97X) = -291.707229229

Zero-point correction=	0.204414
Thermal correction to Energy=	0.211657
Thermal correction to Enthalpy=	0.212601
Thermal correction to Gibbs Free Energy=	0.173394
Sum of electronic and zero-point Energies=	-291.502816
Sum of electronic and thermal Energies=	-291.495573
Sum of electronic and thermal Enthalpies=	-291.494628
Sum of electronic and thermal Free Energies=	-291.533835

1 C	Isotropic =	170.5639	Anisotropy =	10.4679
2 C	Isotropic =	165.4656	Anisotropy =	18.2352
3 C	Isotropic =	139.9831	Anisotropy =	42.5109
4 C	Isotropic =	163.1393	Anisotropy =	19.7908
5 C	Isotropic =	171.0137	Anisotropy =	7.6049

6 C	Isotropic =	171.5283	Anisotropy =	5.5900
7 N	Isotropic =	206.8411	Anisotropy =	39.4465
8 H	Isotropic =	30.1793	Anisotropy =	10.4634
9 H	Isotropic =	30.1651	Anisotropy =	10.4833
10 H	Isotropic =	30.1040	Anisotropy =	9.2098
11 H	Isotropic =	30.2840	Anisotropy =	7.6579
12 H	Isotropic =	28.3922	Anisotropy =	5.8971
13 H	Isotropic =	30.4376	Anisotropy =	8.1182
14 H	Isotropic =	29.7870	Anisotropy =	9.4727
15 H	Isotropic =	30.2896	Anisotropy =	11.0906
16 H	Isotropic =	30.3298	Anisotropy =	9.0317
17 H	Isotropic =	30.5875	Anisotropy =	9.1407
18 H	Isotropic =	30.4165	Anisotropy =	11.0604
19 H	Isotropic =	27.1843	Anisotropy =	16.2945
20 H	Isotropic =	27.6485	Anisotropy =	13.0649
21 H	Isotropic =	27.1634	Anisotropy =	15.5462

Conformer_4

C	-1.604889056849	-1.334793773465	1.199574901227
C	-0.870310390523	0.003107243285	1.162324109945
C	-0.012121714952	0.126429061325	-0.102164102757
C	-0.582269496514	-0.666809761145	-1.283377654226
C	-2.107914109101	-0.680453984320	-1.216432389859
C	-2.598035457518	-1.443687768230	0.028146712396
N	1.373498925540	-0.377817967993	0.185845417183
H	-0.870728957816	-2.148478136948	1.147684496848
H	-2.125567220591	-1.452127130220	2.153747738879
H	-1.596584992874	0.821700902537	1.161658366013
H	-0.244445598980	0.143830377720	2.049834753420
H	0.118344259047	1.176221176218	-0.369766969981
H	-0.212986227125	-1.699605356822	-1.238131153469
H	-0.224835769932	-0.239692945358	-2.224162730995
H	-2.470162652595	0.354039754865	-1.193337385239
H	-2.516586099252	-1.130043830118	-2.125216332525
H	-3.573683563315	-1.050299435582	0.331850330681
H	-2.749668215000	-2.499584773397	-0.219490355959
H	1.962164792104	-0.350241116141	-0.649718770598
H	1.832255802521	0.181955402374	0.907618726571
H	1.349925743724	-1.347447938586	0.513712292446

SCF Done: E(RwB97X) = -291.707757503

Zero-point correction=	0.204457
Thermal correction to Energy=	0.211517

Thermal correction to Enthalpy=	0.212461
Thermal correction to Gibbs Free Energy=	0.173747
Sum of electronic and zero-point Energies=	-291.503300
Sum of electronic and thermal Energies=	-291.496240
Sum of electronic and thermal Enthalpies=	-291.495296
Sum of electronic and thermal Free Energies=	-291.534010

1 C	Isotropic =	175.1111	Anisotropy =	13.6384
2 C	Isotropic =	165.2242	Anisotropy =	13.3553
3 C	Isotropic =	139.6434	Anisotropy =	37.6604
4 C	Isotropic =	164.7396	Anisotropy =	18.4544
5 C	Isotropic =	173.1189	Anisotropy =	8.0967
6 C	Isotropic =	170.1616	Anisotropy =	8.5123
7 N	Isotropic =	208.1862	Anisotropy =	38.7442
8 H	Isotropic =	30.3762	Anisotropy =	8.3141
9 H	Isotropic =	30.4163	Anisotropy =	11.2366
10 H	Isotropic =	30.0315	Anisotropy =	9.4283
11 H	Isotropic =	30.3385	Anisotropy =	9.5533
12 H	Isotropic =	28.1953	Anisotropy =	7.9021
13 H	Isotropic =	30.5440	Anisotropy =	7.1422
14 H	Isotropic =	29.8768	Anisotropy =	10.0488
15 H	Isotropic =	30.5528	Anisotropy =	9.6800
16 H	Isotropic =	30.3599	Anisotropy =	11.1726
17 H	Isotropic =	30.3237	Anisotropy =	10.6373
18 H	Isotropic =	30.2869	Anisotropy =	10.4014
19 H	Isotropic =	27.3055	Anisotropy =	15.7929
20 H	Isotropic =	27.3903	Anisotropy =	16.6592
21 H	Isotropic =	27.2025	Anisotropy =	11.6488

Conformer_5

C	-2.107923552252	-0.680464789210	1.216437122819
C	-0.582278788578	-0.666832998808	1.283382066682
C	-0.012125305544	0.126421156735	0.102181520320
C	-0.870315522390	0.003127059997	-1.162308308556
C	-1.604903434211	-1.334768235944	-1.199580889185
C	-2.598051030579	-1.443673759766	-0.028154843628
N	1.373490978095	-0.377832555518	-0.185837326850
H	-2.516598491234	-1.130067038721	2.125213602180
H	-2.470164460696	0.354032000082	1.193359852967
H	-0.224841536423	-0.239734634965	2.224174175202
H	-0.213003255630	-1.699630602747	1.238118133743
H	0.118349368578	1.176207751368	0.369801786555
H	-0.244450191997	0.143860666347	-2.049816906131
H	-1.596584372779	0.821725815843	-1.161628336489

H	-2.125582010425	-1.452082950816	-2.153755791043
H	-0.870748882044	-2.148458429154	-1.147702919910
H	-3.573695736643	-1.050272184067	-0.331852181073
H	-2.749692613620	-2.499573685260	0.219464416451
H	1.349909098201	-1.347456859634	-0.513720458757
H	1.832252056318	0.181949009743	-0.907601609731
H	1.962157683852	-0.350274735504	0.649726894433

SCF Done: E(RwB97X) = -291.707757503

Zero-point correction=	0.204457
Thermal correction to Energy=	0.211517
Thermal correction to Enthalpy=	0.212461
Thermal correction to Gibbs Free Energy=	0.173747
Sum of electronic and zero-point Energies=	-291.503300
Sum of electronic and thermal Energies=	-291.496240
Sum of electronic and thermal Enthalpies=	-291.495296
Sum of electronic and thermal Free Energies=	-291.534010

1 C	Isotropic =	173.1189	Anisotropy =	8.0968
2 C	Isotropic =	164.7396	Anisotropy =	18.4544
3 C	Isotropic =	139.6434	Anisotropy =	37.6604
4 C	Isotropic =	165.2242	Anisotropy =	13.3552
5 C	Isotropic =	175.1111	Anisotropy =	13.6384
6 C	Isotropic =	170.1615	Anisotropy =	8.5123
7 N	Isotropic =	208.1862	Anisotropy =	38.7442
8 H	Isotropic =	30.3599	Anisotropy =	11.1726
9 H	Isotropic =	30.5528	Anisotropy =	9.6800
10 H	Isotropic =	29.8768	Anisotropy =	10.0488
11 H	Isotropic =	30.5440	Anisotropy =	7.1422
12 H	Isotropic =	28.1953	Anisotropy =	7.9021
13 H	Isotropic =	30.3385	Anisotropy =	9.5533
14 H	Isotropic =	30.0315	Anisotropy =	9.4283
15 H	Isotropic =	30.4163	Anisotropy =	11.2366
16 H	Isotropic =	30.3762	Anisotropy =	8.3141
17 H	Isotropic =	30.3237	Anisotropy =	10.6373
18 H	Isotropic =	30.2869	Anisotropy =	10.4014
19 H	Isotropic =	27.2025	Anisotropy =	11.6488
20 H	Isotropic =	27.3903	Anisotropy =	16.6592
21 H	Isotropic =	27.3055	Anisotropy =	15.7929

Conformer_6

C	-2.097990014671	-0.761440689760	1.173371350381
C	-0.697668183048	-0.172858648156	1.385686792286

C	0.027205939294	0.140064193688	0.063616532087
C	-0.928470372476	0.193688759741	-1.120488965024
C	-1.720211739427	-1.110706276080	-1.310233156964
C	-2.100687182678	-1.774170912132	0.030594440672
N	1.088475412577	-0.897576256727	-0.203982200270
H	-2.437199716357	-1.227449037996	2.102903671148
H	-2.808497740624	0.042744621975	0.948623847482
H	-0.762724206276	0.747651636807	1.971198133214
H	-0.089197685504	-0.868282463318	1.975346351352
H	0.582311363299	1.075061619519	0.141896828599
H	-1.613896026560	1.022624736638	-0.919950551255
H	-0.383050205749	0.453990673772	-2.032979908673
H	-2.621364598646	-0.879771242337	-1.885435435493
H	-1.142736902811	-1.813761561906	-1.920056590100
H	-3.079350305495	-2.254702758592	-0.052909225990
H	-1.389973224515	-2.575576149112	0.272203558395
H	0.706528946456	-1.845238800174	-0.258823702363
H	1.570765507916	-0.708586709147	-1.085883382675
H	1.791730935295	-0.900804736703	0.537801613190

SCF Done: E(RwB97X) = -291.706196945

Zero-point correction=	0.204544
Thermal correction to Energy=	0.211684
Thermal correction to Enthalpy=	0.212629
Thermal correction to Gibbs Free Energy=	0.173683
Sum of electronic and zero-point Energies=	-291.501653
Sum of electronic and thermal Energies=	-291.494513
Sum of electronic and thermal Enthalpies=	-291.493568
Sum of electronic and thermal Free Energies=	-291.532514

1 C	Isotropic =	171.7011	Anisotropy =	2.7589
2 C	Isotropic =	163.4252	Anisotropy =	16.1292
3 C	Isotropic =	139.5986	Anisotropy =	39.1647
4 C	Isotropic =	168.1894	Anisotropy =	10.5034
5 C	Isotropic =	175.4981	Anisotropy =	16.7873
6 C	Isotropic =	171.4907	Anisotropy =	8.6373
7 N	Isotropic =	206.2050	Anisotropy =	41.5195
8 H	Isotropic =	30.4012	Anisotropy =	11.0739
9 H	Isotropic =	30.4091	Anisotropy =	9.5798
10 H	Isotropic =	29.7346	Anisotropy =	10.3965
11 H	Isotropic =	30.3891	Anisotropy =	8.5456
12 H	Isotropic =	28.1730	Anisotropy =	8.6013
13 H	Isotropic =	30.0321	Anisotropy =	9.8175
14 H	Isotropic =	30.1282	Anisotropy =	10.3568
15 H	Isotropic =	30.1584	Anisotropy =	10.8714

16	H	Isotropic =	30.2459	Anisotropy =	9.6061
17	H	Isotropic =	30.1891	Anisotropy =	10.9887
18	H	Isotropic =	30.5366	Anisotropy =	8.4332
19	H	Isotropic =	27.0919	Anisotropy =	10.6716
20	H	Isotropic =	27.3728	Anisotropy =	16.4269
21	H	Isotropic =	27.1773	Anisotropy =	15.8497

Conformer_7

C	-1.720210063170	-1.110699880592	1.310243023131
C	-0.928476792924	0.193698188620	1.120486285383
C	0.027198058661	0.140067117091	-0.063620113998
C	-0.697677336815	-0.172869262239	-1.385686509712
C	-2.097996564362	-0.761453817513	-1.173362648206
C	-2.100687581591	-1.774175532053	-0.030578606650
N	1.088471050705	-0.897567708746	0.203986024555
H	-1.142728428006	-1.813748156132	1.920068028300
H	-2.621361902405	-0.879766256017	1.885447388133
H	-1.613907325077	1.022628614283	0.919941485978
H	-0.383056316704	0.454010869622	2.032973978312
H	0.582300534007	1.075065578540	-0.141909219525
H	-0.762738323124	0.747635839744	-1.971205493401
H	-0.089205438490	-0.868295541458	-1.975341738519
H	-2.808506447476	0.042730772965	-0.948619244369
H	-2.437207298549	-1.227469999029	-2.102890694309
H	-3.079349631237	-2.254708590352	0.052931443286
H	-1.389973799786	-2.575581504959	-0.272184681309
H	1.570761506762	-0.708568507950	1.085884842956
H	0.706527390475	-1.845231331115	0.258835778107
H	1.791724709107	-0.900800892707	-0.537799328143

SCF Done: E(RwB97X) = -291.706196945

Zero-point correction=	0.204544
Thermal correction to Energy=	0.211684
Thermal correction to Enthalpy=	0.212629
Thermal correction to Gibbs Free Energy=	0.173683
Sum of electronic and zero-point Energies=	-291.501653
Sum of electronic and thermal Energies=	-291.494513
Sum of electronic and thermal Enthalpies=	-291.493568
Sum of electronic and thermal Free Energies=	-291.532514

1	C	Isotropic =	175.4981	Anisotropy =	16.7873
2	C	Isotropic =	168.1894	Anisotropy =	10.5034
3	C	Isotropic =	139.5986	Anisotropy =	39.1647

4	C	Isotropic =	163.4252	Anisotropy =	16.1292
5	C	Isotropic =	171.7011	Anisotropy =	2.7589
6	C	Isotropic =	171.4907	Anisotropy =	8.6373
7	N	Isotropic =	206.2051	Anisotropy =	41.5196
8	H	Isotropic =	30.2459	Anisotropy =	9.6061
9	H	Isotropic =	30.1584	Anisotropy =	10.8714
10	H	Isotropic =	30.0321	Anisotropy =	9.8175
11	H	Isotropic =	30.1282	Anisotropy =	10.3568
12	H	Isotropic =	28.1730	Anisotropy =	8.6013
13	H	Isotropic =	29.7346	Anisotropy =	10.3965
14	H	Isotropic =	30.3891	Anisotropy =	8.5456
15	H	Isotropic =	30.4090	Anisotropy =	9.5798
16	H	Isotropic =	30.4012	Anisotropy =	11.0739
17	H	Isotropic =	30.1891	Anisotropy =	10.9888
18	H	Isotropic =	30.5366	Anisotropy =	8.4332
19	H	Isotropic =	27.3728	Anisotropy =	16.4269
20	H	Isotropic =	27.0919	Anisotropy =	10.6715
21	H	Isotropic =	27.1773	Anisotropy =	15.8497

1-phenylethan-1-amine_neutral

Conformer_1

C	-2.363192225551	-0.715605626134	0.084222320201
C	-1.017797158957	-0.956323447885	-0.181990770601
C	-0.065670064554	0.050689769156	-0.025024108082
C	-0.489151916717	1.311716261350	0.400269473938
C	-1.832502921164	1.556744366571	0.664860065624
C	-2.774993911435	0.543231503326	0.508494749098
C	1.402831057175	-0.245553979904	-0.270739983014
C	2.138098544633	-0.482474305271	1.046026539310
N	2.043928974185	0.867760871842	-0.978683893705
H	-3.090667294427	-1.511572708409	-0.046152911557
H	-0.701752394609	-1.940892249012	-0.519088612704
H	0.241400859252	2.106551308382	0.519148779802
H	-2.146621732204	2.543326079743	0.993525541386
H	-3.823707761712	0.735952687494	0.714104386113
H	1.450055906973	-1.176405509139	-0.854479510790
H	3.190564177618	-0.720770738535	0.858326405559
H	1.692744395351	-1.317179981597	1.594878469461
H	2.093891418600	0.411918785267	1.676379412284
H	1.628586772877	0.980417679645	-1.898647102851
H	3.023055274668	0.645969233111	-1.131729249472

SCF Done: E(RwB97X) = -366.234106643

Zero-point correction=	0.175467
Thermal correction to Energy=	0.183911
Thermal correction to Enthalpy=	0.184856
Thermal correction to Gibbs Free Energy=	0.142007
Sum of electronic and zero-point Energies=	-366.058640
Sum of electronic and thermal Energies=	-366.050195
Sum of electronic and thermal Enthalpies=	-366.049251
Sum of electronic and thermal Free Energies=	-366.092100

1 C	Isotropic =	56.1628	Anisotropy =	189.7418
2 C	Isotropic =	57.0367	Anisotropy =	169.4144
3 C	Isotropic =	33.7448	Anisotropy =	207.9637
4 C	Isotropic =	59.3838	Anisotropy =	192.9514
5 C	Isotropic =	55.5087	Anisotropy =	191.4956
6 C	Isotropic =	57.9926	Anisotropy =	187.7741
7 C	Isotropic =	136.9440	Anisotropy =	21.3963
8 C	Isotropic =	163.2008	Anisotropy =	39.6344
9 N	Isotropic =	217.3247	Anisotropy =	44.2630
10 H	Isotropic =	24.0283	Anisotropy =	4.8291
11 H	Isotropic =	24.0710	Anisotropy =	7.5204
12 H	Isotropic =	23.5598	Anisotropy =	9.8422
13 H	Isotropic =	23.9184	Anisotropy =	5.2521
14 H	Isotropic =	24.0962	Anisotropy =	4.4218
15 H	Isotropic =	27.5897	Anisotropy =	7.9659
16 H	Isotropic =	30.4355	Anisotropy =	10.2337
17 H	Isotropic =	30.6605	Anisotropy =	8.4070
18 H	Isotropic =	30.6973	Anisotropy =	6.4207
19 H	Isotropic =	30.5380	Anisotropy =	13.4120
20 H	Isotropic =	30.5972	Anisotropy =	14.4140

Conformer_2

C	-2.292275553442	-0.726120790024	-0.036234693952
C	-0.935125465161	-0.975844562259	-0.222432104100
C	0.013892258274	0.020648872449	0.004811121400
C	-0.424427916122	1.280406107188	0.418663143905
C	-1.779413961776	1.534448414734	0.603401200777
C	-2.718896018068	0.531364528175	0.377280724067
C	1.492191049496	-0.285964040230	-0.154121533521
C	2.143216138580	-0.545389943797	1.202154934523
N	2.184819229321	0.829886286923	-0.807424587273
H	-3.016947074200	-1.513932968164	-0.220583651993
H	-0.607160068645	-1.959240062979	-0.551471699229
H	0.304006296070	2.067186182853	0.591758813950
H	-2.104922318528	2.519937567914	0.924166595912

H	-3.776618518178	0.731127480628	0.520583830143
H	1.567401627164	-1.210125584182	-0.745506615014
H	1.658063492951	-1.382574247202	1.712115367769
H	3.203200279571	-0.790961115182	1.076339451700
H	2.067837333746	0.341695115132	1.839835601508
H	3.169618367656	0.601059611810	-0.902882259387
H	1.827740821291	0.957293146216	-1.749653641184

SCF Done: E(RwB97X) = -366.234106581

Zero-point correction=	0.175466
Thermal correction to Energy=	0.183911
Thermal correction to Enthalpy=	0.184855
Thermal correction to Gibbs Free Energy=	0.142005
Sum of electronic and zero-point Energies=	-366.058641
Sum of electronic and thermal Energies=	-366.050196
Sum of electronic and thermal Enthalpies=	-366.049251
Sum of electronic and thermal Free Energies=	-366.092101

1 C	Isotropic = 56.1629	Anisotropy = 189.7422
2 C	Isotropic = 57.0364	Anisotropy = 169.4208
3 C	Isotropic = 33.7453	Anisotropy = 207.9617
4 C	Isotropic = 59.3863	Anisotropy = 192.9510
5 C	Isotropic = 55.5086	Anisotropy = 191.4955
6 C	Isotropic = 57.9932	Anisotropy = 187.7728
7 C	Isotropic = 136.9448	Anisotropy = 21.4027
8 C	Isotropic = 163.2018	Anisotropy = 39.6366
9 N	Isotropic = 217.3303	Anisotropy = 44.2648
10 H	Isotropic = 24.0283	Anisotropy = 4.8292
11 H	Isotropic = 24.0710	Anisotropy = 7.5212
12 H	Isotropic = 23.5598	Anisotropy = 9.8426
13 H	Isotropic = 23.9184	Anisotropy = 5.2522
14 H	Isotropic = 24.0962	Anisotropy = 4.4217
15 H	Isotropic = 27.5896	Anisotropy = 7.9657
16 H	Isotropic = 30.6605	Anisotropy = 8.4067
17 H	Isotropic = 30.4355	Anisotropy = 10.2338
18 H	Isotropic = 30.6975	Anisotropy = 6.4211
19 H	Isotropic = 30.5972	Anisotropy = 14.4136
20 H	Isotropic = 30.5381	Anisotropy = 13.4125

Conformer_3

C	-1.764079857639	1.606235934447	0.422458936603
C	-0.413092498784	1.318901967507	0.264804652072
C	0.014297873962	0.015087031558	-0.001124111241

C	-0.943678437302	-0.992384554229	-0.101583597287
C	-2.298347435731	-0.709826799644	0.059639613376
C	-2.712727568867	0.590985610483	0.321665258325
C	1.490050685012	-0.301141019454	-0.160041170430
C	2.242037641767	-0.108119601752	1.158789958261
N	2.056957707746	0.484108686967	-1.267065396938
H	-2.078957438692	2.625353646554	0.627656481035
H	0.315805899715	2.121512156038	0.351563124218
H	-0.625999278657	-2.011134876475	-0.310240771446
H	-3.030235066063	-1.508260243314	-0.021828324285
H	-3.767821325890	0.815169591555	0.446990104051
H	1.568505903502	-1.353904448431	-0.450469932117
H	3.296644845760	-0.375926080670	1.036593680507
H	2.190075611727	0.937358118311	1.482697890072
H	1.819959759512	-0.733378579908	1.952308996239
H	2.073181300333	1.468824698556	-1.013541671020
H	3.028721678589	0.216738761902	-1.396173719995

SCF Done: E(RwB97X) = -366.233008264

Zero-point correction=	0.175622
Thermal correction to Energy=	0.184042
Thermal correction to Enthalpy=	0.184986
Thermal correction to Gibbs Free Energy=	0.142330
Sum of electronic and zero-point Energies=	-366.057386
Sum of electronic and thermal Energies=	-366.048966
Sum of electronic and thermal Enthalpies=	-366.048022
Sum of electronic and thermal Free Energies=	-366.090679

1 C	Isotropic =	55.2007	Anisotropy =	192.2087
2 C	Isotropic =	59.6700	Anisotropy =	189.6084
3 C	Isotropic =	34.3449	Anisotropy =	210.9492
4 C	Isotropic =	57.3056	Anisotropy =	164.6764
5 C	Isotropic =	55.7986	Anisotropy =	190.0502
6 C	Isotropic =	58.1439	Anisotropy =	188.6594
7 C	Isotropic =	136.1962	Anisotropy =	18.3496
8 C	Isotropic =	161.3703	Anisotropy =	40.1222
9 N	Isotropic =	214.0676	Anisotropy =	48.0314
10 H	Isotropic =	23.9033	Anisotropy =	5.2749
11 H	Isotropic =	23.8450	Anisotropy =	9.4646
12 H	Isotropic =	24.0710	Anisotropy =	7.2522
13 H	Isotropic =	24.0118	Anisotropy =	4.8057
14 H	Isotropic =	24.0805	Anisotropy =	4.4303
15 H	Isotropic =	28.0412	Anisotropy =	7.4059
16 H	Isotropic =	30.3838	Anisotropy =	9.4363
17 H	Isotropic =	30.3947	Anisotropy =	6.1142

18 H	Isotropic =	30.5875	Anisotropy =	8.9414
19 H	Isotropic =	30.3979	Anisotropy =	11.3327
20 H	Isotropic =	30.4475	Anisotropy =	14.7733

1-phenylethan-1-amine_protonated
Conformer_1

C	0.024779781625	-0.237345724741	-0.070784111427
C	1.522170350906	-0.295907464507	0.177455909208
N	1.880356388966	-1.695684366072	0.600265932185
C	2.020875740732	0.686154072207	1.215536099390
C	3.000463716726	1.614935146738	0.870877771953
C	3.459187212940	2.536567352118	1.807741280232
C	2.946007779843	2.529714336924	3.099668257775
C	1.969752680823	1.601224841433	3.451872628872
C	1.506148189088	0.687010472271	2.513808554915
H	-0.537282353658	-0.447272630201	0.844064178320
H	-0.243530091230	0.761745096386	-0.419768310631
H	-0.267483180203	-0.960941652402	-0.837062456821
H	2.063284411690	-0.134902081673	-0.756108399089
H	2.885218314472	-1.792378389981	0.764401951819
H	1.397078564768	-1.961021394709	1.462748345597
H	1.615817772952	-2.371478700032	-0.120913960774
H	3.404264661249	1.619134778191	-0.138028349838
H	4.220505133541	3.258066932567	1.527512184165
H	3.304353734192	3.246057950073	3.832630176641
H	1.565790475364	1.591595299817	4.459521815649
H	0.738840715213	-0.029573874407	2.797860501859

SCF Done: E(RwB97X) = -366.702165121

Zero-point correction=	0.191365
Thermal correction to Energy=	0.199677
Thermal correction to Enthalpy=	0.200621
Thermal correction to Gibbs Free Energy=	0.158440
Sum of electronic and zero-point Energies=	-366.510800
Sum of electronic and thermal Energies=	-366.502488
Sum of electronic and thermal Enthalpies=	-366.501544
Sum of electronic and thermal Free Energies=	-366.543725

1 C	Isotropic =	169.7602	Anisotropy =	30.8140
2 C	Isotropic =	133.8297	Anisotropy =	23.3295
3 N	Isotropic =	202.6021	Anisotropy =	39.5062
4 C	Isotropic =	45.6093	Anisotropy =	192.6881
5 C	Isotropic =	54.8542	Anisotropy =	171.4939

6	C	Isotropic =	55.2129	Anisotropy =	192.1462
7	C	Isotropic =	54.4173	Anisotropy =	195.0890
8	C	Isotropic =	54.8265	Anisotropy =	194.0729
9	C	Isotropic =	58.4608	Anisotropy =	192.8730
10	H	Isotropic =	29.8909	Anisotropy =	7.5574
11	H	Isotropic =	30.2999	Anisotropy =	9.1178
12	H	Isotropic =	30.0828	Anisotropy =	10.6125
13	H	Isotropic =	27.2433	Anisotropy =	7.4818
14	H	Isotropic =	27.0092	Anisotropy =	13.7395
15	H	Isotropic =	26.7979	Anisotropy =	12.5196
16	H	Isotropic =	26.8259	Anisotropy =	16.0879
17	H	Isotropic =	23.9139	Anisotropy =	7.3924
18	H	Isotropic =	23.8993	Anisotropy =	4.8690
19	H	Isotropic =	23.8454	Anisotropy =	4.6115
20	H	Isotropic =	23.7977	Anisotropy =	5.2845
21	H	Isotropic =	23.6750	Anisotropy =	9.2278

4-methylmorpholine_neutral

Conformer_1

O	-2.502081303201	0.689792089827	-1.238909768602
C	-2.025998523571	1.391681374409	-0.099388214531
C	-0.509317521507	1.384323038910	-0.038298020712
N	-0.009744576575	0.014531478692	-0.027380723087
C	-0.509007838535	-0.696201470375	-1.198540999713
C	-2.025694867978	-0.648440166226	-1.237099824461
C	1.440206829183	-0.015521778197	0.026897177955
H	-2.438879442628	0.935853237763	0.813243782557
H	-2.400674885449	2.414516696515	-0.177678567751
H	-0.180342510260	1.896451482811	0.871656301660
H	-0.107145583748	1.941828380451	-0.905250158306
H	-0.179801474832	-1.739430604794	-1.155960148266
H	-0.106818870328	-0.251547616011	-2.128426729282
H	-2.438563484761	-1.185396534020	-0.369710804848
H	-2.400149011793	-1.119480330715	-2.148477413574
H	1.789787792607	-1.051424465053	0.063154093420
H	1.901468036251	0.473521927800	-0.849926164733
H	1.789557237127	0.498143252524	0.927296179104

SCF Done: E(RwB97X) = -327.124599493

Zero-point correction=	0.164453
Thermal correction to Energy=	0.170979

Thermal correction to Enthalpy=	0.171923
Thermal correction to Gibbs Free Energy=	0.134420
Sum of electronic and zero-point Energies=	-326.960146
Sum of electronic and thermal Energies=	-326.953620
Sum of electronic and thermal Enthalpies=	-326.952676
Sum of electronic and thermal Free Energies=	-326.990180

1 O	Isotropic =	296.9735	Anisotropy =	60.3332
2 C	Isotropic =	123.0613	Anisotropy =	54.0872
3 C	Isotropic =	135.2972	Anisotropy =	36.5239
4 N	Isotropic =	215.3557	Anisotropy =	11.0638
5 C	Isotropic =	135.2972	Anisotropy =	36.5239
6 C	Isotropic =	123.0613	Anisotropy =	54.0873
7 C	Isotropic =	145.7901	Anisotropy =	71.3314
8 H	Isotropic =	28.3210	Anisotropy =	7.9464
9 H	Isotropic =	28.0976	Anisotropy =	8.0962
10 H	Isotropic =	29.3360	Anisotropy =	8.0692
11 H	Isotropic =	29.9015	Anisotropy =	7.2798
12 H	Isotropic =	29.3360	Anisotropy =	8.0692
13 H	Isotropic =	29.9015	Anisotropy =	7.2798
14 H	Isotropic =	28.3210	Anisotropy =	7.9464
15 H	Isotropic =	28.0976	Anisotropy =	8.0962
16 H	Isotropic =	29.4240	Anisotropy =	10.0590
17 H	Isotropic =	30.0252	Anisotropy =	8.7918
18 H	Isotropic =	29.4240	Anisotropy =	10.0590

Conformer_2

O	-2.484916609841	0.611602883529	-1.098674217945
C	-1.675091302961	-0.421556682704	-1.649912417337
C	-0.791009668975	-1.047376262411	-0.577816838060
N	0.043608637776	-0.069868762315	0.123991906578
C	-0.791322274494	1.040742393143	0.586676066501
C	-1.675398153647	1.623738944976	-0.509301876248
C	1.193400606972	0.366156207261	-0.657560791497
H	-1.068618252825	-0.011712222764	-2.471501154951
H	-2.354996981987	-1.168355678261	-2.067045255021
H	-0.150551560729	-1.813906246315	-1.025603117226
H	-1.436634388957	-1.537669789757	0.161437482036
H	-0.151096504571	1.824698832905	1.003557968936
H	-1.436965080768	0.669339174386	1.392232399991
H	-1.068935877695	2.107459785433	-1.289691030373
H	-2.355528021196	2.370945032791	-0.093264942896
H	1.805054113299	1.042367353166	-0.052593018150
H	1.805291571441	-0.503769716765	-0.914827229590

H 0.940609749159 0.888064753702 -1.593503934749

SCF Done: E(RwB97X) = -327.118640894

Zero-point correction= 0.164333
Thermal correction to Energy= 0.170911
Thermal correction to Enthalpy= 0.171855
Thermal correction to Gibbs Free Energy= 0.134254
Sum of electronic and zero-point Energies= -326.954308
Sum of electronic and thermal Energies= -326.947730
Sum of electronic and thermal Enthalpies= -326.946786
Sum of electronic and thermal Free Energies= -326.984387

1 O	Isotropic =	295.4748	Anisotropy =	56.4515
2 C	Isotropic =	130.3235	Anisotropy =	68.1453
3 C	Isotropic =	138.0246	Anisotropy =	28.9912
4 N	Isotropic =	236.7419	Anisotropy =	28.1009
5 C	Isotropic =	138.0245	Anisotropy =	28.9913
6 C	Isotropic =	130.3235	Anisotropy =	68.1452
7 C	Isotropic =	152.7166	Anisotropy =	58.3306
8 H	Isotropic =	27.9117	Anisotropy =	5.9984
9 H	Isotropic =	28.6270	Anisotropy =	8.5283
10 H	Isotropic =	29.3427	Anisotropy =	7.7469
11 H	Isotropic =	28.6938	Anisotropy =	8.6544
12 H	Isotropic =	29.3427	Anisotropy =	7.7469
13 H	Isotropic =	28.6938	Anisotropy =	8.6544
14 H	Isotropic =	27.9117	Anisotropy =	5.9984
15 H	Isotropic =	28.6270	Anisotropy =	8.5282
16 H	Isotropic =	29.5889	Anisotropy =	9.6886
17 H	Isotropic =	29.5889	Anisotropy =	9.6886
18 H	Isotropic =	28.6932	Anisotropy =	7.8712

Conformer_3

O -2.498520976110 0.646025597046 -1.262839300542
C -2.010552680737 1.435162311894 -0.187221496728
C -0.494100842457 1.415333434735 -0.129590622432
N -0.010008118134 0.045601155620 -0.005582245831
C -0.521752102588 -0.755245389107 -1.111366314870
C -2.037680683104 -0.692862231054 -1.149653296586
C 1.439598858203 0.003187444393 0.047683664812
H -2.425371240830 1.061900441801 0.761363339302
H -2.373967299507 2.452138499276 -0.349716369390
H -0.156036166633 1.997816618563 0.733536469959
H -0.088612592547 1.893810027503 -1.041151079892

H	-0.204474416058	-1.795000755827	-0.981849974830
H	-0.117851256695	-0.395325708877	-2.076575649385
H	-2.453444473956	-1.149844135147	-0.238873529344
H	-2.421106154194	-1.234564771676	-2.016980966861
H	1.903287352670	0.411659709682	-0.868328976514
H	1.798081401508	0.586312717585	0.901014907311
H	1.777311391171	-1.030104966411	0.169631441819

SCF Done: E(RwB97X) = -327.124599507

Zero-point correction=	0.164454
Thermal correction to Energy=	0.170979
Thermal correction to Enthalpy=	0.171923
Thermal correction to Gibbs Free Energy=	0.134422
Sum of electronic and zero-point Energies=	-326.960145
Sum of electronic and thermal Energies=	-326.953621
Sum of electronic and thermal Enthalpies=	-326.952676
Sum of electronic and thermal Free Energies=	-326.990178

1 O	Isotropic = 296.9507	Anisotropy = 60.4221
2 C	Isotropic = 123.0613	Anisotropy = 54.0986
3 C	Isotropic = 135.3128	Anisotropy = 36.5103
4 N	Isotropic = 215.3702	Anisotropy = 11.0409
5 C	Isotropic = 135.3159	Anisotropy = 36.5035
6 C	Isotropic = 123.0592	Anisotropy = 54.0967
7 C	Isotropic = 145.7931	Anisotropy = 71.3124
8 H	Isotropic = 28.3210	Anisotropy = 7.9461
9 H	Isotropic = 28.0973	Anisotropy = 8.0972
10 H	Isotropic = 29.3356	Anisotropy = 8.0711
11 H	Isotropic = 29.8998	Anisotropy = 7.2821
12 H	Isotropic = 29.3359	Anisotropy = 8.0719
13 H	Isotropic = 29.8997	Anisotropy = 7.2826
14 H	Isotropic = 28.3210	Anisotropy = 7.9461
15 H	Isotropic = 28.0972	Anisotropy = 8.0972
16 H	Isotropic = 30.0227	Anisotropy = 8.7937
17 H	Isotropic = 29.4222	Anisotropy = 10.0579
18 H	Isotropic = 29.4234	Anisotropy = 10.0580

Conformer_4

O	-2.618342492862	0.299998139136	-0.679050054299
C	-2.003934666381	1.506982609717	-0.232028803259
C	-0.475978387926	1.434839245318	-0.299021748398
N	-0.056681291770	0.067294051896	-0.041839884145
C	-0.500719091736	-0.807493749399	-1.129011036762

C	-1.846620400843	-0.328233399912	-1.686042402765
C	1.371384798535	-0.047643900226	0.175591577438
H	-2.334262328588	1.645485319317	0.800714652164
H	-2.366773924203	2.355131857969	-0.829566822686
H	-0.052833855794	2.096335642845	0.462033322832
H	-0.106022631063	1.789224714214	-1.278483431875
H	-0.578265243513	-1.830604705327	-0.746029379410
H	0.231397855031	-0.816634368964	-1.956307370312
H	-2.429679306647	-1.172006595431	-2.059682840959
H	-1.693092219090	0.367242970474	-2.523021909855
H	1.632483570462	-1.092567184426	0.369954124497
H	1.958759122141	0.291966158932	-0.696754825433
H	1.668780494248	0.546383193866	1.044646833228

SCF Done: E(RwB97X) = -327.112074517

Zero-point correction=	0.164065
Thermal correction to Energy=	0.170890
Thermal correction to Enthalpy=	0.171834
Thermal correction to Gibbs Free Energy=	0.133478
Sum of electronic and zero-point Energies=	-326.948009
Sum of electronic and thermal Energies=	-326.941185
Sum of electronic and thermal Enthalpies=	-326.940241
Sum of electronic and thermal Free Energies=	-326.978597

1 O	Isotropic = 329.6130	Anisotropy = 50.8247
2 C	Isotropic = 124.3088	Anisotropy = 59.8080
3 C	Isotropic = 142.2903	Anisotropy = 44.6213
4 N	Isotropic = 233.6212	Anisotropy = 21.5359
5 C	Isotropic = 137.2573	Anisotropy = 46.0783
6 C	Isotropic = 130.3216	Anisotropy = 58.7132
7 C	Isotropic = 147.0430	Anisotropy = 68.0578
8 H	Isotropic = 27.9135	Anisotropy = 8.7231
9 H	Isotropic = 28.0467	Anisotropy = 8.1863
10 H	Isotropic = 29.4029	Anisotropy = 7.7686
11 H	Isotropic = 29.4436	Anisotropy = 7.6504
12 H	Isotropic = 28.7017	Anisotropy = 9.0891
13 H	Isotropic = 29.9621	Anisotropy = 6.8040
14 H	Isotropic = 28.2478	Anisotropy = 8.1793
15 H	Isotropic = 28.3150	Anisotropy = 7.7212
16 H	Isotropic = 29.3912	Anisotropy = 10.1666
17 H	Isotropic = 30.0184	Anisotropy = 8.8384
18 H	Isotropic = 29.4103	Anisotropy = 10.4490

Conformer_5

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O   -1.959789820305   0.766180621925  -1.544169633072
C   -2.044002005893  -0.608169110375  -1.203985522917
C   -0.691252478785  -1.116599577375  -0.680744233867
N    0.044845701746  -0.077529163984   0.055026054768
C   -0.896957758392   0.855103395874   0.662218591393
C   -1.759176658233   1.577292822196  -0.387848137319
C    1.056267079695   0.595148844210  -0.751215035284
H   -2.339929231707  -1.146231098043  -2.107000900264
H   -2.834444320693  -0.755887082184  -0.453850009970
H   -0.068270614888  -1.455664408927  -1.512841098000
H   -0.869002923548  -1.982349670538  -0.029649332294
H   -0.353752370681   1.591632866540   1.261255831259
H   -1.535431757478   0.288444044748   1.348221744190
H   -1.274354103611   2.491121303399  -0.741540946631
H   -2.729501407248   1.855684842220   0.048961401860
H    1.799987956017  -0.132876606158  -1.087664407651
H    0.652129361478   1.103941672680  -1.639757265714
H    1.571635352527   1.337756303791  -0.133917100487

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SCF Done: E(RwB97X) = -327.109374978

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Zero-point correction=          0.164404
Thermal correction to Energy=    0.171189
Thermal correction to Enthalpy=   0.172134
Thermal correction to Gibbs Free Energy= 0.133932
Sum of electronic and zero-point Energies= -326.944971
Sum of electronic and thermal Energies= -326.938186
Sum of electronic and thermal Enthalpies= -326.937241
Sum of electronic and thermal Free Energies= -326.975443

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1 O  Isotropic = 328.2495  Anisotropy = 54.9936
2 C  Isotropic = 129.5182  Anisotropy = 57.8142
3 C  Isotropic = 139.4841  Anisotropy = 44.6093
4 N  Isotropic = 242.1008  Anisotropy = 43.0884
5 C  Isotropic = 145.4455  Anisotropy = 37.7285
6 C  Isotropic = 128.3189  Anisotropy = 75.4705
7 C  Isotropic = 146.2807  Anisotropy = 66.7469
8 H  Isotropic = 28.2466  Anisotropy = 7.7122
9 H  Isotropic = 28.3830  Anisotropy = 8.5773
10 H  Isotropic = 29.0805  Anisotropy = 7.9450
11 H  Isotropic = 28.9023  Anisotropy = 9.2272
12 H  Isotropic = 29.3271  Anisotropy = 8.3598
13 H  Isotropic = 28.8469  Anisotropy = 8.9250
14 H  Isotropic = 27.7368  Anisotropy = 7.1835
15 H  Isotropic = 28.1820  Anisotropy = 8.5590

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16 H	Isotropic =	29.3187	Anisotropy =	9.8903
17 H	Isotropic =	28.8110	Anisotropy =	8.5653
18 H	Isotropic =	29.4487	Anisotropy =	10.1149

Conformer_6

O	-2.527315013149	0.642529155900	-1.211102922445
C	-2.048523862141	1.324836220070	-0.050746439568
C	-0.535566075685	1.389127752640	-0.018118035443
N	0.031277242731	0.042895449779	0.107386875551
C	-0.808961559704	-0.956407371149	-0.572793636711
C	-1.622452077820	-0.348373540404	-1.701788474223
C	1.410904854171	0.023263706839	-0.346997620041
H	-2.420886003895	0.825371186520	0.854694649286
H	-2.469097425139	2.332844737879	-0.077054942514
H	-0.211945330696	2.008476349661	0.825187095969
H	-0.184304007372	1.885099977975	-0.940100212847
H	-1.496567796758	-1.416084852882	0.147426399074
H	-0.174837024773	-1.755087366707	-0.966951934612
H	-2.225616370538	-1.113729585474	-2.197151194126
H	-0.957235784088	0.097649915599	-2.454527366124
H	1.510295681224	0.255000886338	-1.422652943282
H	1.990333280338	0.766593767157	0.209482062593
H	1.854897273293	-0.958906389742	-0.163291360536

SCF Done: E(RwB97X) = -327.110878119

Zero-point correction=	0.163930
Thermal correction to Energy=	0.170756
Thermal correction to Enthalpy=	0.171700
Thermal correction to Gibbs Free Energy=	0.133282
Sum of electronic and zero-point Energies=	-326.946948
Sum of electronic and thermal Energies=	-326.940122
Sum of electronic and thermal Enthalpies=	-326.939178
Sum of electronic and thermal Free Energies=	-326.977596

1 O	Isotropic =	322.1025	Anisotropy =	67.9593
2 C	Isotropic =	126.8061	Anisotropy =	59.8566
3 C	Isotropic =	138.0789	Anisotropy =	42.7947
4 N	Isotropic =	239.8653	Anisotropy =	40.7950
5 C	Isotropic =	139.8053	Anisotropy =	43.4218
6 C	Isotropic =	130.1546	Anisotropy =	72.0017
7 C	Isotropic =	147.3592	Anisotropy =	65.1407
8 H	Isotropic =	27.7748	Anisotropy =	8.1610
9 H	Isotropic =	28.1091	Anisotropy =	8.2841

10	H	Isotropic =	29.0322	Anisotropy =	9.1930
11	H	Isotropic =	29.1359	Anisotropy =	6.7125
12	H	Isotropic =	28.3896	Anisotropy =	9.2459
13	H	Isotropic =	29.4734	Anisotropy =	7.5715
14	H	Isotropic =	28.3721	Anisotropy =	8.6132
15	H	Isotropic =	27.6226	Anisotropy =	6.4675
16	H	Isotropic =	29.4745	Anisotropy =	8.3396
17	H	Isotropic =	29.5930	Anisotropy =	10.0540
18	H	Isotropic =	29.5073	Anisotropy =	10.1410

Conformer_7

O	-2.527304107158	0.690975059410	-1.184103814118
C	-2.048210979880	-0.654690180400	-1.154670250952
C	-0.535234369198	-0.715895728812	-1.192017267959
N	0.031313174716	-0.115002340280	0.019326970301
C	-0.809236073298	0.988679402497	0.511888565679
C	-1.622728173452	1.629420432371	-0.598869173310
C	1.410882662910	0.282188472552	-0.202597794235
H	-2.468553542769	-1.162179565587	-2.026118580758
H	-2.420577538867	-1.162578561721	-0.253928973339
H	-0.183970427472	-0.192108065964	-2.098485544485
H	-0.211367085744	-1.758775814721	-1.275669522110
H	-0.175341471720	1.743916524601	0.984285609717
H	-1.496857804798	0.617394535369	1.281399166635
H	-0.957503971657	2.035544921704	-1.373856331338
H	-2.226128815824	2.452963400113	-0.208169960298
H	1.510200206790	1.075528918126	-0.965068762493
H	1.854670181193	0.642199731959	0.729593099353
H	1.990548136227	-0.581781141217	-0.542437436289

SCF Done: E(RwB97X) = -327.110878119

Zero-point correction=	0.163930
Thermal correction to Energy=	0.170756
Thermal correction to Enthalpy=	0.171700
Thermal correction to Gibbs Free Energy=	0.133282
Sum of electronic and zero-point Energies=	-326.946948
Sum of electronic and thermal Energies=	-326.940122
Sum of electronic and thermal Enthalpies=	-326.939178
Sum of electronic and thermal Free Energies=	-326.977596

1	O	Isotropic =	322.1026	Anisotropy =	67.9591
2	C	Isotropic =	126.8061	Anisotropy =	59.8567
3	C	Isotropic =	138.0790	Anisotropy =	42.7948

4 N	Isotropic =	239.8653	Anisotropy =	40.7950
5 C	Isotropic =	139.8052	Anisotropy =	43.4218
6 C	Isotropic =	130.1547	Anisotropy =	72.0015
7 C	Isotropic =	147.3592	Anisotropy =	65.1408
8 H	Isotropic =	28.1091	Anisotropy =	8.2841
9 H	Isotropic =	27.7748	Anisotropy =	8.1610
10 H	Isotropic =	29.1359	Anisotropy =	6.7125
11 H	Isotropic =	29.0322	Anisotropy =	9.1930
12 H	Isotropic =	29.4734	Anisotropy =	7.5715
13 H	Isotropic =	28.3896	Anisotropy =	9.2459
14 H	Isotropic =	27.6226	Anisotropy =	6.4675
15 H	Isotropic =	28.3721	Anisotropy =	8.6132
16 H	Isotropic =	29.4745	Anisotropy =	8.3396
17 H	Isotropic =	29.5073	Anisotropy =	10.1410
18 H	Isotropic =	29.5930	Anisotropy =	10.0540

Conformer_8

O	-2.620545167451	0.400044542348	-0.622561427628
C	-1.859921567298	1.589629884943	-0.519982020520
C	-0.517036750315	1.325821144233	0.171751887155
N	-0.059135914713	-0.037474146971	-0.104023935578
C	-0.464497614161	-0.438823849161	-1.440700040081
C	-1.991301862267	-0.544651228512	-1.486077779641
C	1.368449651403	-0.165733742364	0.108920720571
H	-2.453637123590	2.303389837574	0.054094527639
H	-1.702343778127	2.016003593633	-1.520581669170
H	-0.604109409285	1.453657197900	1.255967762236
H	0.211543425047	2.071575377838	-0.193664760243
H	-0.031034214150	-1.414633027717	-1.676806317900
H	-0.094648659853	0.272754679529	-2.201433325890
H	-2.315927221842	-1.528989752704	-1.138884323816
H	-2.347290676466	-0.404832983077	-2.516516177452
H	1.675792786503	-1.207810991453	-0.018320519708
H	1.955933092496	0.458975655727	-0.588187008565
H	1.618911004069	0.142697808235	1.128704408591

SCF Done: E(RwB97X) = -327.112074515

Zero-point correction=	0.164066
Thermal correction to Energy=	0.170890
Thermal correction to Enthalpy=	0.171834
Thermal correction to Gibbs Free Energy=	0.133481
Sum of electronic and zero-point Energies=	-326.948008
Sum of electronic and thermal Energies=	-326.941185

Sum of electronic and thermal Enthalpies= -326.940240
 Sum of electronic and thermal Free Energies= -326.978593

1 O	Isotropic =	329.6032	Anisotropy =	50.7692
2 C	Isotropic =	130.3164	Anisotropy =	58.7067
3 C	Isotropic =	137.2501	Anisotropy =	46.0805
4 N	Isotropic =	233.6184	Anisotropy =	21.5178
5 C	Isotropic =	142.2831	Anisotropy =	44.6243
6 C	Isotropic =	124.3063	Anisotropy =	59.8083
7 C	Isotropic =	147.0421	Anisotropy =	68.0545
8 H	Isotropic =	28.2479	Anisotropy =	8.1798
9 H	Isotropic =	28.3153	Anisotropy =	7.7210
10 H	Isotropic =	28.7018	Anisotropy =	9.0892
11 H	Isotropic =	29.9626	Anisotropy =	6.8035
12 H	Isotropic =	29.4028	Anisotropy =	7.7682
13 H	Isotropic =	29.4441	Anisotropy =	7.6496
14 H	Isotropic =	27.9137	Anisotropy =	8.7240
15 H	Isotropic =	28.0469	Anisotropy =	8.1865
16 H	Isotropic =	29.4101	Anisotropy =	10.4500
17 H	Isotropic =	30.0186	Anisotropy =	8.8379
18 H	Isotropic =	29.3913	Anisotropy =	10.1666

Conformer_9

O	-1.960699489900	0.614744707563	-1.613604020538
C	-2.002417677517	-0.725877279379	-1.152306396461
C	-0.644917373104	-1.132565066344	-0.557327917310
N	0.034390632488	-0.004185920061	0.097110793890
C	-0.955739712803	0.941790033767	0.597424242538
C	-1.817612357679	1.533430264695	-0.531551303530
C	1.039734363436	0.632451848758	-0.745184701522
H	-2.804743060007	-0.836360735781	-0.408432586762
H	-2.256485217946	-1.353819600396	-2.008834176698
H	0.010077935509	-1.519930955508	-1.342422903422
H	-0.806311520575	-1.943106433131	0.165159598985
H	-0.455034689726	1.749339191718	1.139233137108
H	-1.589904180056	0.414290618743	1.317781376951
H	-2.807635804137	1.812773194839	-0.142168271174
H	-1.357565646615	2.429650287952	-0.956268030974
H	1.511768496976	1.447184195927	-0.187027602809
H	1.818053733656	-0.093071953508	-0.998468012744
H	0.638941567998	1.043163600145	-1.684513225529

SCF Done: E(RwB97X) = -327.109374947

Zero-point correction=	0.164406
Thermal correction to Energy=	0.171192
Thermal correction to Enthalpy=	0.172136
Thermal correction to Gibbs Free Energy=	0.133934
Sum of electronic and zero-point Energies=	-326.944969
Sum of electronic and thermal Energies=	-326.938183
Sum of electronic and thermal Enthalpies=	-326.937239
Sum of electronic and thermal Free Energies=	-326.975441

1	O	Isotropic =	328.2572	Anisotropy =	55.0060
2	C	Isotropic =	129.5239	Anisotropy =	57.8077
3	C	Isotropic =	139.4801	Anisotropy =	44.6110
4	N	Isotropic =	242.1047	Anisotropy =	43.0619
5	C	Isotropic =	145.4415	Anisotropy =	37.7268
6	C	Isotropic =	128.3240	Anisotropy =	75.4770
7	C	Isotropic =	146.2903	Anisotropy =	66.7332
8	H	Isotropic =	28.3820	Anisotropy =	8.5772
9	H	Isotropic =	28.2474	Anisotropy =	7.7119
10	H	Isotropic =	29.0810	Anisotropy =	7.9447
11	H	Isotropic =	28.9025	Anisotropy =	9.2273
12	H	Isotropic =	29.3278	Anisotropy =	8.3616
13	H	Isotropic =	28.8460	Anisotropy =	8.9231
14	H	Isotropic =	28.1821	Anisotropy =	8.5596
15	H	Isotropic =	27.7366	Anisotropy =	7.1809
16	H	Isotropic =	29.4494	Anisotropy =	10.1149
17	H	Isotropic =	29.3190	Anisotropy =	9.8906
18	H	Isotropic =	28.8122	Anisotropy =	8.5632

4-methylmorpholine_protonated

Conformer_1

O	-2.498322384802	-0.681527353106	-0.492931875852
C	-2.053640927641	-0.007907548267	-1.657058445956
C	-0.539531525460	0.049671434900	-1.718866604574
N	-0.007054643358	0.719908948102	-0.492916495235
C	-0.539538552605	0.049658448269	0.733022146048
C	-2.053647639086	-0.007920023147	0.671204352364
C	1.474707861697	0.782198792028	-0.492912061073
H	-2.473218943453	1.008224686647	-1.686714365366
H	-2.424436146798	-0.560988232053	-2.520709588640
H	-0.202676130344	0.620305032061	-2.585167331380
H	-0.103011539287	-0.951085960067	-1.744706791453
H	-0.357421592921	1.682857032088	-0.492912260085
H	-0.202689161811	0.620282093008	1.599331394766
H	-0.103019063626	-0.951099423804	0.758854615320

H	-2.424448100059	-0.561009668199	1.534847491693
H	-2.473225937574	1.008211876390	0.700868625180
H	1.862402919403	-0.236505751371	-0.492917944445
H	1.799638232812	1.312019076526	-1.387661283658
H	1.799633274914	1.312006539996	0.401846422348

SCF Done: E(RwB97X) = -327.595275468

Zero-point correction=	0.180160
Thermal correction to Energy=	0.186787
Thermal correction to Enthalpy=	0.187732
Thermal correction to Gibbs Free Energy=	0.149974
Sum of electronic and zero-point Energies=	-327.415115
Sum of electronic and thermal Energies=	-327.408488
Sum of electronic and thermal Enthalpies=	-327.407544
Sum of electronic and thermal Free Energies=	-327.445302

1 O	Isotropic = 298.8959	Anisotropy = 62.9195
2 C	Isotropic = 125.1794	Anisotropy = 60.4287
3 C	Isotropic = 135.1180	Anisotropy = 38.7225
4 N	Isotropic = 201.0433	Anisotropy = 25.5540
5 C	Isotropic = 135.1182	Anisotropy = 38.7223
6 C	Isotropic = 125.1794	Anisotropy = 60.4287
7 C	Isotropic = 146.3288	Anisotropy = 71.4798
8 H	Isotropic = 28.0951	Anisotropy = 7.8468
9 H	Isotropic = 27.8242	Anisotropy = 8.5029
10 H	Isotropic = 28.6004	Anisotropy = 7.9356
11 H	Isotropic = 28.8226	Anisotropy = 7.3895
12 H	Isotropic = 27.2777	Anisotropy = 13.1593
13 H	Isotropic = 28.6004	Anisotropy = 7.9356
14 H	Isotropic = 28.8226	Anisotropy = 7.3895
15 H	Isotropic = 27.8242	Anisotropy = 8.5029
16 H	Isotropic = 28.0951	Anisotropy = 7.8468
17 H	Isotropic = 29.0746	Anisotropy = 8.5723
18 H	Isotropic = 28.8661	Anisotropy = 10.0402
19 H	Isotropic = 28.8661	Anisotropy = 10.0402

Conformer_2

O	-2.476123317205	-0.518635291502	-0.492933592990
C	-1.666218763463	-0.506998767394	-1.656395386655
C	-0.822701341208	0.751182139149	-1.724156755512
N	0.025528946530	0.897250117410	-0.492932400618
C	-0.822686917012	0.751154964836	0.738298462766
C	-1.666206836190	-0.507023351309	0.670520072447

C	1.227164337396	0.020036176938	-0.492949712966
H	-2.331654785476	-0.522360137718	-2.520533311508
H	-1.040748643492	-1.409031271287	-1.688371273850
H	-1.460692745808	1.635638298234	-1.765186147860
H	-0.158920369360	0.739318487145	-2.589274570989
H	0.373405031284	1.857816220644	-0.492923687263
H	-1.460676765492	1.635610997044	0.779355055736
H	-0.158895760223	0.739271665119	1.603408191367
H	-1.040738455486	-1.409057896793	0.702471943840
H	-2.331634089862	-0.522400679838	1.534664504263
H	1.808925205231	0.242711194495	0.400731522961
H	0.929656335195	-1.026820934889	-0.492964609771
H	1.808918934640	0.242738069713	-1.386628303400

SCF Done: E(RwB97X) = -327.591654342

Zero-point correction=	0.180852
Thermal correction to Energy=	0.187332
Thermal correction to Enthalpy=	0.188276
Thermal correction to Gibbs Free Energy=	0.150854
Sum of electronic and zero-point Energies=	-327.410802
Sum of electronic and thermal Energies=	-327.404322
Sum of electronic and thermal Enthalpies=	-327.403378
Sum of electronic and thermal Free Energies=	-327.440801

1 O	Isotropic = 299.0431	Anisotropy = 64.5746
2 C	Isotropic = 130.0832	Anisotropy = 69.0719
3 C	Isotropic = 137.3972	Anisotropy = 34.8656
4 N	Isotropic = 210.6838	Anisotropy = 12.6644
5 C	Isotropic = 137.3972	Anisotropy = 34.8658
6 C	Isotropic = 130.0832	Anisotropy = 69.0719
7 C	Isotropic = 151.7331	Anisotropy = 61.8788
8 H	Isotropic = 28.0171	Anisotropy = 8.8959
9 H	Isotropic = 27.7988	Anisotropy = 6.5339
10 H	Isotropic = 28.2944	Anisotropy = 9.2243
11 H	Isotropic = 28.7673	Anisotropy = 8.2766
12 H	Isotropic = 26.7262	Anisotropy = 15.9154
13 H	Isotropic = 28.2944	Anisotropy = 9.2243
14 H	Isotropic = 28.7673	Anisotropy = 8.2766
15 H	Isotropic = 27.7988	Anisotropy = 6.5340
16 H	Isotropic = 28.0171	Anisotropy = 8.8959
17 H	Isotropic = 29.0271	Anisotropy = 10.1952
18 H	Isotropic = 28.1642	Anisotropy = 6.9205
19 H	Isotropic = 29.0271	Anisotropy = 10.1952

Conformer_3

O	-2.495420533928	-0.680507950883	-0.435195215796
C	-2.039078973340	-0.103175391993	-1.645640324911
C	-0.524613261291	-0.046930239280	-1.695662271424
N	-0.007082400494	0.723275638329	-0.522840338058
C	-0.551484585144	0.153470190761	0.748177062417
C	-2.064581831102	0.086948867628	0.674827927218
C	1.474466337961	0.790352366581	-0.512262477973
H	-2.459900999317	0.906093311911	-1.762741313085
H	-2.399616982783	-0.725847011357	-2.465149899463
H	-0.179135725949	0.452007676203	-2.601942824392
H	-0.085345577934	-1.044946368153	-1.634258578082
H	-0.359866999215	1.681790502627	-0.605388393398
H	-0.225150079370	0.794052289896	1.568408499514
H	-0.112621920759	-0.840368691442	0.859828324156
H	-2.444032462865	-0.394697169559	1.576682401183
H	-2.486123605072	1.101040233897	0.616869128220
H	1.788354051853	1.392589362243	0.339592364934
H	1.807509669524	1.246521643824	-1.443845434790
H	1.864625879222	-0.223669261234	-0.425058636271

SCF Done: E(RwB97X) = -327.595275670

Zero-point correction= 0.180155
Thermal correction to Energy= 0.186782
Thermal correction to Enthalpy= 0.187726
Thermal correction to Gibbs Free Energy= 0.149968
Sum of electronic and zero-point Energies= -327.415121
Sum of electronic and thermal Energies= -327.408494
Sum of electronic and thermal Enthalpies= -327.407549
Sum of electronic and thermal Free Energies= -327.445307

1 O	Isotropic = 298.8808	Anisotropy = 62.8944
2 C	Isotropic = 125.1817	Anisotropy = 60.4264
3 C	Isotropic = 135.0729	Anisotropy = 38.7644
4 N	Isotropic = 200.9718	Anisotropy = 25.5852
5 C	Isotropic = 135.0817	Anisotropy = 38.7596
6 C	Isotropic = 125.1826	Anisotropy = 60.4328
7 C	Isotropic = 146.3338	Anisotropy = 71.4613
8 H	Isotropic = 28.0950	Anisotropy = 7.8454
9 H	Isotropic = 27.8234	Anisotropy = 8.5033
10 H	Isotropic = 28.5987	Anisotropy = 7.9316
11 H	Isotropic = 28.8216	Anisotropy = 7.3860
12 H	Isotropic = 27.2804	Anisotropy = 13.1523
13 H	Isotropic = 28.5989	Anisotropy = 7.9333

14	H	Isotropic =	28.8215	Anisotropy =	7.3871
15	H	Isotropic =	27.8232	Anisotropy =	8.5032
16	H	Isotropic =	28.0949	Anisotropy =	7.8460
17	H	Isotropic =	28.8660	Anisotropy =	10.0398
18	H	Isotropic =	28.8663	Anisotropy =	10.0389
19	H	Isotropic =	29.0743	Anisotropy =	8.5723

Conformer_4

O	-2.608068343813	0.072648955189	-0.544186637365
C	-1.884968692863	-0.561226478723	-1.584799106788
C	-0.542773040769	0.145698480108	-1.781598320972
N	-0.068923490003	0.694326067846	-0.465431809524
C	-0.494071180156	-0.195778855435	0.652333054546
C	-2.023953405297	-0.195924909625	0.726058061246
C	1.393587917766	0.945799641459	-0.469088552641
H	-1.741126634330	-1.624013005637	-1.355926230527
H	-2.477681018495	-0.484054121961	-2.496262426171
H	-0.619696723108	0.994106485693	-2.461681968819
H	0.220567122971	-0.544309861124	-2.144507273153
H	-0.526972377926	1.598853354289	-0.329272283809
H	-0.054113099558	0.177409049616	1.576812253959
H	-0.082363745833	-1.182497466455	0.433578776080
H	-2.361653872597	-1.165878242278	1.109892898806
H	-2.378917959373	0.590180577414	1.394622589133
H	1.661457776819	1.452347434200	0.457273164741
H	1.908535579088	-0.011718703978	-0.544118976200
H	1.632935187477	1.573031599402	-1.327397212543

SCF Done: E(RwB97X) = -327.584681465

Zero-point correction=	0.180508
Thermal correction to Energy=	0.187382
Thermal correction to Enthalpy=	0.188326
Thermal correction to Gibbs Free Energy=	0.149757
Sum of electronic and zero-point Energies=	-327.404174
Sum of electronic and thermal Energies=	-327.397300
Sum of electronic and thermal Enthalpies=	-327.396356
Sum of electronic and thermal Free Energies=	-327.434924

1	O	Isotropic =	329.4776	Anisotropy =	56.5368
2	C	Isotropic =	131.3350	Anisotropy =	61.7592
3	C	Isotropic =	136.4744	Anisotropy =	51.9402
4	N	Isotropic =	211.2352	Anisotropy =	5.1698
5	C	Isotropic =	141.8246	Anisotropy =	50.1852

6	C	Isotropic =	127.8831	Anisotropy =	64.5081
7	C	Isotropic =	147.1929	Anisotropy =	68.3218
8	H	Isotropic =	28.0990	Anisotropy =	8.0625
9	H	Isotropic =	27.9812	Anisotropy =	8.7265
10	H	Isotropic =	28.1302	Anisotropy =	9.0778
11	H	Isotropic =	28.8905	Anisotropy =	7.1281
12	H	Isotropic =	26.9832	Anisotropy =	13.8701
13	H	Isotropic =	28.5693	Anisotropy =	7.9842
14	H	Isotropic =	28.6048	Anisotropy =	7.5196
15	H	Isotropic =	27.8521	Anisotropy =	8.5833
16	H	Isotropic =	27.7822	Anisotropy =	9.0484
17	H	Isotropic =	28.8471	Anisotropy =	10.5175
18	H	Isotropic =	29.0882	Anisotropy =	8.6495
19	H	Isotropic =	28.7802	Anisotropy =	10.0825

Conformer_5

O	-1.888544380536	-0.986825024278	-0.505812707720
C	-1.696921382928	-0.330972173464	0.743702320699
C	-0.915841372016	0.973188295683	0.588176981022
N	0.043915085097	0.855190800135	-0.552040118202
C	-0.704416034310	0.633056382610	-1.845885268703
C	-2.035994167442	-0.060554013829	-1.567022796176
C	1.103177830576	-0.163604399327	-0.311458042350
H	-2.662111741426	-0.102474993090	1.211389341776
H	-1.163298074675	-1.036622963747	1.382964771839
H	-0.348938467379	1.204751130572	1.489356299754
H	-1.567341691971	1.815268163859	0.353548384838
H	0.519110058694	1.755621161481	-0.630586635592
H	-0.060155845648	0.029258450845	-2.483811410225
H	-0.861522267805	1.607554784287	-2.309368003110
H	-2.821858099689	0.667731042828	-1.332702898578
H	-2.343365458723	-0.618038104935	-2.452034629793
H	0.652847436243	-1.154445909148	-0.307914851079
H	1.573189932267	0.049884249150	0.648323232371
H	1.834568641673	-0.088066879633	-1.115023970771

SCF Done: E(RwB97X) = -327.582354274

Zero-point correction=	0.180698
Thermal correction to Energy=	0.187428
Thermal correction to Enthalpy=	0.188372
Thermal correction to Gibbs Free Energy=	0.150268
Sum of electronic and zero-point Energies=	-327.401656
Sum of electronic and thermal Energies=	-327.394927

Sum of electronic and thermal Enthalpies= -327.393982
Sum of electronic and thermal Free Energies= -327.432087

1 O	Isotropic =	333.7319	Anisotropy =	59.6457
2 C	Isotropic =	130.9267	Anisotropy =	72.0881
3 C	Isotropic =	144.5037	Anisotropy =	44.2217
4 N	Isotropic =	214.0380	Anisotropy =	12.7929
5 C	Isotropic =	137.6277	Anisotropy =	51.4833
6 C	Isotropic =	131.8474	Anisotropy =	60.8367
7 C	Isotropic =	145.5752	Anisotropy =	67.9852
8 H	Isotropic =	27.7871	Anisotropy =	8.8852
9 H	Isotropic =	27.6242	Anisotropy =	8.0558
10 H	Isotropic =	28.6772	Anisotropy =	8.8767
11 H	Isotropic =	28.2634	Anisotropy =	9.3341
12 H	Isotropic =	26.7063	Anisotropy =	15.8028
13 H	Isotropic =	28.5181	Anisotropy =	8.2038
14 H	Isotropic =	28.3334	Anisotropy =	9.2248
15 H	Isotropic =	27.9627	Anisotropy =	8.6102
16 H	Isotropic =	27.9659	Anisotropy =	8.6962
17 H	Isotropic =	28.3953	Anisotropy =	7.3636
18 H	Isotropic =	28.9228	Anisotropy =	10.4766
19 H	Isotropic =	28.7273	Anisotropy =	10.1264

Conformer_6

O	-1.888548382148	-0.986828687649	-0.480081985007
C	-2.036002961741	-0.060573544692	0.581140558205
C	-0.704427116211	0.633029840709	0.860027768254
N	0.043921418447	0.855182238687	-0.433806056925
C	-0.915821777718	0.973196518008	-1.574033551162
C	-1.696906042998	-0.330958364526	-1.729584481137
C	1.103187732276	-0.163608519343	-0.674391214110
H	-2.821863170629	0.667717671396	0.346826446514
H	-2.343382758932	-0.618071690227	1.466140699740
H	-0.060173814807	0.029223518238	1.497952895146
H	-0.861538686678	1.607523482089	1.323518695861
H	0.519115961975	1.755611148675	-0.355239246797
H	-0.348905221150	1.204766236258	-2.475202409579
H	-1.567320819184	1.815276122965	-1.339400972906
H	-2.662089261695	-0.102448445241	-2.197280322476
H	-1.163280264702	-1.036603642189	-2.368850839621
H	1.573225949145	0.049911663223	-1.634152901951
H	0.652853466694	-1.154447751810	-0.677980604366
H	1.834555750055	-0.088097794572	0.129197522315

SCF Done: E(RwB97X) = -327.582354272

Zero-point correction=	0.180698
Thermal correction to Energy=	0.187428
Thermal correction to Enthalpy=	0.188372
Thermal correction to Gibbs Free Energy=	0.150268
Sum of electronic and zero-point Energies=	-327.401656
Sum of electronic and thermal Energies=	-327.394927
Sum of electronic and thermal Enthalpies=	-327.393982
Sum of electronic and thermal Free Energies=	-327.432087

1	O	Isotropic =	333.7322	Anisotropy =	59.6459
2	C	Isotropic =	131.8475	Anisotropy =	60.8366
3	C	Isotropic =	137.6275	Anisotropy =	51.4835
4	N	Isotropic =	214.0378	Anisotropy =	12.7930
5	C	Isotropic =	144.5037	Anisotropy =	44.2216
6	C	Isotropic =	130.9268	Anisotropy =	72.0881
7	C	Isotropic =	145.5753	Anisotropy =	67.9849
8	H	Isotropic =	27.9627	Anisotropy =	8.6102
9	H	Isotropic =	27.9659	Anisotropy =	8.6962
10	H	Isotropic =	28.5181	Anisotropy =	8.2038
11	H	Isotropic =	28.3334	Anisotropy =	9.2248
12	H	Isotropic =	26.7063	Anisotropy =	15.8027
13	H	Isotropic =	28.6772	Anisotropy =	8.8767
14	H	Isotropic =	28.2634	Anisotropy =	9.3341
15	H	Isotropic =	27.7871	Anisotropy =	8.8851
16	H	Isotropic =	27.6242	Anisotropy =	8.0558
17	H	Isotropic =	28.9228	Anisotropy =	10.4766
18	H	Isotropic =	28.3953	Anisotropy =	7.3636
19	H	Isotropic =	28.7273	Anisotropy =	10.1264

Conformer_7

O	-1.943369867184	-0.954523328992	-0.362391216194
C	-1.747182905871	-0.395994438651	-1.657684028549
C	-0.937974245140	0.899184190524	-1.602467900664
N	0.026930944645	0.844897386548	-0.461885418677
C	-0.716287056700	0.733167360487	0.848942065097
C	-2.064130534266	0.049690875774	0.629102568654
C	1.063537931134	-0.210534972237	-0.633208624681
H	-2.710810730290	-0.182017988404	-2.135339450738
H	-1.232735963314	-1.157582746061	-2.246486253454
H	-1.570298604028	1.769849512908	-1.427169050541
H	-0.372825052667	1.052031546294	-2.521373218937
H	0.520789610220	1.738609025521	-0.452028753165

H	-0.849373263437	1.741692190400	1.241743432243
H	-0.080262517157	0.163356400239	1.525238084288
H	-2.376836019809	-0.434922765594	1.554242351849
H	-2.836290904881	0.775442205376	0.346416676456
H	0.593142892480	-1.189479431657	-0.562414543164
H	1.531546298954	-0.077406532230	-1.608362611640
H	1.801829987311	-0.092358490247	0.158825891816

SCF Done: E(RwB97X) = -327.582354362

Zero-point correction=	0.180696
Thermal correction to Energy=	0.187426
Thermal correction to Enthalpy=	0.188370
Thermal correction to Gibbs Free Energy=	0.150265
Sum of electronic and zero-point Energies=	-327.401659
Sum of electronic and thermal Energies=	-327.394929
Sum of electronic and thermal Enthalpies=	-327.393985
Sum of electronic and thermal Free Energies=	-327.432090

1 O	Isotropic = 333.7111	Anisotropy = 59.7194
2 C	Isotropic = 130.9194	Anisotropy = 72.0875
3 C	Isotropic = 144.5254	Anisotropy = 44.2231
4 N	Isotropic = 214.0666	Anisotropy = 12.7767
5 C	Isotropic = 137.6348	Anisotropy = 51.4847
6 C	Isotropic = 131.8373	Anisotropy = 60.8310
7 C	Isotropic = 145.5619	Anisotropy = 68.0118
8 H	Isotropic = 27.7864	Anisotropy = 8.8846
9 H	Isotropic = 27.6237	Anisotropy = 8.0545
10 H	Isotropic = 28.2637	Anisotropy = 9.3361
11 H	Isotropic = 28.6777	Anisotropy = 8.8762
12 H	Isotropic = 26.7059	Anisotropy = 15.8054
13 H	Isotropic = 28.3337	Anisotropy = 9.2263
14 H	Isotropic = 28.5185	Anisotropy = 8.2014
15 H	Isotropic = 27.9660	Anisotropy = 8.6959
16 H	Isotropic = 27.9628	Anisotropy = 8.6092
17 H	Isotropic = 28.3949	Anisotropy = 7.3663
18 H	Isotropic = 28.9232	Anisotropy = 10.4781
19 H	Isotropic = 28.7275	Anisotropy = 10.1259

Piperidine_neutral

Conformer_1

C	-0.723505246243	-2.118208442039	-3.504758687264
C	-0.474830919243	-0.615796904498	-3.584845055003
N	0.935524314173	-0.326435651487	-3.324790888278

C	1.806258224401	-0.953366569275	-4.319400496284
C	1.650201240066	-2.469489945870	-4.269151152588
C	0.188676970532	-2.870652611987	-4.474830947287
H	-0.530536010044	-2.456657189067	-2.478793722739
H	-1.775645616091	-2.329240352167	-3.723593666959
H	-0.780105074793	-0.256130315930	-4.584250672247
H	-1.083024998515	-0.086014120248	-2.845686021188
H	1.079182207641	0.676942956359	-3.339776811746
H	1.566147908242	-0.603338692572	-5.339788911755
H	2.840958939203	-0.666714936751	-4.109281141827
H	2.286829840217	-2.930428492649	-5.031818418734
H	1.998345091383	-2.830912834017	-3.293160410547
H	0.067346660357	-3.952409932148	-4.354471158872
H	-0.107623531287	-2.630945965652	-5.505101836682

SCF Done: E(RwB97X) = -251.918445547

Zero-point correction=	0.160480
Thermal correction to Energy=	0.165956
Thermal correction to Enthalpy=	0.166900
Thermal correction to Gibbs Free Energy=	0.131917
Sum of electronic and zero-point Energies=	-251.757965
Sum of electronic and thermal Energies=	-251.752490
Sum of electronic and thermal Enthalpies=	-251.751545
Sum of electronic and thermal Free Energies=	-251.786529

1 C	Isotropic =	163.5228	Anisotropy =	7.7980
2 C	Isotropic =	143.2966	Anisotropy =	29.8254
3 N	Isotropic =	214.5062	Anisotropy =	33.0461
4 C	Isotropic =	143.2966	Anisotropy =	29.8260
5 C	Isotropic =	163.5229	Anisotropy =	7.7975
6 C	Isotropic =	165.3119	Anisotropy =	5.5306
7 H	Isotropic =	30.4923	Anisotropy =	8.6228
8 H	Isotropic =	30.3764	Anisotropy =	10.0907
9 H	Isotropic =	29.3567	Anisotropy =	8.3133
10 H	Isotropic =	28.9916	Anisotropy =	8.9837
11 H	Isotropic =	30.5596	Anisotropy =	15.2878
12 H	Isotropic =	29.3567	Anisotropy =	8.3133
13 H	Isotropic =	28.9916	Anisotropy =	8.9837
14 H	Isotropic =	30.3764	Anisotropy =	10.0907
15 H	Isotropic =	30.4923	Anisotropy =	8.6229
16 H	Isotropic =	30.2485	Anisotropy =	10.0767
17 H	Isotropic =	30.6254	Anisotropy =	8.4776

Conformer_2

```

-----
C      -0.794040203152  -1.948197521552  -4.090150579313
C      -0.467807080574  -0.634530188911  -3.359721964997
N       0.986798002525  -0.464174047410  -3.223698938173
C       1.696786583155  -0.912397898312  -4.419888745317
C       1.635729148820  -2.445558847932  -4.497445534509
C       0.322673274466  -2.970612405401  -3.890348885344
H      -1.754070094033  -2.335921212913  -3.737191201459
H      -0.910216700856  -1.758953465470  -5.163893767233
H      -0.904787832475  -0.643956937015  -2.355033338850
H      -0.923723916115   0.206266248139  -3.905101999371
H       1.194464099291   0.510159812997  -3.041806631037
H       1.263447873569  -0.472967673523  -5.334490944613
H       2.733270523090  -0.569866269052  -4.363586921403
H       2.488934320609  -2.882685373359  -3.967909925422
H       1.718512907551  -2.754644667818  -5.545303816491
H       0.050229775881  -3.929472165154  -4.342101359949
H       0.453399318245  -3.154087387314  -2.818025446520

```

SCF Done: E(RwB97X) = -251.907517123

```

Zero-point correction=          0.160110
Thermal correction to Energy=      0.165927
Thermal correction to Enthalpy=    0.166871
Thermal correction to Gibbs Free Energy=  0.130945
Sum of electronic and zero-point Energies= -251.747408
Sum of electronic and thermal Energies= -251.741591
Sum of electronic and thermal Enthalpies= -251.740646
Sum of electronic and thermal Free Energies= -251.776572

```

```

1 C  Isotropic = 170.4001  Anisotropy = 7.0119
2 C  Isotropic = 147.9942  Anisotropy = 35.8637
3 N  Isotropic = 233.7109  Anisotropy = 60.8558
4 C  Isotropic = 150.7248  Anisotropy = 33.6824
5 C  Isotropic = 166.8590  Anisotropy = 11.2177
6 C  Isotropic = 173.0018  Anisotropy = 6.6524
7 H  Isotropic = 30.3790  Anisotropy = 10.3838
8 H  Isotropic = 30.3157  Anisotropy = 8.6825
9 H  Isotropic = 29.0309  Anisotropy = 9.5616
10 H  Isotropic = 28.9245  Anisotropy = 9.1025
11 H  Isotropic = 31.0542  Anisotropy = 16.2332
12 H  Isotropic = 29.2136  Anisotropy = 8.7683
13 H  Isotropic = 29.2199  Anisotropy = 9.1534
14 H  Isotropic = 30.1231  Anisotropy = 9.8625
15 H  Isotropic = 30.4377  Anisotropy = 9.8574
16 H  Isotropic = 30.4450  Anisotropy = 10.3185

```

17 H Isotropic = 30.3308 Anisotropy = 9.3405

Conformer_3

```
-----  
C      1.478338869244 -2.229097370875 -4.792899857202  
C      1.909279652137 -1.206517711180 -3.744530632551  
N      0.884222906781 -0.176956363887 -3.499307928049  
C     -0.494318809538 -0.635977235467 -3.746765088293  
C     -0.628651570705 -2.107528686298 -3.378681744974  
C      0.224679306953 -2.983789464113 -4.313596023531  
H      1.268046882257 -1.701504599703 -5.731022775496  
H      2.295995487964 -2.926640593836 -5.000712488554  
H      2.129977042301 -1.730962962070 -2.805396433231  
H      2.831233491389 -0.700731007408 -4.044389028002  
H      1.072466966007  0.617442997274 -4.098374569655  
H     -1.183275111940 -0.025517112513 -3.153869319101  
H     -0.780817486865 -0.509129028963 -4.802599913607  
H     -0.307499298585 -2.236995345279 -2.338171097853  
H     -1.680147710723 -2.406089562967 -3.421429817037  
H      0.515383374548 -3.900377656121 -3.789220128648  
H     -0.370913991226 -3.294228296595 -5.178933154216
```

SCF Done: E(RwB97X) = -251.907211898

```
Zero-point correction=          0.160250  
Thermal correction to Energy=      0.166054  
Thermal correction to Enthalpy=     0.166999  
Thermal correction to Gibbs Free Energy= 0.131145  
Sum of electronic and zero-point Energies= -251.746962  
Sum of electronic and thermal Energies= -251.741158  
Sum of electronic and thermal Enthalpies= -251.740213  
Sum of electronic and thermal Free Energies= -251.776067
```

```
1 C Isotropic = 167.7997 Anisotropy = 10.1101  
2 C Isotropic = 149.7915 Anisotropy = 33.1882  
3 N Isotropic = 233.1477 Anisotropy = 63.1199  
4 C Isotropic = 150.2235 Anisotropy = 30.3463  
5 C Isotropic = 169.9415 Anisotropy = 6.3194  
6 C Isotropic = 170.4532 Anisotropy = 5.8494  
7 H Isotropic = 30.2250 Anisotropy = 8.5421  
8 H Isotropic = 30.4345 Anisotropy = 10.1465  
9 H Isotropic = 29.1199 Anisotropy = 8.7510  
10 H Isotropic = 29.2144 Anisotropy = 8.9007  
11 H Isotropic = 30.8854 Anisotropy = 15.4135  
12 H Isotropic = 29.1471 Anisotropy = 9.7243
```

13	H	Isotropic =	28.9327	Anisotropy =	8.2789
14	H	Isotropic =	30.1993	Anisotropy =	8.9419
15	H	Isotropic =	30.3893	Anisotropy =	10.4935
16	H	Isotropic =	30.3007	Anisotropy =	9.9718
17	H	Isotropic =	30.2666	Anisotropy =	9.7398

Piperidine_protonated

Conformer_1

C	0.718878632131	-0.506283132355	-1.093830287317
C	-0.042350253609	0.806967392402	-1.147131473705
N	-1.377163698970	0.649252755375	-0.489085858776
C	-2.210690508154	-0.436113764363	-1.094757378759
C	-1.460100676454	-1.755465046169	-1.041197543897
C	-0.091782554765	-1.644395600574	-1.711978089600
H	1.667811221929	-0.369051763281	-1.618567829883
H	0.957566258230	-0.740805089725	-0.049137579845
H	0.478350319123	1.611130281565	-0.627088091205
H	-0.242016183023	1.115801256663	-2.175725256465
H	-1.239652021791	0.451299703943	0.505695689844
H	-1.885556838541	1.534146982445	-0.534425360115
H	-3.148198437440	-0.467922657940	-0.539492083208
H	-2.413710444200	-0.129203895288	-2.123270454208
H	-1.340284685775	-2.058133997014	0.006366953161
H	-2.076391401052	-2.515557274063	-1.528126840886
H	-0.224890476135	-1.457411320396	-2.784734021648
H	0.451581748494	-2.588054831223	-1.613614493487

SCF Done: E(RwB97X) = -252.393756689

Zero-point correction=	0.175978
Thermal correction to Energy=	0.181591
Thermal correction to Enthalpy=	0.182535
Thermal correction to Gibbs Free Energy=	0.147234
Sum of electronic and zero-point Energies=	-252.217779
Sum of electronic and thermal Energies=	-252.212165
Sum of electronic and thermal Enthalpies=	-252.211221
Sum of electronic and thermal Free Energies=	-252.246523

1	C	Isotropic =	166.3614	Anisotropy =	5.0823
2	C	Isotropic =	142.7805	Anisotropy =	34.5803
3	N	Isotropic =	207.7150	Anisotropy =	16.9221
4	C	Isotropic =	142.7805	Anisotropy =	34.5802
5	C	Isotropic =	166.3614	Anisotropy =	5.0822
6	C	Isotropic =	167.7234	Anisotropy =	6.7663

7 H	Isotropic =	30.0433	Anisotropy =	10.7264
8 H	Isotropic =	30.1500	Anisotropy =	8.8464
9 H	Isotropic =	28.4519	Anisotropy =	9.6052
10 H	Isotropic =	28.7800	Anisotropy =	8.2714
11 H	Isotropic =	27.4920	Anisotropy =	13.7394
12 H	Isotropic =	26.9838	Anisotropy =	16.6120
13 H	Isotropic =	28.4519	Anisotropy =	9.6052
14 H	Isotropic =	28.7800	Anisotropy =	8.2714
15 H	Isotropic =	30.1500	Anisotropy =	8.8464
16 H	Isotropic =	30.0433	Anisotropy =	10.7264
17 H	Isotropic =	30.3252	Anisotropy =	8.9486
18 H	Isotropic =	30.1264	Anisotropy =	10.4619

Conformer_2

C	0.552838030540	-0.328809169416	-1.664230180946
C	0.052089338510	0.578281918466	-0.556791343560
N	-1.439705720724	0.750453518493	-0.677161765919
C	-2.163038142196	-0.437008018390	-1.257065400723
C	-1.430632734937	-1.712335399363	-0.886781375055
C	-0.029240134567	-1.745327211661	-1.520148265307
H	0.277974119920	0.107883709834	-2.630493216470
H	1.644413940153	-0.347457233226	-1.629020391159
H	0.243510297020	0.146900669724	0.426944518543
H	0.490295141892	1.574910563457	-0.595426344410
H	-1.821085566108	0.958554798086	0.246657437697
H	-1.638538041369	1.568914614264	-1.254037319808
H	-3.181574296552	-0.406825298146	-0.871760673003
H	-2.190845003859	-0.294694683229	-2.338472238499
H	-1.365485584746	-1.778542707871	0.204678999762
H	-2.030467760523	-2.563714057140	-1.216138904125
H	-0.075068563522	-2.218030785096	-2.505460941904
H	0.631260681069	-2.360055228787	-0.901892595114

SCF Done: E(RwB97X) = -252.384353116

Zero-point correction=	0.176183
Thermal correction to Energy=	0.182012
Thermal correction to Enthalpy=	0.182956
Thermal correction to Gibbs Free Energy=	0.147013
Sum of electronic and zero-point Energies=	-252.208170
Sum of electronic and thermal Energies=	-252.202341
Sum of electronic and thermal Enthalpies=	-252.201397
Sum of electronic and thermal Free Energies=	-252.237340

1 C	Isotropic =	172.8117	Anisotropy =	7.3611
2 C	Isotropic =	148.1430	Anisotropy =	38.4210
3 N	Isotropic =	216.5483	Anisotropy =	13.8670
4 C	Isotropic =	148.1465	Anisotropy =	38.4221
5 C	Isotropic =	172.8120	Anisotropy =	7.3633
6 C	Isotropic =	172.5471	Anisotropy =	5.7088
7 H	Isotropic =	30.0378	Anisotropy =	9.2303
8 H	Isotropic =	30.1426	Anisotropy =	11.0266
9 H	Isotropic =	28.6241	Anisotropy =	8.6061
10 H	Isotropic =	28.5602	Anisotropy =	9.8923
11 H	Isotropic =	27.0514	Anisotropy =	16.2990
12 H	Isotropic =	27.0513	Anisotropy =	16.2995
13 H	Isotropic =	28.5605	Anisotropy =	9.8927
14 H	Isotropic =	28.6239	Anisotropy =	8.6058
15 H	Isotropic =	30.0380	Anisotropy =	9.2311
16 H	Isotropic =	30.1424	Anisotropy =	11.0262
17 H	Isotropic =	30.1550	Anisotropy =	10.3015
18 H	Isotropic =	30.1552	Anisotropy =	10.3010

Conformer_3

C	0.672610937726	-0.506805282604	-0.937779452413
C	-0.071214796040	0.762148220218	-1.307243699488
N	-1.439733612235	0.750452841774	-0.677288406460
C	-2.039839519625	-0.620863797872	-0.506467197621
C	-1.550094980995	-1.534811638018	-1.613207838623
C	-0.029186613952	-1.745462504622	-1.520321406243
H	0.736553026005	-0.573842420727	0.153709355341
H	1.697642420335	-0.426305130941	-1.306499976049
H	0.430499472740	1.663850394181	-0.958011140151
H	-0.219281451296	0.836001410541	-2.385698189019
H	-1.393611830216	1.204003323405	0.236197003975
H	-2.066193447669	1.323746270903	-1.244009956891
H	-1.728706286927	-0.983097532752	0.474565270567
H	-3.121983533603	-0.495535537441	-0.508745452945
H	-1.823467876744	-1.097415546283	-2.579583046187
H	-2.083604023352	-2.484999206017	-1.538139333171
H	0.365566724684	-1.965117353491	-2.516473884884
H	0.190545391162	-2.613046510254	-0.891502649736

SCF Done: E(RwB97X) = -252.384352956

Zero-point correction=	0.176180
Thermal correction to Energy=	0.182010
Thermal correction to Enthalpy=	0.182954

Thermal correction to Gibbs Free Energy=	0.147008
Sum of electronic and zero-point Energies=	-252.208173
Sum of electronic and thermal Energies=	-252.202343
Sum of electronic and thermal Enthalpies=	-252.201399
Sum of electronic and thermal Free Energies=	-252.237345

1 C	Isotropic =	172.8145	Anisotropy =	7.3562
2 C	Isotropic =	148.1348	Anisotropy =	38.4352
3 N	Isotropic =	216.5424	Anisotropy =	13.8418
4 C	Isotropic =	148.1361	Anisotropy =	38.4357
5 C	Isotropic =	172.8146	Anisotropy =	7.3570
6 C	Isotropic =	172.5632	Anisotropy =	5.7181
7 H	Isotropic =	30.0373	Anisotropy =	9.2306
8 H	Isotropic =	30.1427	Anisotropy =	11.0261
9 H	Isotropic =	28.5601	Anisotropy =	9.8905
10 H	Isotropic =	28.6240	Anisotropy =	8.6052
11 H	Isotropic =	27.0506	Anisotropy =	16.2967
12 H	Isotropic =	27.0506	Anisotropy =	16.2966
13 H	Isotropic =	28.6239	Anisotropy =	8.6051
14 H	Isotropic =	28.5602	Anisotropy =	9.8907
15 H	Isotropic =	30.0374	Anisotropy =	9.2309
16 H	Isotropic =	30.1426	Anisotropy =	11.0260
17 H	Isotropic =	30.1547	Anisotropy =	10.3009
18 H	Isotropic =	30.1546	Anisotropy =	10.3011

Quinuclidine_neutral

Conformer_1

N	0.950385948702	-0.936973994727	-2.533623940657
C	2.021110048526	-0.991140473345	-3.537059657856
C	1.470748015252	-1.346538069439	-4.943957218327
C	-0.055549436052	-1.461532289394	-4.844407259659
C	-0.399874660571	-2.577485697886	-3.849721736656
C	0.261713915979	-2.233063593261	-2.488740879667
C	-0.614086485005	-0.136262156022	-4.310395988567
C	-0.009617557837	0.111038027721	-2.902325388802
H	2.519204573716	-0.016471387367	-3.546341276766
H	2.757052788251	-1.730155691939	-3.205133808726
H	1.741812558320	-0.575429065748	-5.672916363970
H	1.892041825626	-2.292845634880	-5.300017948073
H	-0.484029283419	-1.683915420021	-5.826110789879
H	-1.487292811555	-2.659218892631	-3.745581999643
H	-0.037974037453	-3.540362584095	-4.225893636529
H	0.998795951292	-2.992131208023	-2.208209852460
H	-0.484261450830	-2.192073115039	-1.688902700220

H	-0.354281159150	0.679129583874	-4.994367019809
H	-1.707526316330	-0.181785436742	-4.262571286775
H	-0.792381108758	0.130350940166	-2.137312929103
H	0.508308681296	1.074466158799	-2.861608317855

SCF Done: E(RwB97X) = -329.324801314

Zero-point correction=	0.196640
Thermal correction to Energy=	0.203212
Thermal correction to Enthalpy=	0.204156
Thermal correction to Gibbs Free Energy=	0.165343
Sum of electronic and zero-point Energies=	-329.128161
Sum of electronic and thermal Energies=	-329.121590
Sum of electronic and thermal Enthalpies=	-329.120646
Sum of electronic and thermal Free Energies=	-329.159458

1 N	Isotropic = 235.7203	Anisotropy = 21.5495
2 C	Isotropic = 142.4768	Anisotropy = 44.5275
3 C	Isotropic = 163.0334	Anisotropy = 9.3955
4 C	Isotropic = 168.1725	Anisotropy = 0.8398
5 C	Isotropic = 163.1766	Anisotropy = 9.2742
6 C	Isotropic = 142.5556	Anisotropy = 44.4987
7 C	Isotropic = 163.0920	Anisotropy = 9.3809
8 C	Isotropic = 142.5222	Anisotropy = 44.4717
9 H	Isotropic = 29.0902	Anisotropy = 9.5613
10 H	Isotropic = 29.0511	Anisotropy = 9.6413
11 H	Isotropic = 30.4227	Anisotropy = 9.8311
12 H	Isotropic = 30.4243	Anisotropy = 9.8059
13 H	Isotropic = 30.4159	Anisotropy = 10.8031
14 H	Isotropic = 30.4171	Anisotropy = 9.8108
15 H	Isotropic = 30.4167	Anisotropy = 9.8321
16 H	Isotropic = 29.0837	Anisotropy = 9.5646
17 H	Isotropic = 29.0498	Anisotropy = 9.6421
18 H	Isotropic = 30.4258	Anisotropy = 9.8033
19 H	Isotropic = 30.4111	Anisotropy = 9.8347
20 H	Isotropic = 29.0860	Anisotropy = 9.5742
21 H	Isotropic = 29.0549	Anisotropy = 9.6336

Quinuclidine_protonated

Conformer_1

N	5.635592075965	-6.038083907802	1.385531589587
C	6.217950690770	-5.713210187320	2.728599022883
C	5.240939496936	-6.194189597066	3.814639000642
C	3.901489696898	-6.548978540645	3.156509578592

C	4.105722203694	-7.768644781702	2.249400752893
C	5.286840017306	-7.494487305936	1.304175993371
C	3.444922132293	-5.363979569538	2.296289302954
C	4.423602008189	-5.195334247068	1.121792163198
H	6.334378576874	-5.832066933271	0.671554645803
H	7.189058843592	-6.205110488495	2.783006633946
H	6.367184649482	-4.632913471673	2.746353919024
H	5.646351090767	-7.069614574749	4.329005790102
H	5.106230246187	-5.405317866596	4.557979797254
H	3.153849271120	-6.769797751687	3.920377274211
H	4.316658117133	-8.658677991981	2.846310964792
H	3.196632417178	-7.961837875796	1.673633752870
H	5.054821559545	-7.708831099816	0.261068958325
H	6.186709800006	-8.042807366618	1.585825111197
H	2.438080077462	-5.536062847697	1.909427664407
H	3.418687197189	-4.453365457170	2.900877430755
H	4.767474275112	-4.168297386030	1.001017142813
H	4.008225556303	-5.542390751344	0.174923510381

SCF Done: E(RwB97X) = -329.802883919

Zero-point correction=	0.212640
Thermal correction to Energy=	0.219185
Thermal correction to Enthalpy=	0.220129
Thermal correction to Gibbs Free Energy=	0.182023
Sum of electronic and zero-point Energies=	-329.590244
Sum of electronic and thermal Energies=	-329.583699
Sum of electronic and thermal Enthalpies=	-329.582755
Sum of electronic and thermal Free Energies=	-329.620861

1 N	Isotropic =	212.9790	Anisotropy =	0.2963
2 C	Isotropic =	141.4751	Anisotropy =	52.3094
3 C	Isotropic =	166.2524	Anisotropy =	17.6654
4 C	Isotropic =	169.2764	Anisotropy =	2.4079
5 C	Isotropic =	166.3793	Anisotropy =	17.5883
6 C	Isotropic =	141.4186	Anisotropy =	52.3876
7 C	Isotropic =	166.3377	Anisotropy =	17.5058
8 C	Isotropic =	141.4174	Anisotropy =	52.3676
9 H	Isotropic =	27.4694	Anisotropy =	17.2579
10 H	Isotropic =	28.4849	Anisotropy =	10.0886
11 H	Isotropic =	28.6121	Anisotropy =	9.9286
12 H	Isotropic =	29.9811	Anisotropy =	10.5136
13 H	Isotropic =	29.9743	Anisotropy =	10.7940
14 H	Isotropic =	29.9760	Anisotropy =	11.1650
15 H	Isotropic =	29.9760	Anisotropy =	10.7855
16 H	Isotropic =	29.9847	Anisotropy =	10.5112

17	H	Isotropic =	28.4850	Anisotropy =	10.0720
18	H	Isotropic =	28.6103	Anisotropy =	9.9255
19	H	Isotropic =	29.9711	Anisotropy =	10.7851
20	H	Isotropic =	29.9812	Anisotropy =	10.4985
21	H	Isotropic =	28.4906	Anisotropy =	10.0679
22	H	Isotropic =	28.6162	Anisotropy =	9.9194

Brucine_neutral

Conformer_1

C	-4.435865694007	-1.700714580477	-0.035411506779
N	-4.161635396116	-0.264173775010	0.202570572084
C	-2.765249112268	-0.039012600641	0.127971061091
C	-2.096026751453	-1.243040231347	0.010370861971
C	-0.706632913623	-1.261290320065	-0.093420443613
C	-0.000407898460	-0.065065922582	-0.086818364685
O	1.351517061005	0.029043428131	-0.189746013547
C	2.080534123210	-1.182325490738	-0.316331563169
C	-0.697130660649	1.159878409594	0.038743234179
O	0.071859273145	2.276635569426	0.039891281562
C	-0.585027575854	3.529626448777	0.169603383305
C	-2.083241187211	1.178550268322	0.149292046587
C	-3.055582547829	-2.402518487353	0.113565141948
C	-2.955855576848	-3.133482785207	1.464076235201
C	-3.723896403696	-4.423160983283	1.208978047773
N	-3.420965724931	-4.774042535593	-0.188225603791
C	-4.564524366536	-5.364479724370	-0.893497733646
C	-5.560579651572	-4.314876496609	-1.327686004196
C	-6.857101594108	-4.364452101560	-1.028061509943
C	-7.799383156200	-3.242728895507	-1.373006630258
O	-7.492064254986	-2.049968672492	-0.653016118266
C	-6.531325009300	-1.194986443601	-1.263455000176
C	-6.496826115678	0.061541733731	-0.367014405572
C	-5.129267133247	0.653696434565	-0.090064902065
O	-4.924960404934	1.861902890616	-0.098501056118
C	-5.119250097629	-1.781805503619	-1.404330592946
C	-4.952039051660	-3.144478349200	-2.088999759983
C	-2.836746096039	-3.582394744303	-0.864246899684
C	-3.444606980427	-3.369621065814	-2.244677970004
H	-5.123493156626	-2.069226624906	0.732590877874
H	-0.184518896232	-2.207956065197	-0.177135203201
H	1.794772760094	-1.727834065684	-1.222543884815
H	3.130211118026	-0.897297212350	-0.385358992638
H	1.940509529311	-1.827583679464	0.557938789063
H	-1.275442525446	3.705640375566	-0.662454728785

H	-1.128576732923	3.599726688150	1.117962036251
H	0.201279847002	4.283932214522	0.148048983918
H	-2.630291328098	2.104577710773	0.243084580968
H	-3.364535655984	-2.547559141019	2.291913975588
H	-1.902772118979	-3.345840130134	1.678350745227
H	-4.802316356588	-4.251900333325	1.346999431381
H	-3.430370147349	-5.228665389299	1.889479153769
H	-5.037652813773	-6.097246549846	-0.234709736186
H	-4.198450019231	-5.913983823156	-1.767919605205
H	-7.252781250937	-5.209745265167	-0.467464904063
H	-8.823030491601	-3.502993668319	-1.096072338523
H	-7.790235120852	-3.032903549420	-2.452741483974
H	-6.895095549881	-0.930405431515	-2.265545867543
H	-6.913566803989	-0.230155008460	0.603694071785
H	-7.125949231265	0.857392551077	-0.765184066441
H	-4.591898879380	-1.071423010709	-2.056314482613
H	-5.426373273317	-3.084095819873	-3.076738517835
H	-1.754106592164	-3.728533057640	-0.962720461375
H	-2.976689440211	-2.501706245302	-2.719752935855
H	-3.234945971708	-4.233570943093	-2.881455224031

SCF Done: E(RwB97X) = -1302.52276970

Zero-point correction=	0.470231
Thermal correction to Energy=	0.492267
Thermal correction to Enthalpy=	0.493211
Thermal correction to Gibbs Free Energy=	0.421403
Sum of electronic and zero-point Energies=	-1302.052539
Sum of electronic and thermal Energies=	-1302.030503
Sum of electronic and thermal Enthalpies=	-1302.029559
Sum of electronic and thermal Free Energies=	-1302.101367

1 C	Isotropic =	128.1004	Anisotropy =	40.0787
2 N	Isotropic =	97.3361	Anisotropy =	95.9967
3 C	Isotropic =	49.4437	Anisotropy =	116.0456
4 C	Isotropic =	60.8419	Anisotropy =	134.6967
5 C	Isotropic =	81.3433	Anisotropy =	157.0888
6 C	Isotropic =	39.0750	Anisotropy =	118.3239
7 O	Isotropic =	257.6037	Anisotropy =	91.4170
8 C	Isotropic =	135.6570	Anisotropy =	72.1079
9 C	Isotropic =	36.0843	Anisotropy =	122.6331
10 O	Isotropic =	253.0896	Anisotropy =	99.4903
11 C	Isotropic =	135.6970	Anisotropy =	73.1975
12 C	Isotropic =	87.5577	Anisotropy =	139.8212
13 C	Isotropic =	137.3005	Anisotropy =	27.3284
14 C	Isotropic =	147.8784	Anisotropy =	41.1450

15	C	Isotropic =	140.9048	Anisotropy =	55.2834
16	N	Isotropic =	217.2104	Anisotropy =	60.2432
17	C	Isotropic =	137.9593	Anisotropy =	27.9304
18	C	Isotropic =	36.1771	Anisotropy =	175.1555
19	C	Isotropic =	57.4512	Anisotropy =	135.2416
20	C	Isotropic =	126.3678	Anisotropy =	70.6657
21	O	Isotropic =	271.3251	Anisotropy =	97.0100
22	C	Isotropic =	112.7960	Anisotropy =	54.6757
23	C	Isotropic =	145.8340	Anisotropy =	39.3422
24	C	Isotropic =	11.5777	Anisotropy =	124.3233
25	O	Isotropic =	-60.0134	Anisotropy =	578.5412
26	C	Isotropic =	141.6153	Anisotropy =	20.4840
27	C	Isotropic =	157.3728	Anisotropy =	11.8188
28	C	Isotropic =	129.8682	Anisotropy =	38.4941
29	C	Isotropic =	163.8354	Anisotropy =	13.8288
30	H	Isotropic =	28.1076	Anisotropy =	3.1962
31	H	Isotropic =	24.6422	Anisotropy =	13.2635
32	H	Isotropic =	28.1067	Anisotropy =	7.8968
33	H	Isotropic =	27.7051	Anisotropy =	9.4564
34	H	Isotropic =	28.0559	Anisotropy =	8.1114
35	H	Isotropic =	28.0578	Anisotropy =	8.3583
36	H	Isotropic =	28.0381	Anisotropy =	8.4325
37	H	Isotropic =	27.6443	Anisotropy =	9.6012
38	H	Isotropic =	23.8354	Anisotropy =	11.9979
39	H	Isotropic =	30.1163	Anisotropy =	7.7067
40	H	Isotropic =	30.0457	Anisotropy =	9.3105
41	H	Isotropic =	29.0773	Anisotropy =	6.1834
42	H	Isotropic =	28.8846	Anisotropy =	11.9229
43	H	Isotropic =	29.1660	Anisotropy =	9.0714
44	H	Isotropic =	28.1563	Anisotropy =	10.0148
45	H	Isotropic =	25.6046	Anisotropy =	5.9521
46	H	Isotropic =	27.8074	Anisotropy =	10.4124
47	H	Isotropic =	27.5619	Anisotropy =	7.7686
48	H	Isotropic =	27.7287	Anisotropy =	6.9751
49	H	Isotropic =	29.3074	Anisotropy =	5.2942
50	H	Isotropic =	28.9384	Anisotropy =	8.5447
51	H	Isotropic =	30.8996	Anisotropy =	3.4021
52	H	Isotropic =	28.8026	Anisotropy =	9.3883
53	H	Isotropic =	28.0691	Anisotropy =	10.1161
54	H	Isotropic =	30.6460	Anisotropy =	7.1319
55	H	Isotropic =	29.7013	Anisotropy =	11.2380

Conformer_10

C -4.419793307485 -1.773325496933 -0.066354005848

N	-4.180861686436	-0.360387155327	0.292747485226
C	-2.791737504620	-0.098872295633	0.187500720678
C	-2.101692692160	-1.282403422365	-0.014584440942
C	-0.716844208300	-1.262590244772	-0.162515621976
C	-0.037102551223	-0.051238480039	-0.118634868775
O	1.308538023199	0.079162379071	-0.258198607951
C	2.062972638362	-1.110090632741	-0.435718506852
C	-0.755093485929	1.150091043692	0.088603259075
O	-0.010273798318	2.282458878744	0.117408831887
C	-0.689162348102	3.515637082241	0.309659213860
C	-2.137093065415	1.131250420870	0.246595818331
C	-3.038179308336	-2.464441706075	0.077375914445
C	-2.912862897425	-3.192688455098	1.427600934740
C	-3.657662846816	-4.501851578223	1.192224684372
N	-3.428059189116	-4.836714468279	-0.224502037318
C	-4.639303372909	-5.349121009387	-0.891034632960
C	-5.572117324853	-4.209437855568	-1.233913647899
C	-6.753384632821	-4.081119026621	-0.631431763250
C	-7.711787385847	-2.924743600434	-0.671751428062
O	-7.478353510448	-1.936465655493	-1.659248915316
C	-6.366178459809	-1.061946292205	-1.505500540028
C	-6.509015286822	-0.113418172089	-0.292480706786
C	-5.190092534633	0.538355184710	0.080723429218
O	-5.043126975841	1.749885496941	0.179033459187
C	-4.993865876596	-1.760407738647	-1.486744288792
C	-4.926278512082	-3.147577462339	-2.122308478373
C	-2.825747458386	-3.651268978144	-0.898257369123
C	-3.431996634213	-3.461308547197	-2.282447602926
H	-5.134914808273	-2.207656943154	0.636428215452
H	-0.177740158537	-2.191880865301	-0.309812861060
H	1.952601068192	-1.785261535004	0.419995096906
H	1.774726012342	-1.633647174224	-1.353983799724
H	3.104342250993	-0.798060735650	-0.513429818677
H	-1.202127090552	3.543430102616	1.277104979463
H	0.080487080828	4.286915789886	0.287580235960
H	-1.410687671528	3.702898576638	-0.492950479721
H	-2.701324026283	2.038366650552	0.405705698321
H	-3.322994529622	-2.612258939521	2.258837396154
H	-1.852808139252	-3.379504545956	1.630623636385
H	-4.730127075435	-4.362893041879	1.388315568228
H	-3.305657860644	-5.304187082361	1.848409185880
H	-5.122683350149	-6.061267059872	-0.217944900514
H	-4.347189239104	-5.903884376091	-1.788338462810
H	-7.083653444869	-4.881281401133	0.032487045712
H	-7.757296146208	-2.475717702060	0.332311272054
H	-8.719118701043	-3.301320773151	-0.876086549040

H	-6.416691972074	-0.456399583618	-2.413092011437
H	-6.851362554441	-0.678807743761	0.581125346931
H	-7.238076404985	0.671515669510	-0.491849526359
H	-4.327420588814	-1.113521706050	-2.071121039508
H	-5.412255705353	-3.126766284189	-3.103095119154
H	-1.743846809517	-3.809176981622	-0.987510987558
H	-2.929367845898	-2.638786967100	-2.799961346813
H	-3.267156096393	-4.360767560164	-2.881893062911

SCF Done: E(RwB97X) = -1302.51900705

Zero-point correction=	0.470395
Thermal correction to Energy=	0.492412
Thermal correction to Enthalpy=	0.493356
Thermal correction to Gibbs Free Energy=	0.421500
Sum of electronic and zero-point Energies=	-1302.048612
Sum of electronic and thermal Energies=	-1302.026595
Sum of electronic and thermal Enthalpies=	-1302.025651
Sum of electronic and thermal Free Energies=	-1302.097507

1 C	Isotropic =	126.5666	Anisotropy =	37.8052
2 N	Isotropic =	101.1278	Anisotropy =	102.6243
3 C	Isotropic =	49.4298	Anisotropy =	117.0731
4 C	Isotropic =	60.7889	Anisotropy =	135.1176
5 C	Isotropic =	81.2078	Anisotropy =	157.1980
6 C	Isotropic =	39.0309	Anisotropy =	118.7432
7 O	Isotropic =	257.3944	Anisotropy =	91.2879
8 C	Isotropic =	135.6398	Anisotropy =	72.2433
9 C	Isotropic =	36.0488	Anisotropy =	122.8233
10 O	Isotropic =	253.0682	Anisotropy =	100.4297
11 C	Isotropic =	135.8585	Anisotropy =	73.0418
12 C	Isotropic =	87.9731	Anisotropy =	140.4149
13 C	Isotropic =	137.1849	Anisotropy =	25.6757
14 C	Isotropic =	148.8602	Anisotropy =	42.5129
15 C	Isotropic =	141.7195	Anisotropy =	55.7865
16 N	Isotropic =	213.0022	Anisotropy =	58.0192
17 C	Isotropic =	136.0092	Anisotropy =	26.5745
18 C	Isotropic =	48.4293	Anisotropy =	165.6366
19 C	Isotropic =	56.9541	Anisotropy =	118.9163
20 C	Isotropic =	127.2146	Anisotropy =	57.4267
21 O	Isotropic =	287.6999	Anisotropy =	57.6532
22 C	Isotropic =	117.4936	Anisotropy =	54.4334
23 C	Isotropic =	154.8800	Anisotropy =	45.6412
24 C	Isotropic =	9.8153	Anisotropy =	122.3954
25 O	Isotropic =	-67.2743	Anisotropy =	585.1658
26 C	Isotropic =	139.6067	Anisotropy =	32.3978

27	C	Isotropic =	159.5146	Anisotropy =	10.0801
28	C	Isotropic =	130.0172	Anisotropy =	36.4552
29	C	Isotropic =	162.7662	Anisotropy =	15.2430
30	H	Isotropic =	28.1573	Anisotropy =	2.7612
31	H	Isotropic =	24.6914	Anisotropy =	13.2697
32	H	Isotropic =	28.1163	Anisotropy =	8.0727
33	H	Isotropic =	28.1008	Anisotropy =	7.9358
34	H	Isotropic =	27.7158	Anisotropy =	9.4894
35	H	Isotropic =	28.0327	Anisotropy =	8.4623
36	H	Isotropic =	27.6498	Anisotropy =	9.6124
37	H	Isotropic =	28.0903	Anisotropy =	8.3331
38	H	Isotropic =	23.8995	Anisotropy =	12.0139
39	H	Isotropic =	30.1312	Anisotropy =	7.3271
40	H	Isotropic =	30.2011	Anisotropy =	9.2198
41	H	Isotropic =	29.1570	Anisotropy =	6.1149
42	H	Isotropic =	28.9669	Anisotropy =	11.9919
43	H	Isotropic =	29.3539	Anisotropy =	9.5835
44	H	Isotropic =	28.1304	Anisotropy =	10.1239
45	H	Isotropic =	26.1457	Anisotropy =	5.5554
46	H	Isotropic =	27.1212	Anisotropy =	5.8569
47	H	Isotropic =	27.6394	Anisotropy =	10.2262
48	H	Isotropic =	27.6109	Anisotropy =	6.7590
49	H	Isotropic =	28.4358	Anisotropy =	4.6027
50	H	Isotropic =	29.6163	Anisotropy =	9.7416
51	H	Isotropic =	30.5240	Anisotropy =	3.0097
52	H	Isotropic =	28.8685	Anisotropy =	9.7342
53	H	Isotropic =	28.1312	Anisotropy =	10.1846
54	H	Isotropic =	30.6239	Anisotropy =	7.6843
55	H	Isotropic =	29.6598	Anisotropy =	11.4627

Conformer_11

C	-4.418614975591	-1.777774803145	-0.035029685628
N	-4.166033930496	-0.375131199492	0.354822611403
C	-2.771279186714	-0.141800911181	0.332624426684
C	-2.096364008237	-1.345280032613	0.150796375086
C	-0.711491374382	-1.341699667112	0.070488330294
C	-0.014256932328	-0.144564638864	0.168638735126
O	1.357141774480	-0.163855437806	0.130375680364
C	1.915271546644	0.348443142661	-1.079250882044
C	-0.708180595560	1.064131572095	0.367188693581
O	0.055253364878	2.179513810735	0.476988213335
C	-0.609409770234	3.424722893495	0.652831844730
C	-2.102418116938	1.072806638746	0.448924258551
C	-3.064935526642	-2.503763990025	0.179160994731

C	-3.032756543962	-3.245317002233	1.527412759562
C	-3.795332302804	-4.533553372768	1.238482659387
N	-3.496331454106	-4.861688191530	-0.166874723519
C	-4.681113407742	-5.337204670826	-0.904388057178
C	-5.563644661787	-4.171323975677	-1.291349299069
C	-6.775967485368	-4.018245569881	-0.760603615803
C	-7.701900884113	-2.838246877350	-0.849320132348
O	-7.381764273150	-1.845051062094	-1.807347428851
C	-6.259361950582	-1.001906120776	-1.575235397964
C	-6.451084744253	-0.065963977083	-0.359337744588
C	-5.143312262950	0.550716354406	0.100243321137
O	-4.974806712916	1.755559639770	0.228065822416
C	-4.908786124867	-1.736192788960	-1.485335897602
C	-4.840588138589	-3.119075918382	-2.130191850501
C	-2.826807649176	-3.687190802618	-0.794232232134
C	-3.348648093153	-3.470660140869	-2.208677450302
H	-5.183777418641	-2.200278746320	0.620321120567
H	-0.148542924250	-2.261557687576	-0.063580621047
H	1.668243838204	1.405617474057	-1.211418906871
H	1.558391098964	-0.227248551438	-1.941211707668
H	2.997271523885	0.236563664132	-0.996330668857
H	-1.185935062090	3.440976419226	1.583579963951
H	0.175278892193	4.179094739122	0.702505793568
H	-1.268931207480	3.644321352016	-0.193254981771
H	-2.658007312569	1.986917405367	0.599023475687
H	-3.473870948337	-2.662029000051	2.340573600159
H	-1.990349927628	-3.459486023663	1.786620044898
H	-4.873432787623	-4.369918198064	1.376587341587
H	-3.499286869119	-5.349773205408	1.905081172194
H	-5.220244406209	-6.040365143331	-0.264898669608
H	-4.353276139474	-5.894076415939	-1.787976483886
H	-7.166214761640	-4.814631810511	-0.125285130259
H	-7.802800009699	-2.399620553474	0.155245698326
H	-8.702346795223	-3.187297910595	-1.124197429557
H	-6.240471930114	-0.383127628772	-2.474934874978
H	-6.854697931977	-0.634528981801	0.485656840383
H	-7.150322258141	0.737736702519	-0.588503442895
H	-4.193032091445	-1.102028630005	-2.023706204118
H	-5.269653571438	-3.076368403799	-3.136435435193
H	-1.745695971683	-3.870895281269	-0.823122225445
H	-2.795960198155	-2.657908376448	-2.689514636292
H	-3.173710409675	-4.369690108599	-2.805893961732

SCF Done: E(RwB97X) = -1302.51679778

Zero-point correction= 0.470290

Thermal correction to Energy=	0.492288
Thermal correction to Enthalpy=	0.493233
Thermal correction to Gibbs Free Energy=	0.421579
Sum of electronic and zero-point Energies=	-1302.046507
Sum of electronic and thermal Energies=	-1302.024509
Sum of electronic and thermal Enthalpies=	-1302.023565
Sum of electronic and thermal Free Energies=	-1302.095219

1	C	Isotropic =	126.3669	Anisotropy =	38.2195
2	N	Isotropic =	100.1004	Anisotropy =	100.9954
3	C	Isotropic =	44.7033	Anisotropy =	123.8036
4	C	Isotropic =	59.8931	Anisotropy =	134.7166
5	C	Isotropic =	66.5255	Anisotropy =	152.8951
6	C	Isotropic =	40.1103	Anisotropy =	114.8058
7	O	Isotropic =	282.2465	Anisotropy =	84.7065
8	C	Isotropic =	130.8066	Anisotropy =	89.6843
9	C	Isotropic =	31.2388	Anisotropy =	127.5263
10	O	Isotropic =	250.5830	Anisotropy =	99.1763
11	C	Isotropic =	135.6718	Anisotropy =	73.6175
12	C	Isotropic =	87.7339	Anisotropy =	139.9674
13	C	Isotropic =	137.7013	Anisotropy =	25.5351
14	C	Isotropic =	148.8185	Anisotropy =	42.9872
15	C	Isotropic =	141.7468	Anisotropy =	56.0170
16	N	Isotropic =	213.0569	Anisotropy =	58.0700
17	C	Isotropic =	136.2944	Anisotropy =	26.6126
18	C	Isotropic =	48.5249	Anisotropy =	165.7707
19	C	Isotropic =	56.9284	Anisotropy =	118.8602
20	C	Isotropic =	127.1296	Anisotropy =	57.5230
21	O	Isotropic =	287.8395	Anisotropy =	57.7926
22	C	Isotropic =	117.6914	Anisotropy =	54.6205
23	C	Isotropic =	154.7035	Anisotropy =	45.5975
24	C	Isotropic =	9.5200	Anisotropy =	122.4980
25	O	Isotropic =	-71.3619	Anisotropy =	593.3847
26	C	Isotropic =	139.6559	Anisotropy =	32.3632
27	C	Isotropic =	159.7468	Anisotropy =	9.8809
28	C	Isotropic =	129.9643	Anisotropy =	36.3305
29	C	Isotropic =	162.8107	Anisotropy =	15.1859
30	H	Isotropic =	28.0971	Anisotropy =	2.7113
31	H	Isotropic =	24.4274	Anisotropy =	10.8161
32	H	Isotropic =	27.5153	Anisotropy =	7.7400
33	H	Isotropic =	28.5597	Anisotropy =	8.1497
34	H	Isotropic =	28.0170	Anisotropy =	9.9789
35	H	Isotropic =	27.9894	Anisotropy =	8.4977
36	H	Isotropic =	27.6735	Anisotropy =	9.4258
37	H	Isotropic =	28.0552	Anisotropy =	8.1520
38	H	Isotropic =	23.8646	Anisotropy =	12.2100

39	H	Isotropic =	30.1158	Anisotropy =	7.3122
40	H	Isotropic =	30.2722	Anisotropy =	9.1432
41	H	Isotropic =	29.1334	Anisotropy =	6.1251
42	H	Isotropic =	28.9501	Anisotropy =	12.0031
43	H	Isotropic =	29.3471	Anisotropy =	9.6120
44	H	Isotropic =	28.1284	Anisotropy =	10.0871
45	H	Isotropic =	26.1761	Anisotropy =	5.4286
46	H	Isotropic =	27.1017	Anisotropy =	5.9947
47	H	Isotropic =	27.6211	Anisotropy =	10.2549
48	H	Isotropic =	27.6201	Anisotropy =	6.7331
49	H	Isotropic =	28.3883	Anisotropy =	4.6390
50	H	Isotropic =	29.5897	Anisotropy =	9.6953
51	H	Isotropic =	30.5186	Anisotropy =	3.0837
52	H	Isotropic =	28.8539	Anisotropy =	9.6697
53	H	Isotropic =	28.1364	Anisotropy =	9.9614
54	H	Isotropic =	30.6083	Anisotropy =	7.8537
55	H	Isotropic =	29.6493	Anisotropy =	11.5690

Conformer_12

C	-4.418706885769	-1.760456359664	-0.101172086156
N	-4.202661667505	-0.332875233320	0.209849934088
C	-2.824434569463	-0.042210648364	0.060502944522
C	-2.109549637252	-1.220358976996	-0.127703027429
C	-0.736565850466	-1.186633428421	-0.331815428820
C	-0.077696596281	0.043156023924	-0.355708638605
O	1.254347676435	0.193171789379	-0.578256043233
C	2.027479903669	-0.983998602870	-0.770538086778
C	-0.810329526129	1.226305391930	-0.145011353475
O	-0.185692061675	2.444875441009	-0.202439160593
C	0.623250879397	2.743051263409	0.935555977442
C	-2.183574461352	1.191496404556	0.065364355276
C	-3.019565773084	-2.416479110476	0.028906150750
C	-2.843681089332	-3.091016670830	1.401282486133
C	-3.571951755287	-4.420051470075	1.233842559770
N	-3.372961637874	-4.802978510263	-0.175187128407
C	-4.589482065138	-5.361822738281	-0.792795463133
C	-5.552276974948	-4.254352903038	-1.158914724862
C	-6.725642240811	-4.128590867054	-0.540674132343
C	-7.708799183734	-2.994377697856	-0.606434363143
O	-7.507726394843	-2.033434512422	-1.627427117693
C	-6.410548357011	-1.134109402936	-1.518582602686
C	-6.548667376298	-0.153928711358	-0.330203096359
C	-5.236053750424	0.537818075977	-0.008638661963
O	-5.110896334552	1.753921784081	0.045687810842

C	-5.024242863697	-1.805529579861	-1.507574162212
C	-4.945580412143	-3.212522622890	-2.097474428922
C	-2.807956156571	-3.634228506197	-0.907272619433
C	-3.450210142258	-3.506480627052	-2.281995747784
H	-5.106659291905	-2.188542027498	0.631643918790
H	-0.189105977453	-2.111564896413	-0.476504954792
H	1.978743530354	-1.639878729175	0.105231082559
H	3.054212047467	-0.647724975350	-0.912896688952
H	1.700468807168	-1.533466842990	-1.659732543622
H	0.001234754982	2.824907575035	1.834671238417
H	1.392352533995	1.980367844191	1.085875242468
H	1.099422376554	3.704411651375	0.738468145875
H	-2.724485518006	2.116063905131	0.217972646173
H	-3.241106987914	-2.488029480311	2.222472253167
H	-1.775501317828	-3.253218402601	1.580878377930
H	-4.641229483882	-4.291778571368	1.453574708234
H	-3.188314172800	-5.190822445671	1.909718164117
H	-5.044334485327	-6.055685430731	-0.081762189010
H	-4.307192774661	-5.946742402877	-1.673981347172
H	-7.027555658700	-4.910098775201	0.158056205727
H	-7.752164646366	-2.515154384164	0.383623931008
H	-8.710234545453	-3.397869042490	-0.787404407298
H	-6.489489727601	-0.554948035419	-2.441229533369
H	-6.857481256374	-0.701035432604	0.567146275928
H	-7.299764109361	0.608529555252	-0.535020298423
H	-4.383233279969	-1.167139931157	-2.128696228276
H	-5.453659708154	-3.232387816926	-3.066983854584
H	-1.726055355524	-3.777522852410	-1.016941949898
H	-2.974183896297	-2.696384580924	-2.842490661784
H	-3.283506552551	-4.425344468750	-2.850661678005

SCF Done: E(RwB97X) = -1302.51586172

Zero-point correction=	0.470177
Thermal correction to Energy=	0.492331
Thermal correction to Enthalpy=	0.493275
Thermal correction to Gibbs Free Energy=	0.421048
Sum of electronic and zero-point Energies=	-1302.045685
Sum of electronic and thermal Energies=	-1302.023531
Sum of electronic and thermal Enthalpies=	-1302.022586
Sum of electronic and thermal Free Energies=	-1302.094814

1 C	Isotropic =	126.3352	Anisotropy =	37.9874
2 N	Isotropic =	101.7451	Anisotropy =	104.1845
3 C	Isotropic =	49.8137	Anisotropy =	117.4564
4 C	Isotropic =	53.6455	Anisotropy =	145.1549

5	C	Isotropic = 79.9274	Anisotropy = 158.2454
6	C	Isotropic = 34.7986	Anisotropy = 123.9134
7	O	Isotropic = 254.7752	Anisotropy = 90.2888
8	C	Isotropic = 135.9159	Anisotropy = 72.8342
9	C	Isotropic = 36.9895	Anisotropy = 119.4595
10	O	Isotropic = 279.1229	Anisotropy = 86.1724
11	C	Isotropic = 130.7270	Anisotropy = 89.8551
12	C	Isotropic = 74.4458	Anisotropy = 135.6636
13	C	Isotropic = 136.9783	Anisotropy = 25.9444
14	C	Isotropic = 148.7812	Anisotropy = 42.7282
15	C	Isotropic = 141.6183	Anisotropy = 56.3162
16	N	Isotropic = 213.1393	Anisotropy = 57.8593
17	C	Isotropic = 136.0364	Anisotropy = 26.7297
18	C	Isotropic = 48.4554	Anisotropy = 165.3786
19	C	Isotropic = 57.0038	Anisotropy = 118.9400
20	C	Isotropic = 127.1388	Anisotropy = 57.4550
21	O	Isotropic = 287.9617	Anisotropy = 57.7151
22	C	Isotropic = 117.5790	Anisotropy = 54.4532
23	C	Isotropic = 155.0138	Anisotropy = 45.7406
24	C	Isotropic = 9.9747	Anisotropy = 122.8068
25	O	Isotropic = -70.2847	Anisotropy = 588.2776
26	C	Isotropic = 139.6128	Anisotropy = 32.0816
27	C	Isotropic = 159.4404	Anisotropy = 9.9221
28	C	Isotropic = 130.0474	Anisotropy = 36.2564
29	C	Isotropic = 162.9139	Anisotropy = 14.9186
30	H	Isotropic = 28.1470	Anisotropy = 2.7398
31	H	Isotropic = 24.6757	Anisotropy = 13.3640
32	H	Isotropic = 28.0681	Anisotropy = 7.9892
33	H	Isotropic = 27.6724	Anisotropy = 9.4032
34	H	Isotropic = 28.0769	Anisotropy = 8.1522
35	H	Isotropic = 28.3929	Anisotropy = 8.7393
36	H	Isotropic = 27.6432	Anisotropy = 7.7456
37	H	Isotropic = 27.9850	Anisotropy = 10.0199
38	H	Isotropic = 23.7601	Anisotropy = 10.2018
39	H	Isotropic = 30.0969	Anisotropy = 7.3734
40	H	Isotropic = 30.1935	Anisotropy = 9.2511
41	H	Isotropic = 29.1297	Anisotropy = 6.1609
42	H	Isotropic = 28.9321	Anisotropy = 11.9461
43	H	Isotropic = 29.3342	Anisotropy = 9.5431
44	H	Isotropic = 28.1259	Anisotropy = 10.1360
45	H	Isotropic = 26.1451	Anisotropy = 5.5429
46	H	Isotropic = 27.1505	Anisotropy = 5.9664
47	H	Isotropic = 27.6323	Anisotropy = 10.2369
48	H	Isotropic = 27.6349	Anisotropy = 6.7284
49	H	Isotropic = 28.4766	Anisotropy = 4.5901
50	H	Isotropic = 29.6332	Anisotropy = 9.7700

51	H	Isotropic =	30.5405	Anisotropy =	3.0034
52	H	Isotropic =	28.8741	Anisotropy =	9.7375
53	H	Isotropic =	28.0926	Anisotropy =	10.2305
54	H	Isotropic =	30.6282	Anisotropy =	7.8187
55	H	Isotropic =	29.6626	Anisotropy =	11.4286

Conformer_13

C	-4.415952568538	-1.793310154775	-0.025232724841
N	-4.204933549395	-0.399612852249	0.415576832691
C	-2.818268404819	-0.116178158625	0.366883469922
C	-2.103835775712	-1.284247758736	0.123327301533
C	-0.719705282757	-1.254154165903	0.015928080507
C	-0.047816909757	-0.038219420142	0.147976992873
O	1.301927122485	0.102084248636	0.076910090522
C	2.079590622876	-1.073254027751	-0.107999700800
C	-0.783926017438	1.136668553050	0.390908316065
O	-0.139739551845	2.332181845089	0.575269180585
C	0.379930769765	2.908672744443	-0.623039393054
C	-2.168513397132	1.104871319477	0.505805276099
C	-3.031944935390	-2.476769485644	0.126495332449
C	-2.940532092194	-3.266364676183	1.444609384890
C	-3.670802623462	-4.565901040030	1.124807525791
N	-3.395264674696	-4.832197824554	-0.298214455194
C	-4.579575170587	-5.320499579517	-1.027377346306
C	-5.510556644197	-4.173192409500	-1.350090301541
C	-6.715485171440	-4.084254110181	-0.788917797920
C	-7.685007462551	-2.937011100653	-0.814719466769
O	-7.417517396845	-1.895184579404	-1.736226663185
C	-6.320918236534	-1.022751008801	-1.489653050303
C	-6.516466611128	-0.144490545876	-0.231638966685
C	-5.217175031210	0.500114510808	0.216439281423
O	-5.084339653310	1.705472583885	0.380722729231
C	-4.943221090655	-1.711359330817	-1.460872431945
C	-4.843574414943	-3.064411376349	-2.162982137882
C	-2.779443884154	-3.614636869304	-0.896616288539
C	-3.342762836176	-3.361379017876	-2.288990810576
H	-5.147750179520	-2.270947952549	0.630107426668
H	-0.172112867089	-2.174339655916	-0.156060906200
H	3.119039256273	-0.746129846442	-0.116917110511
H	1.847029689054	-1.560630208337	-1.060953950792
H	1.930310293609	-1.781222864458	0.714099881952
H	0.870360785919	3.840005802453	-0.336695286144
H	1.108459038132	2.245191100561	-1.097379395981
H	-0.432391857873	3.129017934998	-1.325658294536

H	-2.709163603958	2.021876176992	0.699518091692
H	-3.378305080586	-2.727990230693	2.289818874652
H	-1.885942108301	-3.458503332853	1.669277958009
H	-4.749640134170	-4.441590348024	1.293990699787
H	-3.333602746407	-5.396271890771	1.753222045530
H	-5.078789443774	-6.066354588008	-0.404160362194
H	-4.252729757135	-5.830894724712	-1.938943580352
H	-7.062766845938	-4.917357426759	-0.176175140807
H	-7.784055639008	-2.543238978448	0.208143882044
H	-8.676243417018	-3.312440393226	-1.088408289282
H	-6.343072322902	-0.366138008426	-2.362189576532
H	-6.877657270363	-0.759188416271	0.600115868924
H	-7.248223166374	0.642483826561	-0.412118427263
H	-4.263442302693	-1.030355388462	-1.988807077582
H	-5.297621982753	-2.996460911835	-3.156751283842
H	-1.694384335598	-3.762720554683	-0.958605612047
H	-2.829505259846	-2.511740794663	-2.749011017617
H	-3.152367869944	-4.229344638546	-2.925947676619

SCF Done: E(RwB97X) = -1302.51594964

Zero-point correction=	0.470618
Thermal correction to Energy=	0.492560
Thermal correction to Enthalpy=	0.493504
Thermal correction to Gibbs Free Energy=	0.422027
Sum of electronic and zero-point Energies=	-1302.045332
Sum of electronic and thermal Energies=	-1302.023390
Sum of electronic and thermal Enthalpies=	-1302.022446
Sum of electronic and thermal Free Energies=	-1302.093923

1 C	Isotropic = 126.2986	Anisotropy = 38.0597
2 N	Isotropic = 101.5496	Anisotropy = 103.9256
3 C	Isotropic = 49.5793	Anisotropy = 118.1495
4 C	Isotropic = 53.6693	Anisotropy = 145.1747
5 C	Isotropic = 79.9192	Anisotropy = 158.2873
6 C	Isotropic = 34.8817	Anisotropy = 124.1542
7 O	Isotropic = 255.0333	Anisotropy = 90.4660
8 C	Isotropic = 135.8233	Anisotropy = 72.9860
9 C	Isotropic = 37.0999	Anisotropy = 121.2061
10 O	Isotropic = 278.8334	Anisotropy = 87.3360
11 C	Isotropic = 130.6106	Anisotropy = 89.8404
12 C	Isotropic = 74.6158	Anisotropy = 134.8951
13 C	Isotropic = 137.0104	Anisotropy = 26.0717
14 C	Isotropic = 148.8151	Anisotropy = 42.4736
15 C	Isotropic = 141.6724	Anisotropy = 55.9796
16 N	Isotropic = 213.4767	Anisotropy = 58.3099

17	C	Isotropic =	135.8748	Anisotropy =	26.3261
18	C	Isotropic =	48.5874	Anisotropy =	164.8191
19	C	Isotropic =	57.0470	Anisotropy =	119.1504
20	C	Isotropic =	127.1927	Anisotropy =	57.5897
21	O	Isotropic =	288.1908	Anisotropy =	57.6268
22	C	Isotropic =	117.4697	Anisotropy =	54.4783
23	C	Isotropic =	154.8278	Anisotropy =	45.7830
24	C	Isotropic =	9.8583	Anisotropy =	122.1590
25	O	Isotropic =	-70.0013	Anisotropy =	588.6135
26	C	Isotropic =	139.4641	Anisotropy =	32.2442
27	C	Isotropic =	159.4382	Anisotropy =	9.8154
28	C	Isotropic =	129.8491	Anisotropy =	36.1333
29	C	Isotropic =	162.9324	Anisotropy =	14.9928
30	H	Isotropic =	28.0875	Anisotropy =	2.6826
31	H	Isotropic =	24.6419	Anisotropy =	13.3653
32	H	Isotropic =	27.7101	Anisotropy =	9.3510
33	H	Isotropic =	28.0421	Anisotropy =	7.8111
34	H	Isotropic =	28.1206	Anisotropy =	8.1702
35	H	Isotropic =	27.9401	Anisotropy =	10.0340
36	H	Isotropic =	27.5742	Anisotropy =	7.6403
37	H	Isotropic =	28.4782	Anisotropy =	8.4119
38	H	Isotropic =	23.8150	Anisotropy =	9.8322
39	H	Isotropic =	30.0871	Anisotropy =	7.3326
40	H	Isotropic =	30.1655	Anisotropy =	9.3013
41	H	Isotropic =	29.1251	Anisotropy =	6.1569
42	H	Isotropic =	28.9279	Anisotropy =	12.0025
43	H	Isotropic =	29.3409	Anisotropy =	9.5776
44	H	Isotropic =	28.1504	Anisotropy =	10.1004
45	H	Isotropic =	26.1540	Anisotropy =	5.5481
46	H	Isotropic =	27.1414	Anisotropy =	5.9494
47	H	Isotropic =	27.6230	Anisotropy =	10.1802
48	H	Isotropic =	27.5992	Anisotropy =	6.7593
49	H	Isotropic =	28.4597	Anisotropy =	4.6568
50	H	Isotropic =	29.5967	Anisotropy =	9.7917
51	H	Isotropic =	30.4695	Anisotropy =	3.1635
52	H	Isotropic =	28.8327	Anisotropy =	9.6622
53	H	Isotropic =	28.0941	Anisotropy =	10.1833
54	H	Isotropic =	30.6025	Anisotropy =	7.7269
55	H	Isotropic =	29.6879	Anisotropy =	11.3078

Conformer_2

C	-4.415710955690	-1.691480376515	-0.068144853387
N	-4.114351829476	-0.254923835774	0.136445020618
C	-2.725031650175	-0.040425194784	-0.008281720082

C	-2.071812103888	-1.259124719089	-0.143068240155
C	-0.694392978790	-1.279356847650	-0.310987122606
C	0.015643171020	-0.087634618314	-0.356195853045
O	1.369534614134	-0.116895738904	-0.578617629454
C	2.152778879291	0.126514978611	0.588859181797
C	-0.657196211675	1.141535129061	-0.220455897980
O	0.114831592054	2.254202233732	-0.287612880632
C	-0.526573854114	3.516800820138	-0.156214267469
C	-2.041045405703	1.172399703226	-0.038198850997
C	-3.037159666565	-2.406145605606	0.019489697365
C	-2.878707842327	-3.124817407345	1.370806381901
C	-3.671743433808	-4.408161797212	1.166235943215
N	-3.439241455037	-4.776251053098	-0.240010543997
C	-4.620325512780	-5.363997636843	-0.882979986974
C	-5.628395790943	-4.309620666407	-1.276211735950
C	-6.908255856259	-4.344715141616	-0.910242273326
C	-7.857912681072	-3.217544862618	-1.215713705528
O	-7.502764185577	-2.021513280981	-0.523404444448
C	-6.567661231639	-1.180710345059	-1.190430395142
C	-6.475589715349	0.081787419494	-0.306598964447
C	-5.091984488439	0.668727125806	-0.111672004396
O	-4.880262612481	1.874196171384	-0.142187569191
C	-5.169584303010	-1.780924135150	-1.399033345833
C	-5.048591489203	-3.151369097009	-2.077365127165
C	-2.878204652428	-3.597018824337	-0.956349233940
C	-3.553107935284	-3.391483489024	-2.306467595589
H	-5.066776917979	-2.041272914533	0.739267195693
H	-0.149043801697	-2.213970896590	-0.412548819819
H	3.199098281921	0.073777819046	0.284104690972
H	1.945886159023	1.117454127028	1.004010612225
H	1.959794912401	-0.640103717119	1.348682766583
H	-1.016927438673	3.614306253033	0.818094937164
H	0.261826930933	4.264365116259	-0.239624018408
H	-1.260393550957	3.674269116306	-0.953533090723
H	-2.580260812979	2.102061073316	0.064956299048
H	-3.239823114444	-2.526800380654	2.211972441448
H	-1.818524243946	-3.346218071804	1.534614230861
H	-4.740630129432	-4.223956611848	1.353324422072
H	-3.354729320381	-5.209866465361	1.840582697771
H	-5.065807077353	-6.087536669640	-0.195308120603
H	-4.302160846791	-5.923281040693	-1.769868119083
H	-7.281748767019	-5.182321072171	-0.323482305256
H	-8.867394625142	-3.466407913076	-0.882231550001
H	-7.904517251225	-3.017160008177	-2.296287970318
H	-6.980503384204	-0.920566171327	-2.174469701824
H	-6.834786981961	-0.202168844681	0.689127553429

H	-7.123868797750	0.877930571555	-0.671805010055
H	-4.671064317574	-1.081384982184	-2.084486480154
H	-5.569745336049	-3.095024973043	-3.041457506010
H	-1.803335866780	-3.753840516735	-1.107936782792
H	-3.102263137493	-2.532716468267	-2.813536159567
H	-3.383380979243	-4.263315266754	-2.944354195813

SCF Done: E(RwB97X) = -1302.52043936

Zero-point correction=	0.469559
Thermal correction to Energy=	0.491884
Thermal correction to Enthalpy=	0.492828
Thermal correction to Gibbs Free Energy=	0.420016
Sum of electronic and zero-point Energies=	-1302.050880
Sum of electronic and thermal Energies=	-1302.028555
Sum of electronic and thermal Enthalpies=	-1302.027611
Sum of electronic and thermal Free Energies=	-1302.100423

1 C	Isotropic = 127.9566	Anisotropy = 40.3738
2 N	Isotropic = 95.9793	Anisotropy = 94.7218
3 C	Isotropic = 44.8526	Anisotropy = 123.1659
4 C	Isotropic = 59.9523	Anisotropy = 134.1477
5 C	Isotropic = 66.3004	Anisotropy = 153.9449
6 C	Isotropic = 39.9067	Anisotropy = 114.5380
7 O	Isotropic = 284.2475	Anisotropy = 81.8058
8 C	Isotropic = 130.2473	Anisotropy = 90.4426
9 C	Isotropic = 31.2747	Anisotropy = 128.7399
10 O	Isotropic = 250.2294	Anisotropy = 96.2546
11 C	Isotropic = 135.5171	Anisotropy = 73.9000
12 C	Isotropic = 87.4031	Anisotropy = 139.5002
13 C	Isotropic = 137.9258	Anisotropy = 27.3618
14 C	Isotropic = 147.5861	Anisotropy = 41.3427
15 C	Isotropic = 140.8825	Anisotropy = 55.3965
16 N	Isotropic = 217.3320	Anisotropy = 60.5664
17 C	Isotropic = 137.9866	Anisotropy = 27.7823
18 C	Isotropic = 36.1526	Anisotropy = 175.0558
19 C	Isotropic = 57.4631	Anisotropy = 135.2360
20 C	Isotropic = 126.3417	Anisotropy = 70.7838
21 O	Isotropic = 271.5003	Anisotropy = 97.2479
22 C	Isotropic = 112.9345	Anisotropy = 54.7073
23 C	Isotropic = 145.6957	Anisotropy = 39.3886
24 C	Isotropic = 11.3347	Anisotropy = 124.1245
25 O	Isotropic = -64.5427	Anisotropy = 586.0116
26 C	Isotropic = 141.4808	Anisotropy = 20.6599
27 C	Isotropic = 157.6642	Anisotropy = 11.8209
28 C	Isotropic = 129.7670	Anisotropy = 38.3990

29	C	Isotropic =	163.8225	Anisotropy =	13.6604
30	H	Isotropic =	28.0942	Anisotropy =	3.2079
31	H	Isotropic =	24.3944	Anisotropy =	10.9609
32	H	Isotropic =	28.0035	Anisotropy =	10.0041
33	H	Isotropic =	27.7162	Anisotropy =	8.0871
34	H	Isotropic =	28.4670	Anisotropy =	8.4294
35	H	Isotropic =	27.9838	Anisotropy =	8.3540
36	H	Isotropic =	27.6379	Anisotropy =	9.4844
37	H	Isotropic =	28.0229	Anisotropy =	8.4761
38	H	Isotropic =	23.7929	Anisotropy =	12.2061
39	H	Isotropic =	30.1109	Anisotropy =	7.5226
40	H	Isotropic =	30.0508	Anisotropy =	9.4891
41	H	Isotropic =	29.0999	Anisotropy =	6.0982
42	H	Isotropic =	28.8802	Anisotropy =	11.9289
43	H	Isotropic =	29.1592	Anisotropy =	9.0654
44	H	Isotropic =	28.1607	Anisotropy =	10.0928
45	H	Isotropic =	25.5753	Anisotropy =	5.9665
46	H	Isotropic =	27.8042	Anisotropy =	10.4218
47	H	Isotropic =	27.5716	Anisotropy =	7.7532
48	H	Isotropic =	27.7217	Anisotropy =	6.9712
49	H	Isotropic =	29.2956	Anisotropy =	5.2205
50	H	Isotropic =	28.9108	Anisotropy =	8.5311
51	H	Isotropic =	30.8881	Anisotropy =	3.4637
52	H	Isotropic =	28.8052	Anisotropy =	9.3609
53	H	Isotropic =	28.1502	Anisotropy =	9.7227
54	H	Isotropic =	30.6471	Anisotropy =	7.1739
55	H	Isotropic =	29.7141	Anisotropy =	11.3046

Conformer_3

C	-4.436445683759	-1.684004558189	-0.083733419220
N	-4.184980508008	-0.235810167679	0.101052866875
C	-2.796202056627	0.015703666257	-0.006570870124
C	-2.102583957624	-1.182972946011	-0.101971597963
C	-0.721113248542	-1.190930642939	-0.245609528725
C	-0.031227549265	0.019841296211	-0.302939394690
O	1.312816441742	0.127337919653	-0.472227633412
C	2.057419674688	-1.075926669916	-0.606188553053
C	-0.743872281659	1.228239923963	-0.187773042642
O	-0.090310111464	2.429275683727	-0.281690846131
C	0.691083669365	2.765160928174	0.865138182513
C	-2.125043198980	1.234174237444	-0.037578058430
C	-3.039911586198	-2.353926616488	0.059205311169
C	-2.896604941117	-3.032318622535	1.433086428973
C	-3.646037571811	-4.343247180247	1.240883943039

N	-3.363277224916	-4.741088182011	-0.147973432906
C	-4.510195097898	-5.377990740547	-0.806469775428
C	-5.535561924777	-4.361954027621	-1.251625803642
C	-6.821551412250	-4.423466272768	-0.912192234598
C	-7.797351202216	-3.333761962447	-1.265933015054
O	-7.489832597129	-2.107009090127	-0.605798234438
C	-6.565560368581	-1.260974329749	-1.281685584646
C	-6.535397822953	0.038319972741	-0.447868372939
C	-5.172590419415	0.657025801467	-0.205198255881
O	-4.985687744642	1.866755067592	-0.249547455791
C	-5.146151581648	-1.825419109566	-1.433653638127
C	-4.967969540602	-3.209827617656	-2.070481444124
C	-2.817759447717	-3.564145173354	-0.880049825845
C	-3.460296733522	-3.412452409104	-2.252852207028
H	-5.100461408987	-2.038640508098	0.711092856848
H	-0.191258587338	-2.134349312489	-0.317335979816
H	3.097173406666	-0.773726233873	-0.728923880813
H	1.966046650153	-1.703185349445	0.286901220642
H	1.739314129436	-1.643276212687	-1.487386723430
H	1.181179065375	3.713856119843	0.642537542219
H	0.045971610703	2.888620274274	1.742920598145
H	1.448417391563	2.002418480985	1.066039449257
H	-2.648962123494	2.177052575653	0.040718945214
H	-3.297974385630	-2.424117698864	2.248284807106
H	-1.835388910850	-3.218280619164	1.630714642033
H	-4.724514703296	-4.185413235802	1.393214597055
H	-3.324972596947	-5.117134226984	1.945092892536
H	-4.953931666978	-6.096414165368	-0.112282127734
H	-4.152888289193	-5.950830152268	-1.669379931983
H	-7.183523250495	-5.256351822713	-0.311676869340
H	-8.804357512298	-3.602535999168	-0.940400478266
H	-7.833111999230	-3.166979250098	-2.352639929834
H	-6.962025577510	-1.052698610562	-2.284720797352
H	-6.946813491871	-0.206259531131	0.537973611049
H	-7.171742165888	0.809304963920	-0.881973424338
H	-4.646112671825	-1.130195362473	-2.122445596153
H	-5.464916200897	-3.196925707593	-3.048837687450
H	-1.735088891127	-3.693475937605	-0.997695032146
H	-3.019630823305	-2.554250882765	-2.769880179813
H	-3.248330969209	-4.295219773801	-2.862367031370

SCF Done: E(RwB97X) = -1302.51947490

Zero-point correction=	0.469431
Thermal correction to Energy=	0.491770
Thermal correction to Enthalpy=	0.492714

Thermal correction to Gibbs Free Energy=	0.419799
Sum of electronic and zero-point Energies=	-1302.050044
Sum of electronic and thermal Energies=	-1302.027705
Sum of electronic and thermal Enthalpies=	-1302.026761
Sum of electronic and thermal Free Energies=	-1302.099676

1 C	Isotropic =	127.9601	Anisotropy =	40.2854
2 N	Isotropic =	97.9456	Anisotropy =	97.8796
3 C	Isotropic =	49.6847	Anisotropy =	116.2105
4 C	Isotropic =	53.7033	Anisotropy =	144.6509
5 C	Isotropic =	80.0557	Anisotropy =	157.9031
6 C	Isotropic =	34.7618	Anisotropy =	123.2615
7 O	Isotropic =	254.8375	Anisotropy =	90.3406
8 C	Isotropic =	135.8293	Anisotropy =	72.6978
9 C	Isotropic =	36.8968	Anisotropy =	119.0088
10 O	Isotropic =	278.5010	Anisotropy =	87.2200
11 C	Isotropic =	130.8853	Anisotropy =	89.7708
12 C	Isotropic =	74.2968	Anisotropy =	134.7570
13 C	Isotropic =	137.1270	Anisotropy =	27.4276
14 C	Isotropic =	147.5915	Anisotropy =	41.4295
15 C	Isotropic =	140.8364	Anisotropy =	55.4908
16 N	Isotropic =	217.0026	Anisotropy =	60.2844
17 C	Isotropic =	137.8446	Anisotropy =	27.9285
18 C	Isotropic =	36.2146	Anisotropy =	174.6777
19 C	Isotropic =	57.3293	Anisotropy =	134.7274
20 C	Isotropic =	126.2803	Anisotropy =	70.8467
21 O	Isotropic =	271.4479	Anisotropy =	97.3378
22 C	Isotropic =	112.8352	Anisotropy =	54.4920
23 C	Isotropic =	145.8520	Anisotropy =	39.5837
24 C	Isotropic =	11.7262	Anisotropy =	124.5553
25 O	Isotropic =	-62.8547	Anisotropy =	581.2773
26 C	Isotropic =	141.6427	Anisotropy =	20.3201
27 C	Isotropic =	157.2386	Anisotropy =	11.3504
28 C	Isotropic =	129.6827	Anisotropy =	38.3229
29 C	Isotropic =	163.8264	Anisotropy =	13.6634
30 H	Isotropic =	28.0814	Anisotropy =	3.2365
31 H	Isotropic =	24.5875	Anisotropy =	13.4640
32 H	Isotropic =	27.6723	Anisotropy =	9.3490
33 H	Isotropic =	27.9968	Anisotropy =	8.0012
34 H	Isotropic =	28.0856	Anisotropy =	8.0862
35 H	Isotropic =	27.9836	Anisotropy =	9.9929
36 H	Isotropic =	28.4003	Anisotropy =	8.7356
37 H	Isotropic =	27.5738	Anisotropy =	7.6443
38 H	Isotropic =	23.6834	Anisotropy =	10.2860
39 H	Isotropic =	30.0908	Anisotropy =	7.7281
40 H	Isotropic =	30.0370	Anisotropy =	9.2922

41	H	Isotropic =	29.0399	Anisotropy =	6.1233
42	H	Isotropic =	28.8636	Anisotropy =	11.8751
43	H	Isotropic =	29.1349	Anisotropy =	9.0808
44	H	Isotropic =	28.1426	Anisotropy =	10.0398
45	H	Isotropic =	25.5764	Anisotropy =	5.9735
46	H	Isotropic =	27.7954	Anisotropy =	10.4552
47	H	Isotropic =	27.6164	Anisotropy =	7.7591
48	H	Isotropic =	27.7629	Anisotropy =	6.9534
49	H	Isotropic =	29.3221	Anisotropy =	5.3605
50	H	Isotropic =	28.9154	Anisotropy =	8.5672
51	H	Isotropic =	30.8906	Anisotropy =	3.3512
52	H	Isotropic =	28.8035	Anisotropy =	9.3976
53	H	Isotropic =	28.0336	Anisotropy =	10.1943
54	H	Isotropic =	30.6420	Anisotropy =	7.2076
55	H	Isotropic =	29.7130	Anisotropy =	11.2261

Conformer_4

C	-4.438154150493	-1.713887582203	0.002319253959
N	-4.188013188784	-0.285381639581	0.304015374612
C	-2.794290220268	-0.041083729910	0.291201303917
C	-2.103089985504	-1.236081012378	0.145838460259
C	-0.714927203155	-1.248008322766	0.093634702782
C	-0.015067823761	-0.044964018240	0.186803117310
O	1.339546859451	0.057840663935	0.161123756726
C	2.090108233409	-1.143663089134	0.047225136960
C	-0.728014637050	1.159178006981	0.337909502741
O	-0.056976438653	2.344599805024	0.489866196941
C	0.497401780721	2.862080715495	-0.719401140650
C	-2.116043271449	1.169416663168	0.392768309172
C	-3.055321850790	-2.406578425905	0.167865849624
C	-2.989856840963	-3.186496677062	1.492945387263
C	-3.736097493825	-4.472392578125	1.165084995327
N	-3.384739084101	-4.767908124570	-0.233655208346
C	-4.498623753423	-5.343008660309	-0.997220179763
C	-5.492576864623	-4.287607446763	-1.421856177133
C	-6.796625304309	-4.361599731174	-1.163212297039
C	-7.742208981114	-3.237463553870	-1.491159684573
O	-7.467110054608	-2.068693895802	-0.720395085154
C	-6.499081712722	-1.182795122680	-1.272245928376
C	-6.505280380249	0.043860434794	-0.334744263069
C	-5.152677880663	0.635610241756	0.008448307569
O	-4.955471153831	1.843877000846	0.047788054421
C	-5.076910965274	-1.749453340126	-1.389557208401
C	-4.873601804081	-3.083208018330	-2.118955462250

C	-2.792269380126	-3.546743163156	-0.846027599409
C	-3.359772057373	-3.287958986447	-2.235853422609
H	-5.145011015190	-2.117722126494	0.734040003142
H	-0.187397336335	-2.190151774202	-0.006479750052
H	3.138093071044	-0.844860329875	0.054907818836
H	1.900433260559	-1.813061899452	0.893042983928
H	1.870426295634	-1.664104414007	-0.891191373942
H	-0.296562430151	3.073131836120	-1.445515064753
H	1.004190023918	3.792521541169	-0.459765914907
H	1.218761567351	2.164050191735	-1.154125319932
H	-2.638433175406	2.108754105399	0.513576235552
H	-3.430539875148	-2.635998553830	2.328540634822
H	-1.942093329490	-3.397704526236	1.732273479002
H	-4.820140151624	-4.316985271783	1.274520901466
H	-3.455525736083	-5.299367731375	1.824860594377
H	-4.983086459265	-6.105855373834	-0.382219046096
H	-4.098781174770	-5.853581873075	-1.880402978984
H	-7.198157626289	-5.233014453005	-0.648677253496
H	-8.769252474381	-3.518716812977	-1.249469039324
H	-7.709048756014	-2.988043652315	-2.562014376261
H	-6.835231143710	-0.888842655129	-2.275737529770
H	-6.951649115735	-0.282584927299	0.611465709552
H	-7.127245272582	0.847833516331	-0.727716418864
H	-4.536479492448	-1.009922149414	-1.996894277682
H	-5.317071660609	-2.989436450180	-3.118362311034
H	-1.705627659370	-3.678575996380	-0.915588248962
H	-2.886794701354	-2.398799528358	-2.664352745152
H	-3.121930024944	-4.126047105004	-2.896770764277

SCF Done: E(RwB97X) = -1302.51968290

Zero-point correction=	0.469909
Thermal correction to Energy=	0.492032
Thermal correction to Enthalpy=	0.492976
Thermal correction to Gibbs Free Energy=	0.420977
Sum of electronic and zero-point Energies=	-1302.049774
Sum of electronic and thermal Energies=	-1302.027651
Sum of electronic and thermal Enthalpies=	-1302.026707
Sum of electronic and thermal Free Energies=	-1302.098706

1 C	Isotropic =	128.2736	Anisotropy =	40.0456
2 N	Isotropic =	97.7973	Anisotropy =	97.6177
3 C	Isotropic =	49.5763	Anisotropy =	116.6282
4 C	Isotropic =	53.4489	Anisotropy =	144.8221
5 C	Isotropic =	80.1009	Anisotropy =	157.9570
6 C	Isotropic =	34.8524	Anisotropy =	124.3017

7	O	Isotropic = 255.3199	Anisotropy = 90.2521
8	C	Isotropic = 135.7134	Anisotropy = 72.9624
9	C	Isotropic = 37.0736	Anisotropy = 120.9341
10	O	Isotropic = 279.6609	Anisotropy = 86.8104
11	C	Isotropic = 130.3877	Anisotropy = 89.9089
12	C	Isotropic = 74.0684	Anisotropy = 134.6201
13	C	Isotropic = 137.1101	Anisotropy = 27.5727
14	C	Isotropic = 147.5496	Anisotropy = 41.4996
15	C	Isotropic = 140.9895	Anisotropy = 55.5727
16	N	Isotropic = 217.2721	Anisotropy = 60.8634
17	C	Isotropic = 137.8654	Anisotropy = 27.8178
18	C	Isotropic = 36.2675	Anisotropy = 174.5747
19	C	Isotropic = 57.4073	Anisotropy = 134.9243
20	C	Isotropic = 126.3521	Anisotropy = 70.7845
21	O	Isotropic = 271.6345	Anisotropy = 97.2576
22	C	Isotropic = 112.8317	Anisotropy = 54.5333
23	C	Isotropic = 145.6752	Anisotropy = 39.5069
24	C	Isotropic = 11.8036	Anisotropy = 124.2597
25	O	Isotropic = -62.3867	Anisotropy = 581.4125
26	C	Isotropic = 141.4944	Anisotropy = 20.4647
27	C	Isotropic = 157.2444	Anisotropy = 11.4903
28	C	Isotropic = 129.5410	Anisotropy = 38.2153
29	C	Isotropic = 163.6529	Anisotropy = 13.7294
30	H	Isotropic = 28.0967	Anisotropy = 3.1819
31	H	Isotropic = 24.5739	Anisotropy = 13.4083
32	H	Isotropic = 27.6979	Anisotropy = 9.3394
33	H	Isotropic = 28.0597	Anisotropy = 8.2124
34	H	Isotropic = 28.0356	Anisotropy = 7.7851
35	H	Isotropic = 28.4413	Anisotropy = 8.4159
36	H	Isotropic = 27.9355	Anisotropy = 10.0113
37	H	Isotropic = 27.6309	Anisotropy = 7.7066
38	H	Isotropic = 23.7257	Anisotropy = 9.9614
39	H	Isotropic = 30.0768	Anisotropy = 7.6324
40	H	Isotropic = 30.0132	Anisotropy = 9.3826
41	H	Isotropic = 29.0531	Anisotropy = 6.1617
42	H	Isotropic = 28.8432	Anisotropy = 11.9335
43	H	Isotropic = 29.1274	Anisotropy = 9.1196
44	H	Isotropic = 28.1541	Anisotropy = 9.9810
45	H	Isotropic = 25.6141	Anisotropy = 5.9366
46	H	Isotropic = 27.8112	Anisotropy = 10.4021
47	H	Isotropic = 27.5875	Anisotropy = 7.7623
48	H	Isotropic = 27.7344	Anisotropy = 6.9824
49	H	Isotropic = 29.3121	Anisotropy = 5.3386
50	H	Isotropic = 28.9021	Anisotropy = 8.6251
51	H	Isotropic = 30.8425	Anisotropy = 3.4607
52	H	Isotropic = 28.7514	Anisotropy = 9.3456

53	H	Isotropic =	28.0455	Anisotropy =	10.1578
54	H	Isotropic =	30.6125	Anisotropy =	7.1949
55	H	Isotropic =	29.6563	Anisotropy =	11.1733

Conformer_5

C	-4.515020947894	-1.639960716050	-0.177736723394
N	-4.211764180984	-0.204723786430	-0.007507016362
C	-2.811646860383	-0.020172349049	0.033499640192
C	-2.171336529927	-1.244511600338	-0.021526316510
C	-0.778320237496	-1.298275156118	-0.000988250322
C	-0.042238108994	-0.122338565711	0.068757518958
O	1.315663367245	-0.066096767194	0.088995157233
C	2.019692363821	-1.296637418197	0.021696203630
C	-0.712255038479	1.122466948653	0.128760126916
O	0.084261820070	2.217741271775	0.198741691769
C	-0.547755201086	3.487381495920	0.280587300594
C	-2.100984613539	1.178865947148	0.112980460937
C	-3.158381354580	-2.393801308305	-0.020591915101
C	-3.121557597281	-3.209640168034	1.306573134610
C	-2.749391527009	-4.642908170010	0.896136433760
N	-3.132404894576	-4.800136888346	-0.503719026001
C	-4.488193195251	-5.316415653293	-0.767710711544
C	-5.539222536330	-4.271834516696	-1.079852681644
C	-6.761259054221	-4.297816718968	-0.549753527348
C	-7.811270386062	-3.265859651176	-0.874750231169
O	-7.476398767531	-1.962045928712	-0.402329432517
C	-6.656959348190	-1.196304291506	-1.281129462941
C	-6.539990141373	0.205394965710	-0.644542246836
C	-5.148309417927	0.730873890567	-0.319581373055
O	-4.913405046273	1.935501147022	-0.319602805680
C	-5.259318668834	-1.779869468645	-1.501733822052
C	-5.119450635304	-3.193441158631	-2.070290878670
C	-2.855515892309	-3.493968739221	-1.113143369276
C	-3.635068826320	-3.359564190867	-2.413305859439
H	-5.189788484965	-1.949243042416	0.623046466151
H	-0.275663307870	-2.258708673525	-0.035212151391
H	1.794316464710	-1.836630251409	-0.904710784491
H	3.078888305240	-1.039891885921	0.037836342203
H	1.792178120295	-1.935621883299	0.882187708117
H	-1.155689775612	3.687820618619	-0.608256442415
H	-1.171788861049	3.566055460967	1.177352539129
H	0.257104387043	4.219964351428	0.337280967225
H	-2.630645041872	2.118869303909	0.154464342055
H	-4.106195074674	-3.194068691566	1.781711781130

H	-2.407024402767	-2.792607708591	2.020711286864
H	-3.223435529022	-5.405510756360	1.518333850618
H	-1.664091218658	-4.782400949658	0.972390297502
H	-4.804204743549	-5.931333628901	0.078593079347
H	-4.430748345361	-5.985246484215	-1.637213877314
H	-7.022705571234	-5.074264073271	0.167422711238
H	-8.755070272340	-3.523083188288	-0.389693765314
H	-7.996581407732	-3.221974538686	-1.958468600949
H	-7.169232356084	-1.120876907551	-2.249759261924
H	-7.097567694864	0.190959564191	0.298172596344
H	-7.007780837345	0.964728134918	-1.272557238542
H	-4.782128141927	-1.110942108611	-2.230415212840
H	-5.732817668140	-3.275937283671	-2.976425568840
H	-1.778990760074	-3.446444387085	-1.314064844564
H	-3.283090389279	-2.499401796964	-2.989363003951
H	-3.459345935849	-4.251611649343	-3.022395234124

SCF Done: E(RwB97X) = -1302.51538432

Zero-point correction=	0.469839
Thermal correction to Energy=	0.492191
Thermal correction to Enthalpy=	0.493136
Thermal correction to Gibbs Free Energy=	0.419852
Sum of electronic and zero-point Energies=	-1302.045546
Sum of electronic and thermal Energies=	-1302.023193
Sum of electronic and thermal Enthalpies=	-1302.022249
Sum of electronic and thermal Free Energies=	-1302.095533

1 C	Isotropic = 122.8307	Anisotropy = 38.9791
2 N	Isotropic = 98.3010	Anisotropy = 101.6279
3 C	Isotropic = 50.4756	Anisotropy = 113.2127
4 C	Isotropic = 56.0380	Anisotropy = 138.8456
5 C	Isotropic = 80.7902	Anisotropy = 154.7633
6 C	Isotropic = 39.0800	Anisotropy = 118.8564
7 O	Isotropic = 257.1813	Anisotropy = 91.4353
8 C	Isotropic = 135.4501	Anisotropy = 72.2779
9 C	Isotropic = 36.3714	Anisotropy = 122.0603
10 O	Isotropic = 253.8729	Anisotropy = 99.7720
11 C	Isotropic = 135.7168	Anisotropy = 73.1914
12 C	Isotropic = 88.4114	Anisotropy = 138.8388
13 C	Isotropic = 136.9765	Anisotropy = 23.9367
14 C	Isotropic = 137.4317	Anisotropy = 62.9891
15 C	Isotropic = 133.6946	Anisotropy = 66.2026
16 N	Isotropic = 196.9214	Anisotropy = 70.9267
17 C	Isotropic = 134.1367	Anisotropy = 37.9505
18 C	Isotropic = 32.2980	Anisotropy = 177.5900

19	C	Isotropic =	60.3239	Anisotropy =	132.1366
20	C	Isotropic =	125.5913	Anisotropy =	70.3712
21	O	Isotropic =	276.4872	Anisotropy =	93.3094
22	C	Isotropic =	112.7158	Anisotropy =	53.3941
23	C	Isotropic =	146.3347	Anisotropy =	40.5822
24	C	Isotropic =	13.7332	Anisotropy =	121.7628
25	O	Isotropic =	-47.8275	Anisotropy =	567.4917
26	C	Isotropic =	139.6023	Anisotropy =	23.7350
27	C	Isotropic =	157.6013	Anisotropy =	10.5262
28	C	Isotropic =	124.0619	Anisotropy =	39.0612
29	C	Isotropic =	161.3244	Anisotropy =	14.4335
30	H	Isotropic =	27.8059	Anisotropy =	3.2714
31	H	Isotropic =	24.5690	Anisotropy =	13.2725
32	H	Isotropic =	28.0837	Anisotropy =	7.8667
33	H	Isotropic =	27.6885	Anisotropy =	9.4349
34	H	Isotropic =	28.0430	Anisotropy =	8.0429
35	H	Isotropic =	28.0426	Anisotropy =	8.3961
36	H	Isotropic =	28.0538	Anisotropy =	8.3977
37	H	Isotropic =	27.6606	Anisotropy =	9.5593
38	H	Isotropic =	23.8328	Anisotropy =	12.0117
39	H	Isotropic =	29.7781	Anisotropy =	5.8526
40	H	Isotropic =	29.9545	Anisotropy =	6.4116
41	H	Isotropic =	28.7817	Anisotropy =	9.8989
42	H	Isotropic =	28.4987	Anisotropy =	11.1681
43	H	Isotropic =	28.8359	Anisotropy =	7.5336
44	H	Isotropic =	27.9290	Anisotropy =	9.6887
45	H	Isotropic =	25.6148	Anisotropy =	5.8345
46	H	Isotropic =	27.7913	Anisotropy =	10.4862
47	H	Isotropic =	27.6919	Anisotropy =	7.5893
48	H	Isotropic =	27.7660	Anisotropy =	6.8131
49	H	Isotropic =	29.3585	Anisotropy =	5.9311
50	H	Isotropic =	28.9212	Anisotropy =	8.3601
51	H	Isotropic =	30.7250	Anisotropy =	3.5427
52	H	Isotropic =	28.8485	Anisotropy =	9.3326
53	H	Isotropic =	28.2141	Anisotropy =	8.9410
54	H	Isotropic =	30.3573	Anisotropy =	7.5516
55	H	Isotropic =	29.5355	Anisotropy =	11.1703

Conformer_6

C	-4.495421801762	-1.628964909086	-0.202360889703
N	-4.164797808755	-0.195100326238	-0.071253186482
C	-2.765813000899	-0.022683057382	-0.105541322175
C	-2.142215236374	-1.262547574665	-0.175611100262
C	-0.756019399650	-1.320396994878	-0.228415284952

C	-0.010029783700	-0.150182359071	-0.220696912834
O	1.356506316301	-0.220831661697	-0.324629155619
C	2.042194902369	0.012879240086	0.904455433250
C	-0.654718951096	1.099277879187	-0.151325555733
O	0.153381751405	2.188410932849	-0.160220754153
C	-0.460389033102	3.469416614410	-0.090654572888
C	-2.047056312395	1.170665306077	-0.087064265373
C	-3.142003100475	-2.397661856324	-0.106830277256
C	-3.045260264035	-3.199057694105	1.226327010269
C	-2.706427577320	-4.639770114925	0.812868162223
N	-3.164898034302	-4.808666333507	-0.562533693044
C	-4.537888907127	-5.313174408944	-0.748047722830
C	-5.593245232476	-4.260921469981	-1.017363631479
C	-6.786275735133	-4.267381148172	-0.424432319991
C	-7.841804412770	-3.228966202280	-0.708639960783
O	-7.471780345266	-1.922631900875	-0.270383928492
C	-6.688548711364	-1.175441749788	-1.196713592881
C	-6.522794925484	0.229624562483	-0.578172440169
C	-5.110009960513	0.747135389266	-0.345891227117
O	-4.862897184671	1.947525530496	-0.380478350804
C	-5.310945959833	-1.777313430956	-1.483130253883
C	-5.215289930365	-3.198709927845	-2.041600091353
C	-2.907677919229	-3.512710510147	-1.200585558139
C	-3.752447626097	-3.383980044906	-2.459618164394
H	-5.129586251781	-1.916639068342	0.638672740299
H	-0.229594171116	-2.270228836301	-0.277141461922
H	1.841024723566	1.019259355150	1.283953265545
H	1.749333178548	-0.730335954260	1.655418552469
H	3.108182844195	-0.088670849246	0.695550213692
H	0.353321928560	4.193874820946	-0.110542030827
H	-1.116987352659	3.641430986151	-0.949950954366
H	-1.029602177801	3.588688927766	0.837190591995
H	-2.567779026730	2.115315577364	-0.035837334412
H	-4.004770531356	-3.169292492701	1.749870747102
H	-2.291943759353	-2.780510638816	1.898415011783
H	-3.152423222640	-5.391546614025	1.468053243704
H	-1.619711593474	-4.786978863930	0.832911396528
H	-4.815115495602	-5.914281680386	0.121442888125
H	-4.533167609233	-5.992906094908	-1.610954056186
H	-7.018245427819	-5.032422207070	0.314801060212
H	-8.761644083950	-3.470915747164	-0.172531086973
H	-8.081715935110	-3.197501583645	-1.782031262431
H	-7.248138244556	-1.101182765523	-2.138833985199
H	-7.016208946406	0.222666740594	0.399836246199
H	-7.026223019427	0.988339318966	-1.178458334543
H	-4.866120037378	-1.122219809308	-2.244196600197

H	-5.877063990948	-3.284740995198	-2.912735650855
H	-1.842812264658	-3.477354448329	-1.457454074249
H	-3.422535660307	-2.533441776902	-3.062405676033
H	-3.617699688449	-4.283947079966	-3.067499842417

SCF Done: E(RwB97X) = -1302.51311533

Zero-point correction=	0.469373
Thermal correction to Energy=	0.491892
Thermal correction to Enthalpy=	0.492836
Thermal correction to Gibbs Free Energy=	0.419272
Sum of electronic and zero-point Energies=	-1302.043742
Sum of electronic and thermal Energies=	-1302.021223
Sum of electronic and thermal Enthalpies=	-1302.020279
Sum of electronic and thermal Free Energies=	-1302.093844

1 C	Isotropic = 122.5254	Anisotropy = 39.2641
2 N	Isotropic = 96.9330	Anisotropy = 100.4968
3 C	Isotropic = 45.6811	Anisotropy = 120.2478
4 C	Isotropic = 54.9689	Anisotropy = 138.2667
5 C	Isotropic = 65.8512	Anisotropy = 150.9977
6 C	Isotropic = 39.8532	Anisotropy = 114.8331
7 O	Isotropic = 283.5859	Anisotropy = 81.8530
8 C	Isotropic = 130.1188	Anisotropy = 90.5628
9 C	Isotropic = 31.5149	Anisotropy = 127.9309
10 O	Isotropic = 251.1602	Anisotropy = 96.8009
11 C	Isotropic = 135.5878	Anisotropy = 73.8602
12 C	Isotropic = 88.3023	Anisotropy = 138.0281
13 C	Isotropic = 137.5007	Anisotropy = 23.9745
14 C	Isotropic = 137.1944	Anisotropy = 63.3372
15 C	Isotropic = 133.7894	Anisotropy = 66.2869
16 N	Isotropic = 196.7149	Anisotropy = 70.9227
17 C	Isotropic = 134.3012	Anisotropy = 37.7772
18 C	Isotropic = 32.3021	Anisotropy = 177.9477
19 C	Isotropic = 60.3205	Anisotropy = 132.1107
20 C	Isotropic = 125.6506	Anisotropy = 70.2664
21 O	Isotropic = 276.6085	Anisotropy = 93.7253
22 C	Isotropic = 112.9640	Anisotropy = 53.2543
23 C	Isotropic = 146.1686	Anisotropy = 40.3047
24 C	Isotropic = 13.2688	Anisotropy = 122.0827
25 O	Isotropic = -53.6951	Anisotropy = 576.1561
26 C	Isotropic = 139.3881	Anisotropy = 23.7571
27 C	Isotropic = 157.7261	Anisotropy = 10.6924
28 C	Isotropic = 123.7590	Anisotropy = 39.1956
29 C	Isotropic = 161.4050	Anisotropy = 14.1565
30 H	Isotropic = 27.7836	Anisotropy = 3.2273

31	H	Isotropic =	24.3269	Anisotropy =	11.1387
32	H	Isotropic =	27.6675	Anisotropy =	8.0174
33	H	Isotropic =	28.4807	Anisotropy =	8.3236
34	H	Isotropic =	27.9891	Anisotropy =	9.9734
35	H	Isotropic =	27.6545	Anisotropy =	9.4558
36	H	Isotropic =	28.0203	Anisotropy =	8.5004
37	H	Isotropic =	27.9862	Anisotropy =	8.2768
38	H	Isotropic =	23.8260	Anisotropy =	12.1774
39	H	Isotropic =	29.7678	Anisotropy =	5.7542
40	H	Isotropic =	29.9536	Anisotropy =	6.5175
41	H	Isotropic =	28.7926	Anisotropy =	9.8663
42	H	Isotropic =	28.5166	Anisotropy =	11.2035
43	H	Isotropic =	28.8490	Anisotropy =	7.5041
44	H	Isotropic =	27.9287	Anisotropy =	9.6977
45	H	Isotropic =	25.6283	Anisotropy =	5.8008
46	H	Isotropic =	27.7903	Anisotropy =	10.4693
47	H	Isotropic =	27.6838	Anisotropy =	7.6334
48	H	Isotropic =	27.7227	Anisotropy =	6.8864
49	H	Isotropic =	29.3295	Anisotropy =	5.8692
50	H	Isotropic =	28.8954	Anisotropy =	8.3440
51	H	Isotropic =	30.7133	Anisotropy =	3.5769
52	H	Isotropic =	28.8189	Anisotropy =	9.3585
53	H	Isotropic =	28.3158	Anisotropy =	8.4883
54	H	Isotropic =	30.3646	Anisotropy =	7.5864
55	H	Isotropic =	29.5327	Anisotropy =	11.2388

Conformer_7

C	-4.506902397900	-1.616154263328	-0.250867815663
N	-4.213087059992	-0.173401124049	-0.160230482974
C	-2.816350934848	0.027858534129	-0.147269610886
C	-2.161300506378	-1.196773711735	-0.166274973766
C	-0.772430993791	-1.249999210260	-0.168252098654
C	-0.038262436589	-0.063961338512	-0.154260808762
O	1.318936973491	-0.001265053105	-0.169281232668
C	2.035211103740	-1.227885104552	-0.214735658980
C	-0.716781374887	1.168783232911	-0.125914297486
O	-0.010272143590	2.343865321471	-0.148120517836
C	0.564572374926	2.691460894358	1.111017247576
C	-2.104216942200	1.223069536107	-0.120770553902
C	-3.140134425790	-2.352273726210	-0.110158159553
C	-3.060088966923	-3.127486077975	1.239195107450
C	-2.611371001738	-4.544882291137	0.860788656239
N	-3.063223104961	-4.773858936225	-0.508497519556
C	-4.428621852680	-5.313810031903	-0.665627316804

C	-5.509636380043	-4.295915128383	-0.966574865556
C	-6.695222243293	-4.302833214714	-0.358677515375
C	-7.783767006822	-3.307112038440	-0.673914501060
O	-7.450415885341	-1.968812305946	-0.308814901007
C	-6.694684512204	-1.250395325624	-1.280112705948
C	-6.564826958876	0.193752499404	-0.749804355030
C	-5.168235466153	0.740905985824	-0.478027121146
O	-4.943707001524	1.946161005874	-0.527166722394
C	-5.301871002811	-1.828481157953	-1.534258558205
C	-5.164884781428	-3.267194406839	-2.035435716741
C	-2.853262771202	-3.484378889841	-1.178489336381
C	-3.696350926441	-3.424761750325	-2.444187151182
H	-5.145260361189	-1.890758326264	0.591007124453
H	-0.270873949881	-2.211690894865	-0.178858312179
H	3.091263325564	-0.959064415219	-0.223572676850
H	1.828187790514	-1.844448502518	0.666504004664
H	1.798897237229	-1.792849160846	-1.122864814743
H	1.097274265992	3.632346782638	0.966402862969
H	-0.218820383894	2.831872804248	1.865079819022
H	1.268169934218	1.924352394593	1.448249082651
H	-2.603183623819	2.182868838552	-0.103691906216
H	-4.048752789506	-3.161145491359	1.705546031264
H	-2.376992954735	-2.651418354389	1.947097078994
H	-2.995325192929	-5.314310660131	1.534458428917
H	-1.516355527786	-4.607437672882	0.872799846605
H	-4.687258367585	-5.888466338519	0.227187255691
H	-4.413878394997	-6.024117632596	-1.503203928261
H	-6.900300801161	-5.041678969469	0.414412704411
H	-8.686115583468	-3.549224123192	-0.109041066088
H	-8.044315866436	-3.337774734431	-1.742616730656
H	-7.260309171457	-1.247621626982	-2.221751829660
H	-7.117475929872	0.257235226619	0.193701993601
H	-7.032432561726	0.904223061276	-1.432995835207
H	-4.864488321474	-1.191264544823	-2.314432168928
H	-5.821770756090	-3.409670450245	-2.902568163749
H	-1.789419058676	-3.415323912737	-1.431433880540
H	-3.389157554683	-2.587897590449	-3.077083038216
H	-3.532316775904	-4.342457629036	-3.017308395696

SCF Done: E(RwB97X) = -1302.51217754

Zero-point correction=	0.469006
Thermal correction to Energy=	0.491603
Thermal correction to Enthalpy=	0.492547
Thermal correction to Gibbs Free Energy=	0.418527
Sum of electronic and zero-point Energies=	-1302.043171

Sum of electronic and thermal Energies= -1302.020574
Sum of electronic and thermal Enthalpies= -1302.019630
Sum of electronic and thermal Free Energies= -1302.093651

1 C	Isotropic =	123.2378	Anisotropy =	39.6823
2 N	Isotropic =	98.7301	Anisotropy =	104.0303
3 C	Isotropic =	50.7250	Anisotropy =	113.3493
4 C	Isotropic =	48.3793	Anisotropy =	149.3916
5 C	Isotropic =	79.4884	Anisotropy =	155.1830
6 C	Isotropic =	34.5693	Anisotropy =	124.4613
7 O	Isotropic =	255.1362	Anisotropy =	90.1148
8 C	Isotropic =	135.7191	Anisotropy =	72.7640
9 C	Isotropic =	37.0151	Anisotropy =	119.7025
10 O	Isotropic =	280.6299	Anisotropy =	83.0618
11 C	Isotropic =	130.1259	Anisotropy =	90.7944
12 C	Isotropic =	74.6509	Anisotropy =	134.2310
13 C	Isotropic =	137.1986	Anisotropy =	22.9200
14 C	Isotropic =	137.0510	Anisotropy =	62.1121
15 C	Isotropic =	133.4019	Anisotropy =	64.6953
16 N	Isotropic =	194.5846	Anisotropy =	68.6532
17 C	Isotropic =	134.5433	Anisotropy =	37.2700
18 C	Isotropic =	32.0586	Anisotropy =	178.9049
19 C	Isotropic =	60.2732	Anisotropy =	131.9106
20 C	Isotropic =	125.5386	Anisotropy =	70.0833
21 O	Isotropic =	277.3482	Anisotropy =	90.3754
22 C	Isotropic =	112.7024	Anisotropy =	53.1220
23 C	Isotropic =	146.3428	Anisotropy =	40.4112
24 C	Isotropic =	14.1558	Anisotropy =	120.9918
25 O	Isotropic =	-48.7844	Anisotropy =	568.2827
26 C	Isotropic =	139.4616	Anisotropy =	24.1068
27 C	Isotropic =	157.3254	Anisotropy =	10.3714
28 C	Isotropic =	123.2360	Anisotropy =	38.9232
29 C	Isotropic =	161.1628	Anisotropy =	14.5350
30 H	Isotropic =	27.7267	Anisotropy =	3.4052
31 H	Isotropic =	24.4871	Anisotropy =	13.5799
32 H	Isotropic =	27.7067	Anisotropy =	9.2773
33 H	Isotropic =	28.0281	Anisotropy =	7.7792
34 H	Isotropic =	28.0722	Anisotropy =	8.0005
35 H	Isotropic =	27.9428	Anisotropy =	10.0267
36 H	Isotropic =	28.3803	Anisotropy =	8.6201
37 H	Isotropic =	27.6965	Anisotropy =	7.9109
38 H	Isotropic =	23.6917	Anisotropy =	10.3872
39 H	Isotropic =	29.8148	Anisotropy =	5.8275
40 H	Isotropic =	29.9287	Anisotropy =	6.3999
41 H	Isotropic =	28.8207	Anisotropy =	10.0334
42 H	Isotropic =	28.5501	Anisotropy =	11.0453

43	H	Isotropic =	28.8764	Anisotropy =	7.4672
44	H	Isotropic =	27.9562	Anisotropy =	9.6728
45	H	Isotropic =	25.6446	Anisotropy =	5.8878
46	H	Isotropic =	27.7705	Anisotropy =	10.4408
47	H	Isotropic =	27.6605	Anisotropy =	7.6751
48	H	Isotropic =	27.7700	Anisotropy =	6.8361
49	H	Isotropic =	29.3397	Anisotropy =	6.0781
50	H	Isotropic =	28.8896	Anisotropy =	8.4232
51	H	Isotropic =	30.6414	Anisotropy =	3.5814
52	H	Isotropic =	28.8613	Anisotropy =	9.4957
53	H	Isotropic =	28.1885	Anisotropy =	8.8508
54	H	Isotropic =	30.3599	Anisotropy =	7.6327
55	H	Isotropic =	29.5337	Anisotropy =	11.0918

Brucine_protonated

Conformer_1

C	-3.581114631630	-1.384042835073	1.134836815916
N	-3.197083461089	0.043806282073	1.096679724414
C	-1.789090119342	0.153168493408	1.093603909649
C	-1.215866934857	-1.097294652421	1.279588261291
C	0.165936780932	-1.224213166148	1.301297561420
C	0.963437075175	-0.104176156942	1.121484924924
O	2.326800496699	-0.245366909094	1.086782865234
C	2.985522374310	0.193315900534	2.274869063321
C	0.372551923389	1.160759508239	0.929609947897
O	1.228145262871	2.194513576757	0.750845800730
C	0.674237794325	3.490293194264	0.551816753911
C	-1.016224766622	1.298773321259	0.921280152087
C	-2.280100814675	-2.136257738136	1.539752022959
C	-2.316024766838	-2.574803910101	3.014663655141
C	-3.161924998806	-3.832548446975	2.994559575005
N	-2.803504626571	-4.508907350384	1.694198706610
C	-3.983936525861	-5.157423614200	1.022825704269
C	-4.822555176111	-4.118401024647	0.335833511202
C	-6.130929298916	-4.021507361187	0.553978346612
C	-6.963649234639	-2.943399738662	-0.086872056531
O	-6.593009288524	-1.650373067314	0.382342915731
C	-5.539957406741	-1.011067893234	-0.331785981172
C	-5.456256999937	0.405136437032	0.276892042600
C	-4.066326430694	0.947284077124	0.544126068554
O	-3.760109659531	2.108526240535	0.314358198263
C	-4.173302932026	-1.704603310020	-0.241425841218
C	-4.078127581679	-3.189451829567	-0.612007102580

C	-2.073805416976	-3.482125269839	0.814841679053
C	-2.589110118161	-3.547553345151	-0.610212308352
H	-4.485896771517	-3.316359542747	-1.621585395585
H	-3.548633457043	-1.186122569420	-0.981053976263
H	-4.348768109524	-1.531055146998	1.900654062603
H	-5.826972434173	-0.950424137878	-1.389565358696
H	0.646720620076	-2.187042679928	1.452997584968
H	4.053102619043	0.028132323412	2.122731924368
H	2.805500466747	1.256953609013	2.456543703946
H	2.649445878960	-0.391791531614	3.139003191301
H	0.053222609962	3.521336187172	-0.349294896362
H	0.082608625712	3.806042735459	1.417350301629
H	1.522071668866	4.163441846567	0.428753736618
H	-1.491509060530	2.256862790289	0.773885429151
H	-2.740022184497	-1.808630605100	3.666591518757
H	-1.298753032072	-2.796982639751	3.350555859930
H	-4.227839209619	-3.601773848466	2.957157023688
H	-2.973343988744	-4.527706852158	3.810999439325
H	-2.136730268195	-5.252629948393	1.900899177126
H	-3.578382554812	-5.878645096261	0.310519952182
H	-4.538500089382	-5.696544357173	1.790894158405
H	-6.617634277719	-4.703844212242	1.247487550983
H	-8.015457441677	-3.069141474445	0.175085476275
H	-6.883853261078	-2.982395681558	-1.182803250970
H	-5.964523918917	0.364927052475	1.247014912334
H	-5.981859095038	1.137370634239	-0.335203337259
H	-1.018693308854	-3.752928303570	0.868882656385
H	-2.406150685330	-4.538194112830	-1.032919051945
H	-2.021969858117	-2.832713850219	-1.212047309834

SCF Done: E(RwB97X) = -1302.99357382

Zero-point correction=	0.485481
Thermal correction to Energy=	0.507819
Thermal correction to Enthalpy=	0.508763
Thermal correction to Gibbs Free Energy=	0.435926
Sum of electronic and zero-point Energies=	-1302.508092
Sum of electronic and thermal Energies=	-1302.485755
Sum of electronic and thermal Enthalpies=	-1302.484811
Sum of electronic and thermal Free Energies=	-1302.557647

1 C	Isotropic =	128.9724	Anisotropy =	39.7119
2 N	Isotropic =	97.8624	Anisotropy =	96.6745
3 C	Isotropic =	44.6730	Anisotropy =	123.3871
4 C	Isotropic =	64.2869	Anisotropy =	124.7376
5 C	Isotropic =	66.2259	Anisotropy =	155.0185

6	C	Isotropic = 39.6627	Anisotropy = 115.1230
7	O	Isotropic = 283.5159	Anisotropy = 82.5460
8	C	Isotropic = 130.1856	Anisotropy = 90.6320
9	C	Isotropic = 30.0442	Anisotropy = 130.7031
10	O	Isotropic = 247.3136	Anisotropy = 101.0746
11	C	Isotropic = 135.2604	Anisotropy = 74.2623
12	C	Isotropic = 87.1536	Anisotropy = 139.8952
13	C	Isotropic = 137.4584	Anisotropy = 25.9129
14	C	Isotropic = 149.1309	Anisotropy = 40.1591
15	C	Isotropic = 137.6615	Anisotropy = 61.9772
16	N	Isotropic = 187.7341	Anisotropy = 37.5024
17	C	Isotropic = 136.2202	Anisotropy = 31.0033
18	C	Isotropic = 46.9440	Anisotropy = 161.7697
19	C	Isotropic = 47.1089	Anisotropy = 152.2116
20	C	Isotropic = 126.6925	Anisotropy = 70.0441
21	O	Isotropic = 275.8116	Anisotropy = 94.4825
22	C	Isotropic = 113.1991	Anisotropy = 54.9525
23	C	Isotropic = 145.8571	Anisotropy = 39.0456
24	C	Isotropic = 11.6030	Anisotropy = 123.3454
25	O	Isotropic = -68.6792	Anisotropy = 593.9252
26	C	Isotropic = 142.2925	Anisotropy = 20.1797
27	C	Isotropic = 158.7879	Anisotropy = 11.8772
28	C	Isotropic = 124.9378	Anisotropy = 49.2858
29	C	Isotropic = 165.3298	Anisotropy = 12.4418
30	H	Isotropic = 28.5740	Anisotropy = 9.6176
31	H	Isotropic = 30.7054	Anisotropy = 3.7192
32	H	Isotropic = 27.8553	Anisotropy = 3.1600
33	H	Isotropic = 27.6321	Anisotropy = 7.0615
34	H	Isotropic = 24.3180	Anisotropy = 10.9345
35	H	Isotropic = 27.9876	Anisotropy = 9.9794
36	H	Isotropic = 27.6903	Anisotropy = 8.0626
37	H	Isotropic = 28.4678	Anisotropy = 8.4332
38	H	Isotropic = 28.0036	Anisotropy = 8.4680
39	H	Isotropic = 27.9612	Anisotropy = 8.3496
40	H	Isotropic = 27.6193	Anisotropy = 9.4605
41	H	Isotropic = 23.7537	Anisotropy = 12.1867
42	H	Isotropic = 29.7685	Anisotropy = 8.0026
43	H	Isotropic = 29.7906	Anisotropy = 9.3618
44	H	Isotropic = 28.4352	Anisotropy = 6.1525
45	H	Isotropic = 28.1360	Anisotropy = 11.6062
46	H	Isotropic = 25.8810	Anisotropy = 16.8862
47	H	Isotropic = 27.6768	Anisotropy = 10.0270
48	H	Isotropic = 28.3783	Anisotropy = 9.2866
49	H	Isotropic = 25.0477	Anisotropy = 6.3663
50	H	Isotropic = 27.6649	Anisotropy = 10.5740
51	H	Isotropic = 27.5064	Anisotropy = 7.8158

52	H	Isotropic =	29.2360	Anisotropy =	5.3963
53	H	Isotropic =	28.8268	Anisotropy =	8.6106
54	H	Isotropic =	27.5095	Anisotropy =	8.9063
55	H	Isotropic =	29.4899	Anisotropy =	11.5412
56	H	Isotropic =	30.3015	Anisotropy =	7.7053

Conformer_2

C	-3.604400457172	-1.384597008897	1.166595173460
N	-3.253377051017	0.051556416502	1.161235485701
C	-1.846400037819	0.186931085367	1.234230801302
C	-1.257216069314	-1.045846234735	1.438036786081
C	0.128895792116	-1.156091225781	1.530822644156
C	0.915144847351	-0.019055129707	1.406672969623
O	2.271164601005	-0.011900724046	1.472475830501
C	2.920110699184	-1.256890312527	1.684356998145
C	0.300303334898	1.240261661628	1.201676279696
O	1.143828992130	2.293628804660	1.095992314185
C	0.572953888242	3.579652657934	0.892980287598
C	-1.082849168745	1.349458140311	1.117376128932
C	-2.309831823199	-2.110988765229	1.634974487680
C	-2.416200435282	-2.561423339229	3.103003914878
C	-3.238672844946	-3.832649799410	3.028331195503
N	-2.793007857690	-4.494756674601	1.747767752443
C	-3.918232383906	-5.165687391371	1.007940357802
C	-4.741296326961	-4.140220858038	0.282607371641
C	-6.061102174706	-4.072445351391	0.432003435323
C	-6.881887606835	-3.005866822729	-0.242431132955
O	-6.563897233584	-1.709261181107	0.254695540143
C	-5.489601793916	-1.042809604103	-0.400932255414
C	-5.468152171148	0.373183390138	0.213875470464
C	-4.106153494317	0.939202667911	0.564561191564
O	-3.810798804744	2.108509856648	0.357076416657
C	-4.115128849166	-1.707364813591	-0.241429035545
C	-3.967916247723	-3.187039359524	-0.616961233785
C	-2.037867244083	-3.447607356498	0.914569085531
C	-2.473458813330	-3.512535078787	-0.536729320104
H	-4.319452850701	-3.314509494867	-1.647427701547
H	-3.463439308134	-1.170205969002	-0.943514553431
H	-4.407322947253	-1.558737080077	1.889546730244
H	-5.722486343240	-0.984331589781	-1.472084873074
H	0.585460124111	-2.125110440711	1.699258794625
H	3.988031900577	-1.040789461140	1.705054797712
H	2.710172607595	-1.95995720187	0.870800645872
H	2.625531520361	-1.703920152742	2.640188077978

H	0.007630867167	3.619970516986	-0.044234176175
H	-0.077521063765	3.863426706361	1.727078786648
H	1.411039063019	4.273769019216	0.836278055620
H	-1.566220030406	2.301801222953	0.959662188821
H	-2.887806739088	-1.807248752535	3.735998793609
H	-1.415056331199	-2.769857528171	3.492192253821
H	-4.304288850491	-3.619146045230	2.929166483573
H	-3.086972145387	-4.529347337791	3.851122957683
H	-2.122082592386	-5.224101158676	1.989488228161
H	-3.456311958516	-5.872736493732	0.316149973601
H	-4.502326293939	-5.722264924727	1.740789021716
H	-6.568921984360	-4.770699328500	1.093784719142
H	-7.943138910994	-3.155556344057	-0.037174835944
H	-6.744067458475	-3.033210811887	-1.332905173172
H	-6.035896885171	0.323381317597	1.149910219849
H	-5.966975690763	1.097462825503	-0.429487820172
H	-0.982106577738	-3.698753521936	1.024611310341
H	-2.245502541823	-4.494823628762	-0.957050672255
H	-1.890721844324	-2.779413473900	-1.100577174457

SCF Done: E(RwB97X) = -1302.99595767

Zero-point correction=	0.485952
Thermal correction to Energy=	0.508032
Thermal correction to Enthalpy=	0.508976
Thermal correction to Gibbs Free Energy=	0.437063
Sum of electronic and zero-point Energies=	-1302.510005
Sum of electronic and thermal Energies=	-1302.487926
Sum of electronic and thermal Enthalpies=	-1302.486982
Sum of electronic and thermal Free Energies=	-1302.558894

1 C	Isotropic =	129.1797	Anisotropy =	39.4354
2 N	Isotropic =	99.2510	Anisotropy =	97.6972
3 C	Isotropic =	49.0786	Anisotropy =	116.5150
4 C	Isotropic =	65.2561	Anisotropy =	125.2121
5 C	Isotropic =	81.5449	Anisotropy =	157.3940
6 C	Isotropic =	38.7822	Anisotropy =	118.9089
7 O	Isotropic =	256.4051	Anisotropy =	93.9665
8 C	Isotropic =	135.5833	Anisotropy =	72.2923
9 C	Isotropic =	34.8016	Anisotropy =	124.6054
10 O	Isotropic =	250.1393	Anisotropy =	104.5381
11 C	Isotropic =	135.4462	Anisotropy =	73.5556
12 C	Isotropic =	87.4240	Anisotropy =	140.1701
13 C	Isotropic =	136.8479	Anisotropy =	25.8930
14 C	Isotropic =	149.5436	Anisotropy =	39.5635
15 C	Isotropic =	137.8233	Anisotropy =	61.5704

16	N	Isotropic =	187.7105	Anisotropy =	37.3549
17	C	Isotropic =	136.2756	Anisotropy =	30.9407
18	C	Isotropic =	46.9894	Anisotropy =	161.8250
19	C	Isotropic =	47.0227	Anisotropy =	152.1312
20	C	Isotropic =	126.6656	Anisotropy =	70.0315
21	O	Isotropic =	275.6527	Anisotropy =	93.9770
22	C	Isotropic =	112.9972	Anisotropy =	54.9903
23	C	Isotropic =	146.0366	Anisotropy =	39.0165
24	C	Isotropic =	11.8577	Anisotropy =	123.5634
25	O	Isotropic =	-64.2128	Anisotropy =	586.5779
26	C	Isotropic =	142.4151	Anisotropy =	20.0333
27	C	Isotropic =	158.4673	Anisotropy =	11.9533
28	C	Isotropic =	124.9476	Anisotropy =	49.6240
29	C	Isotropic =	165.3325	Anisotropy =	12.6832
30	H	Isotropic =	28.5740	Anisotropy =	9.6564
31	H	Isotropic =	30.7156	Anisotropy =	3.6507
32	H	Isotropic =	27.8725	Anisotropy =	3.1821
33	H	Isotropic =	27.6421	Anisotropy =	7.0473
34	H	Isotropic =	24.5933	Anisotropy =	13.1998
35	H	Isotropic =	27.6764	Anisotropy =	9.4608
36	H	Isotropic =	28.0955	Anisotropy =	7.9030
37	H	Isotropic =	28.0587	Anisotropy =	8.1233
38	H	Isotropic =	28.0396	Anisotropy =	8.3542
39	H	Isotropic =	28.0131	Anisotropy =	8.4257
40	H	Isotropic =	27.6224	Anisotropy =	9.5841
41	H	Isotropic =	23.8159	Anisotropy =	11.9559
42	H	Isotropic =	29.7854	Anisotropy =	8.2137
43	H	Isotropic =	29.7835	Anisotropy =	9.2175
44	H	Isotropic =	28.4134	Anisotropy =	6.1692
45	H	Isotropic =	28.1539	Anisotropy =	11.6358
46	H	Isotropic =	25.8646	Anisotropy =	16.8663
47	H	Isotropic =	27.6685	Anisotropy =	9.9742
48	H	Isotropic =	28.3756	Anisotropy =	9.3328
49	H	Isotropic =	25.0819	Anisotropy =	6.3455
50	H	Isotropic =	27.6622	Anisotropy =	10.5615
51	H	Isotropic =	27.5000	Anisotropy =	7.8299
52	H	Isotropic =	29.2533	Anisotropy =	5.4778
53	H	Isotropic =	28.8561	Anisotropy =	8.6166
54	H	Isotropic =	27.4371	Anisotropy =	9.3288
55	H	Isotropic =	29.4742	Anisotropy =	11.4968
56	H	Isotropic =	30.3083	Anisotropy =	7.6322

Conformer_4

C -3.643085598742 -1.411437576304 1.175251375127

N	-3.293955897931	0.025453590203	1.200551720658
C	-1.891134455608	0.171597351685	1.253302334806
C	-1.289559830839	-1.075054111603	1.409583501963
C	0.088332281127	-1.177094431403	1.470359593735
C	0.872244529531	-0.030163996749	1.367311872602
O	2.237713083346	-0.156772662646	1.415989241834
C	2.822547053574	0.312047721241	2.632216974069
C	0.259209913503	1.220022070278	1.197198516736
O	0.974953605542	2.382005641124	1.121890843610
C	1.947609349462	2.470363963052	0.075943415161
C	-1.131342106711	1.328298166792	1.149589412534
C	-2.337469004915	-2.146514540496	1.596094186492
C	-2.409573086605	-2.636124753379	3.053549307648
C	-3.220016183274	-3.914215418154	2.962406667303
N	-2.801833980284	-4.534799239845	1.652219373732
C	-3.941162023387	-5.188895876642	0.918570150454
C	-4.785369145877	-4.146187419712	0.243438081353
C	-6.101461163143	-4.088392178930	0.426102615502
C	-6.942840256718	-3.007769828682	-0.199078112318
O	-6.616297269678	-1.723576937776	0.324598856686
C	-5.562080781732	-1.035605334723	-0.340620110371
C	-5.530531242558	0.364738965193	0.308779819308
C	-4.163186818793	0.926925407243	0.642920617158
O	-3.872776626251	2.099826069673	0.459480369736
C	-4.182027979606	-1.697863186852	-0.229790938735
C	-4.036543707489	-3.165728452927	-0.647707064639
C	-2.072255756468	-3.460263080401	0.833011081030
C	-2.539528210783	-3.487127884439	-0.609771147342
H	-4.409606813946	-3.267203077244	-1.673456977700
H	-3.547382296795	-1.138422624960	-0.930104812780
H	-4.431049308883	-1.603363766763	1.909852271072
H	-5.820943302155	-0.951876233218	-1.404051178381
H	0.582282305935	-2.135055702893	1.609193455295
H	2.457857292931	-0.274247875831	3.483267090754
H	3.900242309093	0.175634841990	2.535001402234
H	2.603023115072	1.371607583035	2.798902573478
H	2.854797267626	1.911149983884	0.317042316953
H	1.530166837681	2.101449273445	-0.866702971390
H	2.187486195266	3.529159949023	-0.027346835156
H	-1.586123604853	2.300429471076	1.019435048858
H	-2.875387387666	-1.904651158914	3.716669137815
H	-1.398803704142	-2.844358794841	3.416263605365
H	-4.290495436471	-3.711901287717	2.899528510385
H	-3.036769161681	-4.631870308693	3.760371681864
H	-2.122752444455	-5.268044989365	1.856660100269
H	-3.492500434395	-5.870961665251	0.193743555999

H	-4.505053185748	-5.771125087708	1.647431549683
H	-6.590254716071	-4.807703683340	1.079534378974
H	-7.997783106543	-3.167264501310	0.029792627713
H	-6.833054045416	-3.005421217293	-1.293100661233
H	-6.073948754299	0.288535899899	1.257480425352
H	-6.047717513687	1.103433445267	-0.302800472894
H	-1.012818472325	-3.705848773702	0.912589462113
H	-2.317708922909	-4.457273387526	-1.060330688630
H	-1.971481399857	-2.737598345869	-1.166857151848

SCF Done: E(RwB97X) = -1302.98944996

Zero-point correction=	0.485134
Thermal correction to Energy=	0.507682
Thermal correction to Enthalpy=	0.508627
Thermal correction to Gibbs Free Energy=	0.435102
Sum of electronic and zero-point Energies=	-1302.504316
Sum of electronic and thermal Energies=	-1302.481768
Sum of electronic and thermal Enthalpies=	-1302.480823
Sum of electronic and thermal Free Energies=	-1302.554348

1 C	Isotropic = 129.1362	Anisotropy = 39.5844
2 N	Isotropic = 98.3497	Anisotropy = 98.6345
3 C	Isotropic = 44.9745	Anisotropy = 123.1798
4 C	Isotropic = 58.2178	Anisotropy = 132.8705
5 C	Isotropic = 65.5610	Anisotropy = 154.0181
6 C	Isotropic = 36.2668	Anisotropy = 118.9636
7 O	Isotropic = 278.9975	Anisotropy = 84.0162
8 C	Isotropic = 131.5020	Anisotropy = 89.5488
9 C	Isotropic = 29.9957	Anisotropy = 130.8216
10 O	Isotropic = 268.6311	Anisotropy = 99.5114
11 C	Isotropic = 132.0602	Anisotropy = 89.8762
12 C	Isotropic = 75.5411	Anisotropy = 131.1127
13 C	Isotropic = 137.4528	Anisotropy = 25.8558
14 C	Isotropic = 148.8879	Anisotropy = 40.5652
15 C	Isotropic = 137.6074	Anisotropy = 62.2760
16 N	Isotropic = 187.8207	Anisotropy = 37.7111
17 C	Isotropic = 136.1700	Anisotropy = 30.8159
18 C	Isotropic = 47.1960	Anisotropy = 161.2684
19 C	Isotropic = 47.1191	Anisotropy = 152.0510
20 C	Isotropic = 126.5877	Anisotropy = 70.1878
21 O	Isotropic = 276.0515	Anisotropy = 94.5916
22 C	Isotropic = 113.2594	Anisotropy = 54.9393
23 C	Isotropic = 145.7615	Anisotropy = 39.0440
24 C	Isotropic = 11.7942	Anisotropy = 123.2635
25 O	Isotropic = -71.2765	Anisotropy = 596.6841

26	C	Isotropic =	142.3554	Anisotropy =	20.1827
27	C	Isotropic =	158.5595	Anisotropy =	11.6753
28	C	Isotropic =	124.7622	Anisotropy =	49.2503
29	C	Isotropic =	165.2082	Anisotropy =	12.4283
30	H	Isotropic =	28.5567	Anisotropy =	9.6104
31	H	Isotropic =	30.6886	Anisotropy =	3.7595
32	H	Isotropic =	27.8539	Anisotropy =	3.1482
33	H	Isotropic =	27.6524	Anisotropy =	7.0632
34	H	Isotropic =	24.3681	Anisotropy =	11.0899
35	H	Isotropic =	28.4107	Anisotropy =	8.6204
36	H	Isotropic =	27.9704	Anisotropy =	9.9651
37	H	Isotropic =	27.6828	Anisotropy =	8.3551
38	H	Isotropic =	27.0861	Anisotropy =	7.6489
39	H	Isotropic =	28.5092	Anisotropy =	8.7275
40	H	Isotropic =	27.8055	Anisotropy =	9.9517
41	H	Isotropic =	23.7423	Anisotropy =	10.2772
42	H	Isotropic =	29.7308	Anisotropy =	8.0190
43	H	Isotropic =	29.7750	Anisotropy =	9.4322
44	H	Isotropic =	28.4009	Anisotropy =	6.1647
45	H	Isotropic =	28.1028	Anisotropy =	11.6045
46	H	Isotropic =	25.8515	Anisotropy =	16.8430
47	H	Isotropic =	27.6766	Anisotropy =	9.9810
48	H	Isotropic =	28.3484	Anisotropy =	9.3541
49	H	Isotropic =	25.0675	Anisotropy =	6.3326
50	H	Isotropic =	27.6622	Anisotropy =	10.5728
51	H	Isotropic =	27.5312	Anisotropy =	7.7918
52	H	Isotropic =	29.2418	Anisotropy =	5.5024
53	H	Isotropic =	28.8014	Anisotropy =	8.6903
54	H	Isotropic =	27.5041	Anisotropy =	8.9569
55	H	Isotropic =	29.4621	Anisotropy =	11.5119
56	H	Isotropic =	30.3108	Anisotropy =	7.7933

Conformer_5

C	-3.573697255603	-1.461847808039	1.124162629898
N	-3.235657527624	-0.028513736905	1.202594519114
C	-1.829985385259	0.110294112492	1.152325030417
C	-1.227419151069	-1.139153264700	1.247417026150
C	0.155619496357	-1.238202199560	1.202443920583
C	0.923541181171	-0.093595707372	1.043658512119
O	2.285927055130	-0.205902401622	0.937526940498
C	2.996036377989	0.193850113882	2.109761210751
C	0.302540681330	1.167808736826	0.945818989020
O	1.130144045486	2.226100893339	0.779984402494
C	0.548601718066	3.524230775727	0.722648066689

C	-1.087736645898	1.278294408853	1.008773731692
C	-2.267424381529	-2.202629033402	1.517084874732
C	-2.266019635458	-2.630695602798	2.996149330825
C	-3.089003984915	-3.905402170746	3.017657973892
N	-2.822596730601	-4.565867742343	1.685510376990
C	-4.073478467019	-5.121311181114	1.042695653315
C	-4.840446957120	-3.992243704110	0.413086979138
C	-6.038254614615	-3.658852425101	0.888852116847
C	-6.899376427889	-2.489640823286	0.513347796041
O	-6.519337753201	-1.761109138981	-0.637655174655
C	-5.354994113378	-0.944528564641	-0.583696359579
C	-5.495410233547	0.249752457433	0.388405465454
C	-4.154616074787	0.874458020800	0.727787233517
O	-3.911889928639	2.063988436663	0.592889029175
C	-4.048398664337	-1.712619718967	-0.311582613210
C	-4.060321079906	-3.204603508845	-0.636762027486
C	-2.073881355418	-3.557305586548	0.801654627525
C	-2.592596059128	-3.651740610469	-0.620815908504
H	-4.485608669664	-3.366569821694	-1.631111086831
H	-3.294342883353	-1.253244359403	-0.962185415888
H	-4.365508281297	-1.682746133082	1.843225674774
H	-5.298089366105	-0.547990770184	-1.599299125394
H	0.659583752694	-2.197550606125	1.285283460565
H	2.721464981178	-0.441223045281	2.960187110923
H	4.057530864860	0.066092802385	1.893219944487
H	2.799215906852	1.242044260931	2.353189624437
H	1.378644341829	4.218414863888	0.595154893728
H	-0.133980580680	3.615801129063	-0.128324070059
H	0.016622387293	3.758938779466	1.650471670957
H	-1.587440731320	2.232891598439	0.935082545170
H	-2.687786848367	-1.864524394725	3.649839222713
H	-1.236717635433	-2.828167443882	3.308946021907
H	-4.157531112200	-3.695828780575	3.068569865041
H	-2.823193508299	-4.604478742231	3.808777558257
H	-2.194907357889	-5.354717100529	1.840630473834
H	-3.746122683895	-5.863101938739	0.312983074016
H	-4.638256333416	-5.624142185317	1.827344716004
H	-6.465073883599	-4.263503102886	1.688894448367
H	-6.983659463192	-1.833500884229	1.392879231813
H	-7.912800198729	-2.848389357432	0.309006662625
H	-5.941886383813	-0.088195160237	1.329986048576
H	-6.139044196797	1.022386800181	-0.030666154831
H	-1.021799728598	-3.839459230977	0.864445042487
H	-2.461431497227	-4.668599382948	-0.998597176597
H	-1.990649019422	-2.997350820344	-1.255958614522

SCF Done: E(RwB97X) = -1302.99078274

Zero-point correction=	0.486217
Thermal correction to Energy=	0.508402
Thermal correction to Enthalpy=	0.509346
Thermal correction to Gibbs Free Energy=	0.436699
Sum of electronic and zero-point Energies=	-1302.504566
Sum of electronic and thermal Energies=	-1302.482381
Sum of electronic and thermal Enthalpies=	-1302.481436
Sum of electronic and thermal Free Energies=	-1302.554084

1	C	Isotropic =	127.0744	Anisotropy =	37.5757
2	N	Isotropic =	101.6206	Anisotropy =	103.1583
3	C	Isotropic =	44.6705	Anisotropy =	124.2548
4	C	Isotropic =	64.3183	Anisotropy =	125.4030
5	C	Isotropic =	66.0782	Anisotropy =	155.2303
6	C	Isotropic =	39.6154	Anisotropy =	115.4079
7	O	Isotropic =	283.5424	Anisotropy =	82.6772
8	C	Isotropic =	130.2841	Anisotropy =	90.4782
9	C	Isotropic =	30.0177	Anisotropy =	130.5914
10	O	Isotropic =	247.2233	Anisotropy =	102.2473
11	C	Isotropic =	135.4369	Anisotropy =	74.0017
12	C	Isotropic =	87.2691	Anisotropy =	140.4111
13	C	Isotropic =	137.3457	Anisotropy =	24.4629
14	C	Isotropic =	150.3974	Anisotropy =	40.9427
15	C	Isotropic =	138.5212	Anisotropy =	62.8694
16	N	Isotropic =	185.3312	Anisotropy =	38.2175
17	C	Isotropic =	134.2600	Anisotropy =	30.6020
18	C	Isotropic =	57.4072	Anisotropy =	152.9054
19	C	Isotropic =	44.4203	Anisotropy =	140.2583
20	C	Isotropic =	126.6076	Anisotropy =	55.1448
21	O	Isotropic =	289.1439	Anisotropy =	57.7652
22	C	Isotropic =	117.9636	Anisotropy =	54.8693
23	C	Isotropic =	154.9683	Anisotropy =	45.4371
24	C	Isotropic =	9.9193	Anisotropy =	121.5994
25	O	Isotropic =	-76.9359	Anisotropy =	601.4009
26	C	Isotropic =	139.8763	Anisotropy =	32.8276
27	C	Isotropic =	160.7671	Anisotropy =	10.3333
28	C	Isotropic =	125.2693	Anisotropy =	46.8021
29	C	Isotropic =	164.3179	Anisotropy =	14.5651
30	H	Isotropic =	28.6305	Anisotropy =	9.9654
31	H	Isotropic =	30.3747	Anisotropy =	3.1824
32	H	Isotropic =	27.8486	Anisotropy =	2.7719
33	H	Isotropic =	27.5216	Anisotropy =	6.8437
34	H	Isotropic =	24.3536	Anisotropy =	10.8992
35	H	Isotropic =	28.4854	Anisotropy =	8.4553

36	H	Isotropic =	28.0068	Anisotropy =	9.9942
37	H	Isotropic =	27.6932	Anisotropy =	8.0285
38	H	Isotropic =	27.6232	Anisotropy =	9.4476
39	H	Isotropic =	27.9637	Anisotropy =	8.4322
40	H	Isotropic =	28.0181	Anisotropy =	8.4157
41	H	Isotropic =	23.8286	Anisotropy =	12.1668
42	H	Isotropic =	29.8093	Anisotropy =	7.6429
43	H	Isotropic =	29.9391	Anisotropy =	9.2943
44	H	Isotropic =	28.4445	Anisotropy =	6.3513
45	H	Isotropic =	28.1717	Anisotropy =	11.6017
46	H	Isotropic =	25.9154	Anisotropy =	16.9371
47	H	Isotropic =	27.6367	Anisotropy =	10.0335
48	H	Isotropic =	28.5190	Anisotropy =	9.5752
49	H	Isotropic =	25.5098	Anisotropy =	5.7092
50	H	Isotropic =	27.0611	Anisotropy =	6.2142
51	H	Isotropic =	27.4715	Anisotropy =	10.3454
52	H	Isotropic =	28.3963	Anisotropy =	4.6392
53	H	Isotropic =	29.5024	Anisotropy =	9.8091
54	H	Isotropic =	27.5304	Anisotropy =	8.9885
55	H	Isotropic =	29.4958	Anisotropy =	11.6669
56	H	Isotropic =	30.2853	Anisotropy =	8.1156

Conformer_6

C	-3.592170549145	-1.463657035674	1.156824988206
N	-3.291885906844	-0.024307197941	1.266563035685
C	-1.885547188561	0.141154744170	1.296675807573
C	-1.263829205227	-1.089007030549	1.416376975104
C	0.125981401982	-1.171057072403	1.460504326788
C	0.882877244906	-0.010714535171	1.368372137042
O	2.239801832226	0.024998442214	1.395903885201
C	2.921039446401	-1.209136192216	1.566525813457
C	0.235294574189	1.242610942582	1.241818946876
O	1.053051158919	2.317613631894	1.156796901257
C	0.451798444986	3.597926154615	1.013525892949
C	-1.152474651563	1.324600105169	1.209686723364
C	-2.292148826284	-2.180166545735	1.612615115005
C	-2.363179077998	-2.630597580104	3.083261045463
C	-3.157964953046	-3.922223018063	3.040350191670
N	-2.797629554833	-4.558977202675	1.719468213384
C	-3.995413205488	-5.137292383254	1.000367740245
C	-4.755386960425	-4.016845273443	0.348268615755
C	-5.983055359551	-3.717702250013	0.767090887544
C	-6.850286822657	-2.561149877330	0.367298532020
O	-6.434239796440	-1.809610971398	-0.756233136927

C	-5.292495484331	-0.968137690954	-0.637249441579
C	-5.508997718877	0.213338437014	0.336155226069
C	-4.200285342521	0.862118944382	0.749409077983
O	-3.975229759711	2.058140383895	0.632443621965
C	-3.984073287396	-1.708459175758	-0.304779997184
C	-3.940859635011	-3.195813681621	-0.648288634745
C	-2.026950110284	-3.519955668467	0.891294862776
C	-2.465026417588	-3.606604430852	-0.558675266546
H	-4.308536526299	-3.355509647797	-1.665835079532
H	-3.208294884681	-1.222276707025	-0.908404428484
H	-4.416220669406	-1.711047382362	1.830126604307
H	-5.193899303070	-0.561246161123	-1.645567758465
H	0.607016405911	-2.137112196847	1.566944974191
H	3.983681219178	-0.967798617590	1.579172097877
H	2.649509738794	-1.687299152123	2.514090550153
H	2.717842745425	-1.896102861350	0.737699894113
H	1.275170689004	4.308869038195	0.950109250766
H	-0.146798545611	3.655838821116	0.098205835824
H	-0.174183223980	3.843911796941	1.877880337958
H	-1.661857760162	2.272333291243	1.115984626671
H	-2.837407956376	-1.883368875510	3.722833510153
H	-1.348977455029	-2.811479520199	3.451073734790
H	-4.231688919345	-3.734312082614	3.028738565413
H	-2.926277147780	-4.625566896508	3.838362689407
H	-2.158773506976	-5.332971339033	1.901282326262
H	-3.609161310850	-5.858337783684	0.278821119409
H	-4.588206688743	-5.667753456034	1.745097555062
H	-6.435462860391	-4.344787290403	1.535191411488
H	-6.987156805243	-1.919067863700	1.250683210140
H	-7.845965949550	-2.937509020796	0.113461859199
H	-5.997560900610	-0.142390865773	1.249916756100
H	-6.146288925073	0.976132770895	-0.109833496846
H	-0.973239771256	-3.778188688618	1.008980010725
H	-2.287590428688	-4.614226166248	-0.942264046092
H	-1.846985549021	-2.927920115368	-1.151524196991

SCF Done: E(RwB97X) = -1302.99302628

Zero-point correction=	0.486217
Thermal correction to Energy=	0.508261
Thermal correction to Enthalpy=	0.509205
Thermal correction to Gibbs Free Energy=	0.437297
Sum of electronic and zero-point Energies=	-1302.506809
Sum of electronic and thermal Energies=	-1302.484765
Sum of electronic and thermal Enthalpies=	-1302.483821
Sum of electronic and thermal Free Energies=	-1302.555730

1	C	Isotropic = 127.3358	Anisotropy = 37.3310
2	N	Isotropic = 102.8147	Anisotropy = 104.1732
3	C	Isotropic = 49.2260	Anisotropy = 117.3974
4	C	Isotropic = 65.1083	Anisotropy = 125.5934
5	C	Isotropic = 81.3514	Anisotropy = 157.6123
6	C	Isotropic = 38.7114	Anisotropy = 119.3230
7	O	Isotropic = 256.1558	Anisotropy = 93.8503
8	C	Isotropic = 135.5208	Anisotropy = 72.5052
9	C	Isotropic = 34.7389	Anisotropy = 124.8041
10	O	Isotropic = 250.1034	Anisotropy = 105.5796
11	C	Isotropic = 135.6315	Anisotropy = 73.3854
12	C	Isotropic = 87.8013	Anisotropy = 140.6641
13	C	Isotropic = 136.7263	Anisotropy = 24.1507
14	C	Isotropic = 150.6204	Anisotropy = 40.7277
15	C	Isotropic = 138.7536	Anisotropy = 62.1906
16	N	Isotropic = 185.3412	Anisotropy = 38.1222
17	C	Isotropic = 134.3711	Anisotropy = 30.5288
18	C	Isotropic = 57.5207	Anisotropy = 152.7728
19	C	Isotropic = 44.3849	Anisotropy = 140.2800
20	C	Isotropic = 126.7178	Anisotropy = 54.9818
21	O	Isotropic = 288.7214	Anisotropy = 58.0208
22	C	Isotropic = 117.8436	Anisotropy = 54.5746
23	C	Isotropic = 155.0771	Anisotropy = 45.2356
24	C	Isotropic = 10.1791	Anisotropy = 121.4484
25	O	Isotropic = -71.9343	Anisotropy = 593.5170
26	C	Isotropic = 139.8985	Anisotropy = 32.9058
27	C	Isotropic = 160.6137	Anisotropy = 10.0844
28	C	Isotropic = 125.1752	Anisotropy = 47.0321
29	C	Isotropic = 164.2599	Anisotropy = 14.7811
30	H	Isotropic = 28.6110	Anisotropy = 9.9432
31	H	Isotropic = 30.3608	Anisotropy = 3.1585
32	H	Isotropic = 27.8779	Anisotropy = 2.8826
33	H	Isotropic = 27.5281	Anisotropy = 6.8430
34	H	Isotropic = 24.6354	Anisotropy = 13.2150
35	H	Isotropic = 27.6901	Anisotropy = 9.4870
36	H	Isotropic = 28.1227	Anisotropy = 8.0756
37	H	Isotropic = 28.0834	Anisotropy = 7.9345
38	H	Isotropic = 27.6233	Anisotropy = 9.6018
39	H	Isotropic = 28.0712	Anisotropy = 8.3353
40	H	Isotropic = 28.0085	Anisotropy = 8.4618
41	H	Isotropic = 23.8865	Anisotropy = 11.9709
42	H	Isotropic = 29.8041	Anisotropy = 7.8249
43	H	Isotropic = 29.9201	Anisotropy = 9.1348
44	H	Isotropic = 28.4261	Anisotropy = 6.3696
45	H	Isotropic = 28.2074	Anisotropy = 11.6457

46	H	Isotropic =	25.8973	Anisotropy =	16.9281
47	H	Isotropic =	27.6261	Anisotropy =	10.0166
48	H	Isotropic =	28.5215	Anisotropy =	9.6598
49	H	Isotropic =	25.5147	Anisotropy =	5.7654
50	H	Isotropic =	27.0714	Anisotropy =	6.1613
51	H	Isotropic =	27.4925	Anisotropy =	10.3243
52	H	Isotropic =	28.4251	Anisotropy =	4.6987
53	H	Isotropic =	29.5257	Anisotropy =	9.8265
54	H	Isotropic =	27.4771	Anisotropy =	9.3389
55	H	Isotropic =	29.4694	Anisotropy =	11.6172
56	H	Isotropic =	30.2890	Anisotropy =	8.0589

Conformer_7

C	-3.582773622544	-1.458258077572	1.115927084609
N	-3.298157341326	-0.013167135265	1.172322212890
C	-1.895048408125	0.171966533469	1.145746783861
C	-1.249630890085	-1.051092770059	1.280002881179
C	0.136277049215	-1.130110450754	1.253666137072
C	0.881388702558	0.035382115744	1.078645176005
O	2.236204662238	0.073108059730	1.004222129769
C	2.939065203549	-1.155234182356	1.141450829878
C	0.217008657993	1.272125490102	0.961154939949
O	0.931190763160	2.420529823702	0.749338199033
C	1.628268655442	2.901283554420	1.899850012968
C	-1.169276058112	1.348502321724	0.995753125973
C	-2.260208079028	-2.143943479924	1.551194990727
C	-2.277899293280	-2.537275012669	3.039734017317
C	-3.069304801821	-3.831699826512	3.071066956526
N	-2.743986972358	-4.518392116070	1.765989869268
C	-3.956552440354	-5.134712695121	1.105127749715
C	-4.747483571388	-4.047782260635	0.432587988288
C	-5.967383226555	-3.747118908151	0.872652808295
C	-6.858723603309	-2.616311738859	0.452853115533
O	-6.476865415588	-1.897867029704	-0.703973344145
C	-5.343034084897	-1.040461723850	-0.640039180261
C	-5.546686508943	0.167071244931	0.304163793405
C	-4.233943609927	0.845256371395	0.654173944915
O	-4.025828576678	2.038129928567	0.489752543690
C	-4.016729866246	-1.756472972843	-0.323283342913
C	-3.970520440424	-3.255108128400	-0.615705339652
C	-2.006799162442	-3.508188111572	0.873976208230
C	-2.489490513806	-3.651912366983	-0.556925686184
H	-4.366805885094	-3.451938265445	-1.615845691238
H	-3.264532789584	-1.285673589054	-0.967623194630

H	-4.380618999611	-1.695191213052	1.823195091639
H	-5.276496775477	-0.661378832254	-1.661694270737
H	0.626772206172	-2.091403899207	1.361445948276
H	3.996962300582	-0.904186641971	1.070166132423
H	2.740931823315	-1.620062523128	2.113090907903
H	2.678012206966	-1.853279557140	0.338968602063
H	2.190071232895	3.779725449094	1.580250553071
H	0.917171914175	3.190942970114	2.682205670765
H	2.319705847155	2.148255257406	2.287538377074
H	-1.654469104741	2.310407543464	0.897052083990
H	-2.732926419766	-1.768392977646	3.667439507213
H	-1.251221157309	-2.702706703044	3.378784498497
H	-4.143812151465	-3.647299235251	3.083122793986
H	-2.811514608022	-4.501766667051	3.889446983998
H	-2.093332771624	-5.279699365028	1.960011415412
H	-3.583570277483	-5.880389420497	0.401802299181
H	-4.522159404192	-5.641196132149	1.886875323719
H	-6.392256962183	-4.350012559439	1.675077548025
H	-6.985982633232	-1.947197994389	1.317367622589
H	-7.854150790069	-3.013960809452	0.232331987797
H	-6.000637751958	-0.167199281689	1.243442378889
H	-6.208319985305	0.907645936188	-0.143898157042
H	-0.948464111520	-3.756240253463	0.968100210223
H	-2.316144656700	-4.672055314327	-0.907502586791
H	-1.894987502842	-2.992492378071	-1.193978642238

SCF Done: E(RwB97X) = -1302.98947454

Zero-point correction=	0.485833
Thermal correction to Energy=	0.508008
Thermal correction to Enthalpy=	0.508952
Thermal correction to Gibbs Free Energy=	0.436741
Sum of electronic and zero-point Energies=	-1302.503642
Sum of electronic and thermal Energies=	-1302.481466
Sum of electronic and thermal Enthalpies=	-1302.480522
Sum of electronic and thermal Free Energies=	-1302.552734

1 C	Isotropic =	127.1439	Anisotropy =	37.3522
2 N	Isotropic =	103.4512	Anisotropy =	105.7548
3 C	Isotropic =	49.6550	Anisotropy =	117.7406
4 C	Isotropic =	58.0680	Anisotropy =	135.6057
5 C	Isotropic =	79.8790	Anisotropy =	158.9386
6 C	Isotropic =	34.4635	Anisotropy =	124.5686
7 O	Isotropic =	253.5731	Anisotropy =	92.9737
8 C	Isotropic =	135.8143	Anisotropy =	72.9689
9 C	Isotropic =	35.5984	Anisotropy =	121.6167

10	O	Isotropic = 277.4027	Anisotropy = 87.7890
11	C	Isotropic = 130.6833	Anisotropy = 90.0427
12	C	Isotropic = 74.0755	Anisotropy = 136.7259
13	C	Isotropic = 136.5789	Anisotropy = 24.3919
14	C	Isotropic = 150.6338	Anisotropy = 40.7126
15	C	Isotropic = 138.6287	Anisotropy = 62.4601
16	N	Isotropic = 185.3682	Anisotropy = 38.0229
17	C	Isotropic = 134.3550	Anisotropy = 30.7358
18	C	Isotropic = 57.6244	Anisotropy = 152.4722
19	C	Isotropic = 44.4032	Anisotropy = 140.3248
20	C	Isotropic = 126.6378	Anisotropy = 55.1102
21	O	Isotropic = 288.9281	Anisotropy = 57.8965
22	C	Isotropic = 117.9384	Anisotropy = 54.5823
23	C	Isotropic = 155.2004	Anisotropy = 45.3218
24	C	Isotropic = 10.3027	Anisotropy = 121.7537
25	O	Isotropic = -75.0424	Anisotropy = 596.6305
26	C	Isotropic = 140.0191	Anisotropy = 32.6009
27	C	Isotropic = 160.5396	Anisotropy = 9.8224
28	C	Isotropic = 125.2118	Anisotropy = 47.0818
29	C	Isotropic = 164.3954	Anisotropy = 14.4701
30	H	Isotropic = 28.6198	Anisotropy = 9.9816
31	H	Isotropic = 30.3839	Anisotropy = 3.1613
32	H	Isotropic = 27.8649	Anisotropy = 2.8391
33	H	Isotropic = 27.5578	Anisotropy = 6.8304
34	H	Isotropic = 24.6038	Anisotropy = 13.3321
35	H	Isotropic = 27.6458	Anisotropy = 9.3943
36	H	Isotropic = 28.0572	Anisotropy = 7.9797
37	H	Isotropic = 28.0716	Anisotropy = 8.1431
38	H	Isotropic = 27.9517	Anisotropy = 9.9985
39	H	Isotropic = 28.3810	Anisotropy = 8.7502
40	H	Isotropic = 27.6023	Anisotropy = 7.7478
41	H	Isotropic = 23.7235	Anisotropy = 10.1705
42	H	Isotropic = 29.7721	Anisotropy = 7.9369
43	H	Isotropic = 29.9115	Anisotropy = 9.1801
44	H	Isotropic = 28.4074	Anisotropy = 6.3535
45	H	Isotropic = 28.1782	Anisotropy = 11.6039
46	H	Isotropic = 25.8826	Anisotropy = 16.8616
47	H	Isotropic = 27.6144	Anisotropy = 10.0219
48	H	Isotropic = 28.5068	Anisotropy = 9.6318
49	H	Isotropic = 25.5209	Anisotropy = 5.7337
50	H	Isotropic = 27.0993	Anisotropy = 6.2495
51	H	Isotropic = 27.4910	Anisotropy = 10.3268
52	H	Isotropic = 28.4643	Anisotropy = 4.6908
53	H	Isotropic = 29.5420	Anisotropy = 9.8526
54	H	Isotropic = 27.4424	Anisotropy = 9.4109
55	H	Isotropic = 29.4720	Anisotropy = 11.5576

56 H Isotropic = 30.2968 Anisotropy = 8.1893

Conformer_8

C	-3.625443402006	-1.498311884310	1.168427363534
N	-3.331342980129	-0.061836631594	1.320687645098
C	-1.930814237097	0.120249082084	1.325075464112
C	-1.292658704909	-1.119898487438	1.380875657268
C	0.087959367020	-1.186036605307	1.374563644493
C	0.837079101892	-0.012895479679	1.301929881831
O	2.206258967577	-0.104379102957	1.288054543472
C	2.825858314652	0.311798776454	2.506287838827
C	0.187156129622	1.228107489873	1.230363673921
O	0.865296754403	2.413207288599	1.189658221987
C	1.829789829603	2.577121177657	0.145293240750
C	-1.207212161562	1.300567264021	1.254092326480
C	-2.312470963838	-2.219965253218	1.572515348189
C	-2.347447933100	-2.703947514689	3.034012196931
C	-3.142968977678	-3.994957084762	2.978011028742
N	-2.812649903114	-4.599091883566	1.633457894650
C	-4.024495910477	-5.161228552355	0.924674770372
C	-4.801221822364	-4.027939094497	0.315045505254
C	-6.023043201091	-3.746471872807	0.762188698476
C	-6.903494875770	-2.586432511142	0.404171230655
O	-6.504202230569	-1.799132064697	-0.700669064392
C	-5.365937420190	-0.954988737153	-0.571959904268
C	-5.571753558148	0.191510492852	0.445335918516
C	-4.260775997370	0.836754776585	0.856845445115
O	-4.047101749751	2.036850016015	0.785724841446
C	-4.047613129492	-1.700110321766	-0.290509612105
C	-4.008940235287	-3.177915136661	-0.675406601369
C	-2.061078710306	-3.540933934317	0.813472064884
C	-2.531420367231	-3.589405680748	-0.628444106145
H	-4.397518574452	-3.309446389515	-1.689067415873
H	-3.286617607841	-1.194424368162	-0.897346633735
H	-4.432901976024	-1.771547600510	1.850611860983
H	-5.287112169996	-0.512155739918	-1.566682531478
H	0.611628766038	-2.136005131529	1.440409802971
H	2.523767490265	-0.342214893824	3.331974024730
H	3.902877019312	0.229975541671	2.355208234291
H	2.570748059656	1.348211516782	2.750789824230
H	2.768346147163	2.067251277921	0.374497125061
H	1.434212464865	2.202942442448	-0.804463465950
H	2.009279920239	3.649610492434	0.062483628388
H	-1.692791633662	2.265645852392	1.201968026110

H	-2.806382822838	-1.973372994338	3.703184414387
H	-1.324882860459	-2.893271456141	3.372579713042
H	-4.217119776330	-3.808851019816	2.996938302335
H	-2.890577427682	-4.717384808807	3.752355411740
H	-2.170824729719	-5.377518834997	1.783932334485
H	-3.649813891190	-5.861807319611	0.177121160505
H	-4.600630044550	-5.712838036672	1.667271818132
H	-6.458874595533	-4.394636964065	1.522282996473
H	-7.038068741001	-1.971810012489	1.307007541684
H	-7.898344875352	-2.963553857097	0.147927987907
H	-6.039465282020	-0.197479075708	1.356677239896
H	-6.222407677133	0.964260477994	0.037511038842
H	-1.004899380399	-3.799924284134	0.900950563170
H	-2.363348026005	-4.586302193870	-1.042619430642
H	-1.925587768643	-2.894941150914	-1.215478728406

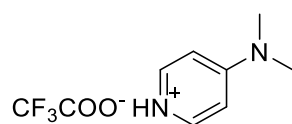
SCF Done: E(RwB97X) = -1302.98660078

Zero-point correction=	0.485910
Thermal correction to Energy=	0.508095
Thermal correction to Enthalpy=	0.509039
Thermal correction to Gibbs Free Energy=	0.436786
Sum of electronic and zero-point Energies=	-1302.500691
Sum of electronic and thermal Energies=	-1302.478506
Sum of electronic and thermal Enthalpies=	-1302.477562
Sum of electronic and thermal Free Energies=	-1302.549815

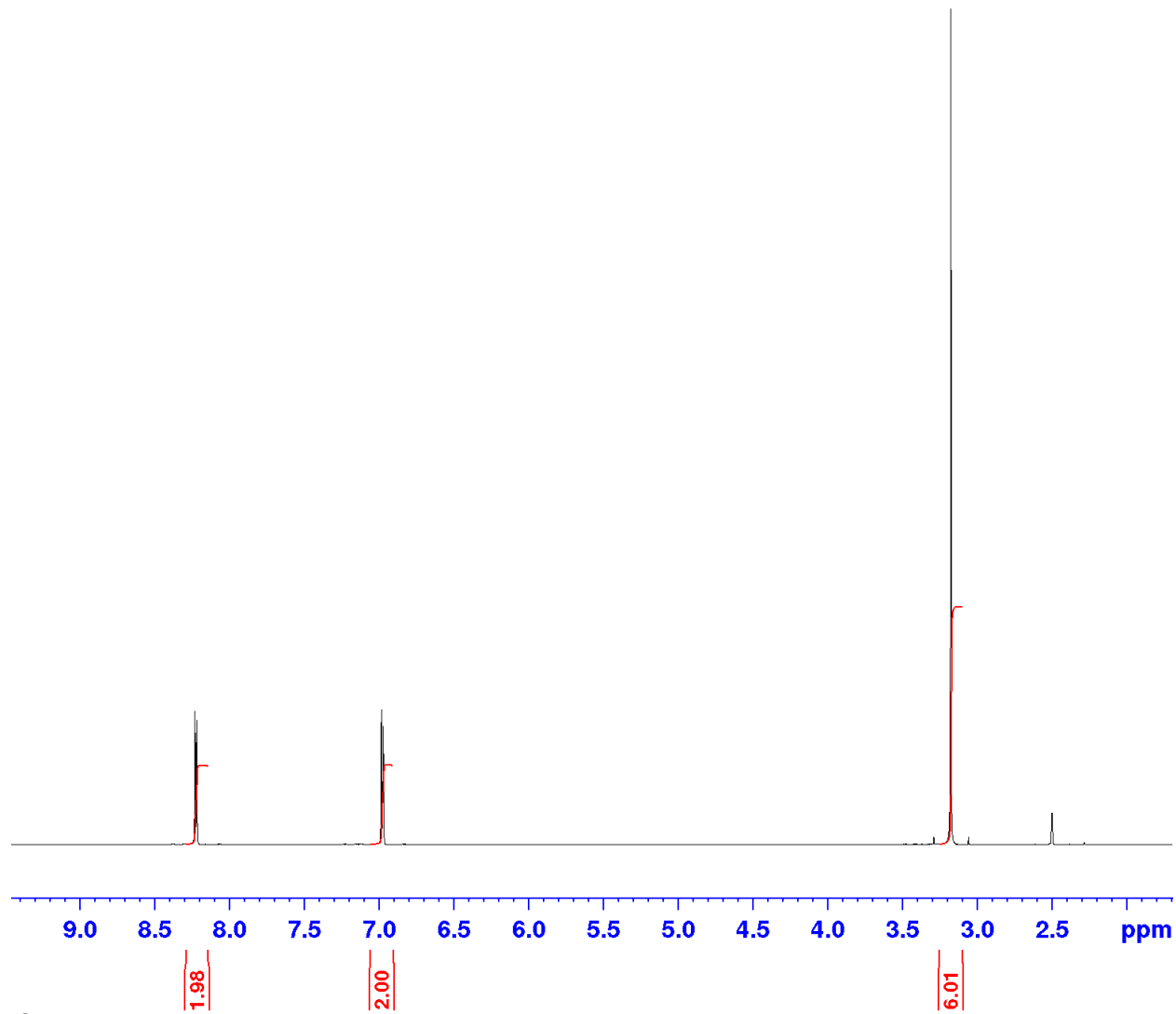
1 C	Isotropic = 126.9081	Anisotropy = 37.7539
2 N	Isotropic = 102.1805	Anisotropy = 104.3520
3 C	Isotropic = 45.0797	Anisotropy = 124.7724
4 C	Isotropic = 58.7137	Anisotropy = 133.2561
5 C	Isotropic = 65.3510	Anisotropy = 154.7256
6 C	Isotropic = 36.4486	Anisotropy = 118.0877
7 O	Isotropic = 279.5963	Anisotropy = 83.1195
8 C	Isotropic = 131.5720	Anisotropy = 89.4375
9 C	Isotropic = 30.1478	Anisotropy = 131.0047
10 O	Isotropic = 266.6894	Anisotropy = 101.6812
11 C	Isotropic = 131.9967	Anisotropy = 89.5997
12 C	Isotropic = 75.9965	Anisotropy = 131.3720
13 C	Isotropic = 137.3455	Anisotropy = 24.4898
14 C	Isotropic = 150.2810	Anisotropy = 41.1977
15 C	Isotropic = 138.3563	Anisotropy = 62.8778
16 N	Isotropic = 185.5423	Anisotropy = 38.1353
17 C	Isotropic = 134.1364	Anisotropy = 30.5123
18 C	Isotropic = 57.5430	Anisotropy = 152.4937
19 C	Isotropic = 44.4511	Anisotropy = 140.6008

20	C	Isotropic = 126.7483	Anisotropy = 55.0851
21	O	Isotropic = 289.2136	Anisotropy = 57.7475
22	C	Isotropic = 117.9806	Anisotropy = 54.9569
23	C	Isotropic = 154.9513	Anisotropy = 45.6928
24	C	Isotropic = 10.1246	Anisotropy = 121.0030
25	O	Isotropic = -79.0412	Anisotropy = 603.8444
26	C	Isotropic = 139.8204	Anisotropy = 32.5853
27	C	Isotropic = 160.6290	Anisotropy = 9.9344
28	C	Isotropic = 125.2865	Anisotropy = 46.6261
29	C	Isotropic = 164.4473	Anisotropy = 14.3427
30	H	Isotropic = 28.6055	Anisotropy = 9.8878
31	H	Isotropic = 30.3197	Anisotropy = 3.3696
32	H	Isotropic = 27.8474	Anisotropy = 2.7193
33	H	Isotropic = 27.5176	Anisotropy = 6.8503
34	H	Isotropic = 24.3756	Anisotropy = 11.0949
35	H	Isotropic = 28.4094	Anisotropy = 8.5972
36	H	Isotropic = 27.9969	Anisotropy = 10.0181
37	H	Isotropic = 27.7380	Anisotropy = 8.3197
38	H	Isotropic = 27.1228	Anisotropy = 7.6024
39	H	Isotropic = 28.4979	Anisotropy = 8.7333
40	H	Isotropic = 27.8329	Anisotropy = 9.8975
41	H	Isotropic = 23.8182	Anisotropy = 10.2253
42	H	Isotropic = 29.7666	Anisotropy = 7.7140
43	H	Isotropic = 29.9300	Anisotropy = 9.2997
44	H	Isotropic = 28.4122	Anisotropy = 6.3378
45	H	Isotropic = 28.1711	Anisotropy = 11.5890
46	H	Isotropic = 25.8940	Anisotropy = 16.9169
47	H	Isotropic = 27.6358	Anisotropy = 9.9955
48	H	Isotropic = 28.5181	Anisotropy = 9.6409
49	H	Isotropic = 25.5053	Anisotropy = 5.7718
50	H	Isotropic = 27.0842	Anisotropy = 6.1907
51	H	Isotropic = 27.4780	Anisotropy = 10.2869
52	H	Isotropic = 28.4471	Anisotropy = 4.6355
53	H	Isotropic = 29.4751	Anisotropy = 9.8835
54	H	Isotropic = 27.4949	Anisotropy = 9.0576
55	H	Isotropic = 29.4998	Anisotropy = 11.5140
56	H	Isotropic = 30.2652	Anisotropy = 8.2074

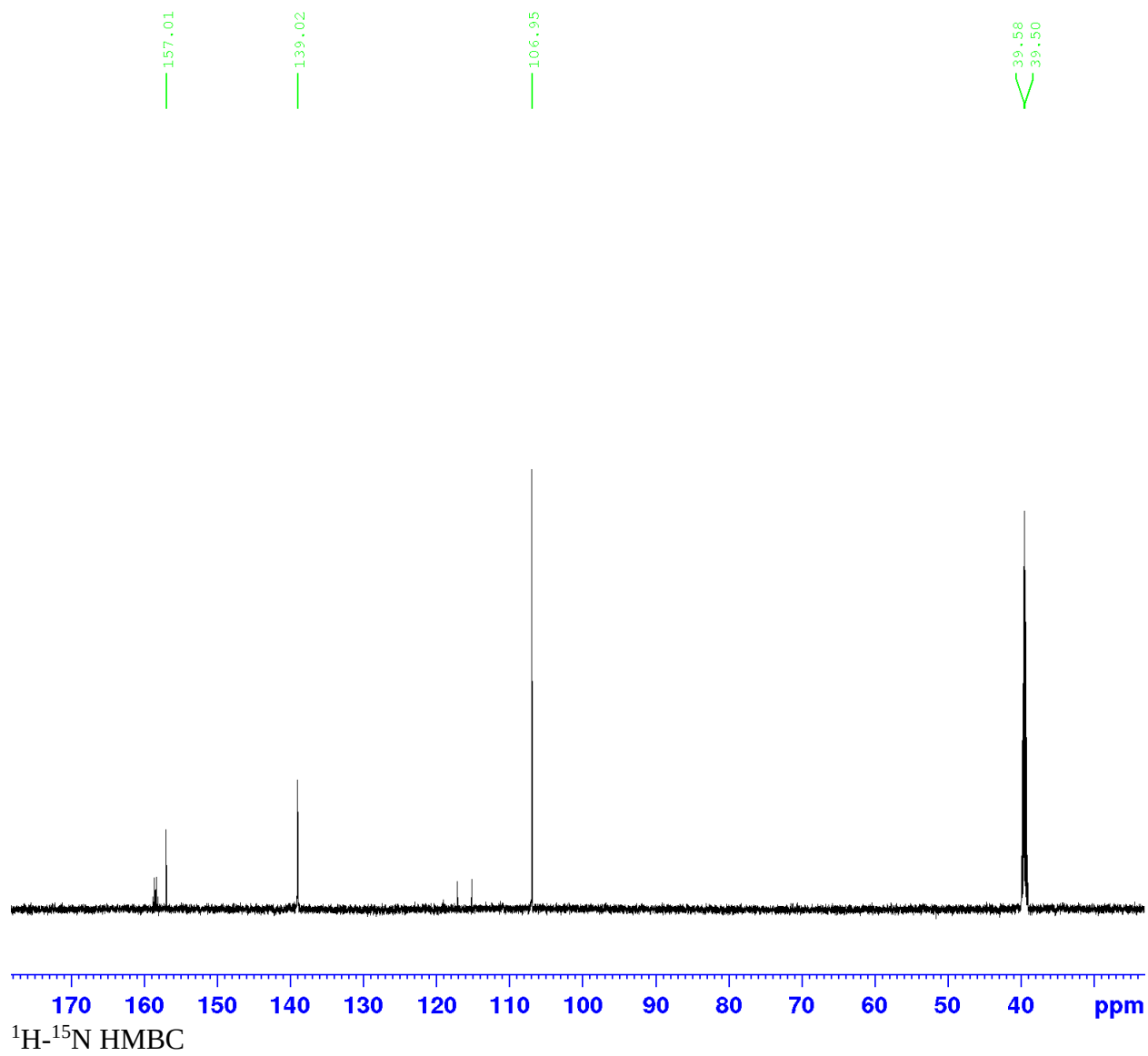
8. NMR Spectra of Protonated Model Compounds

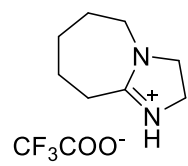
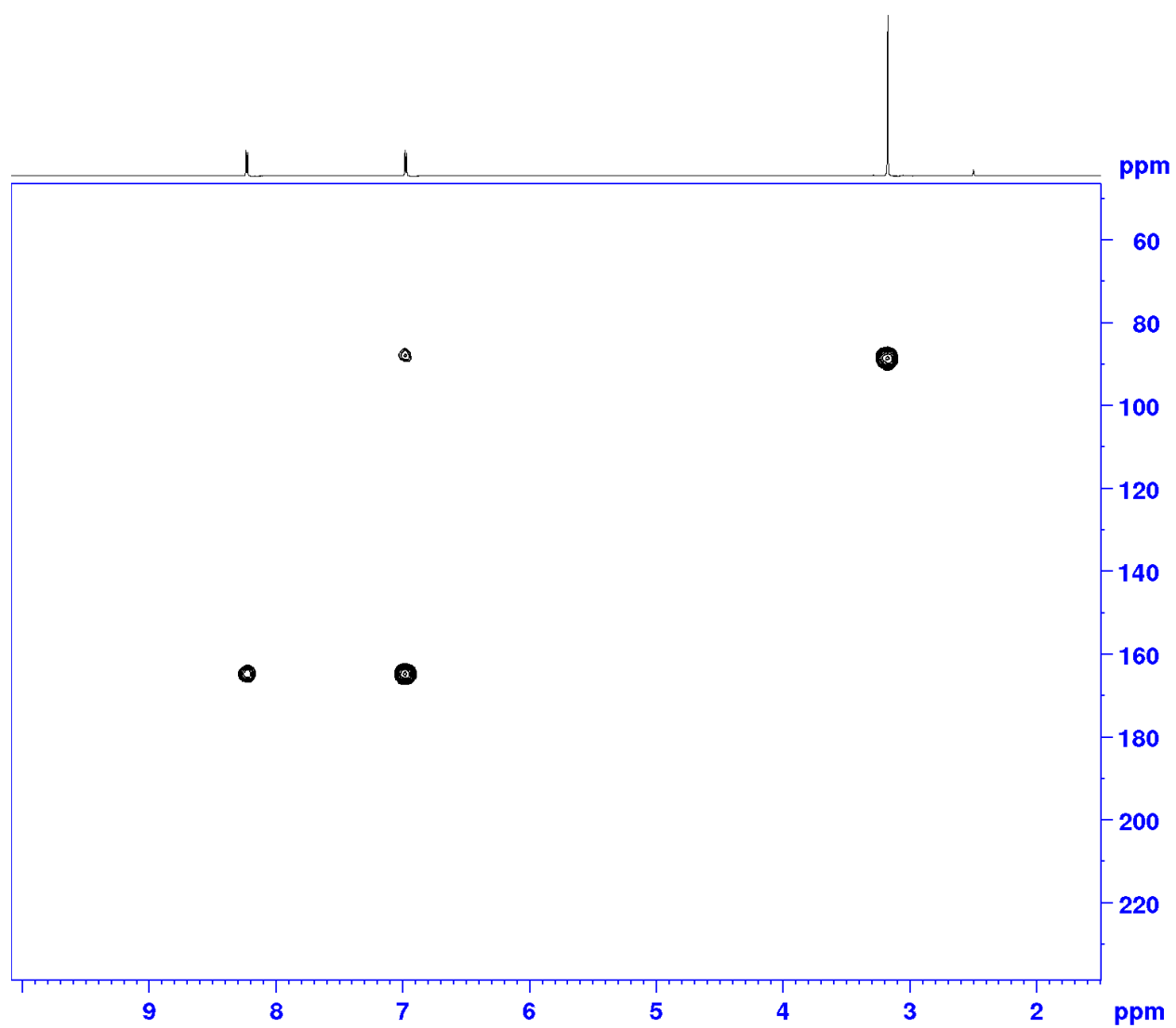


^1H spectrum

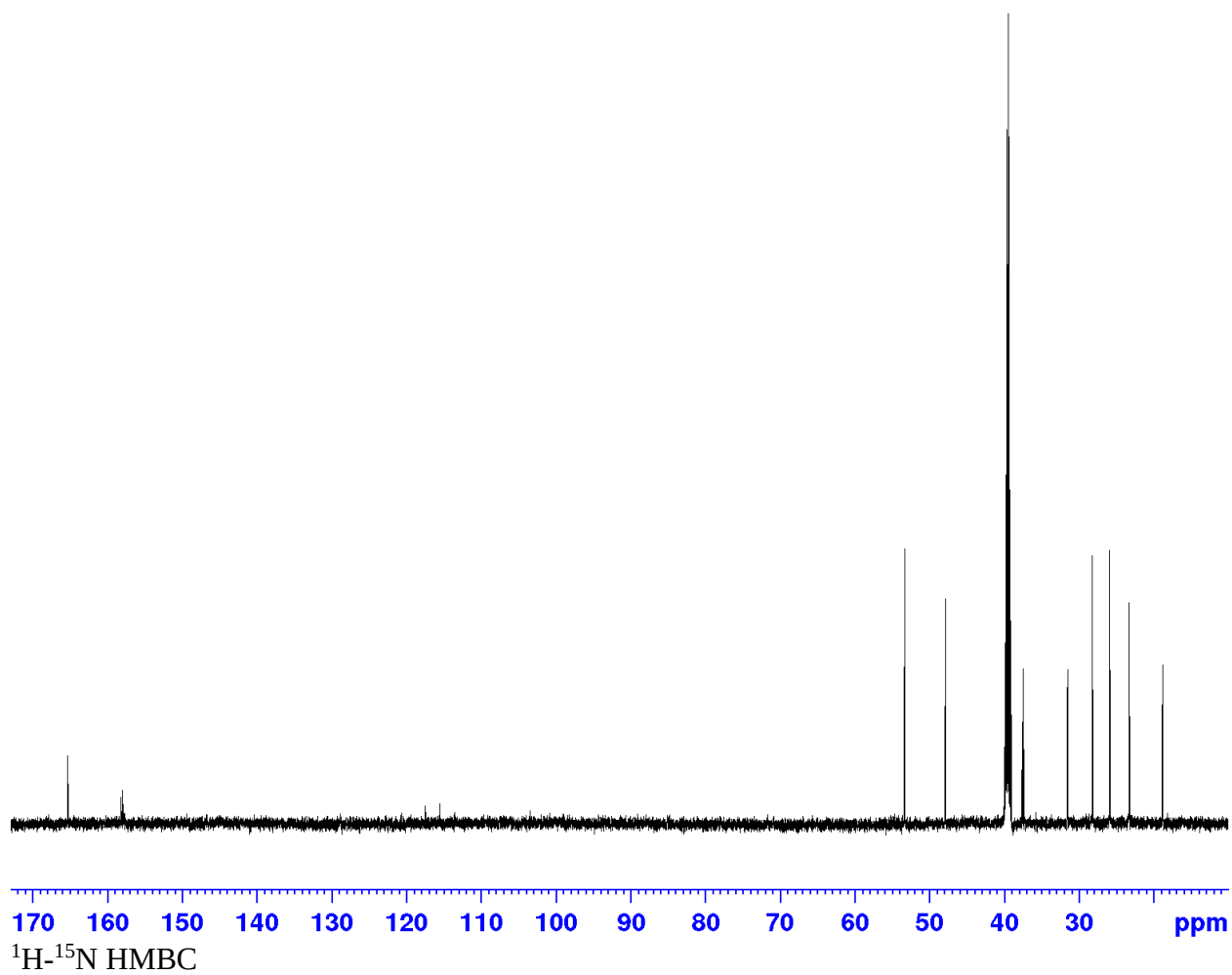
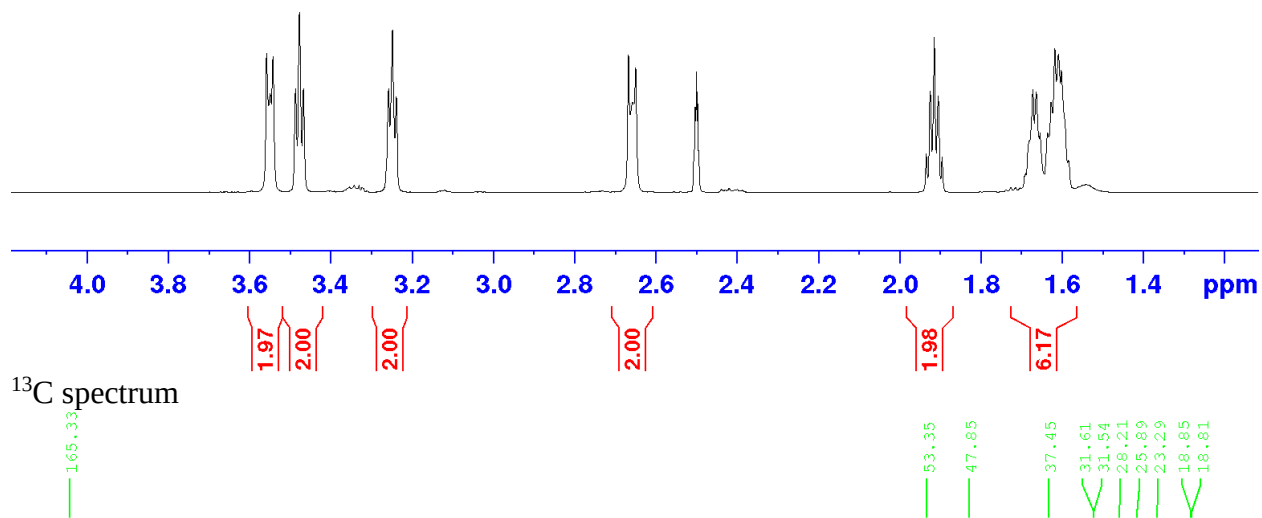


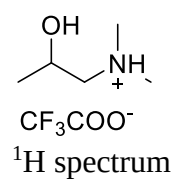
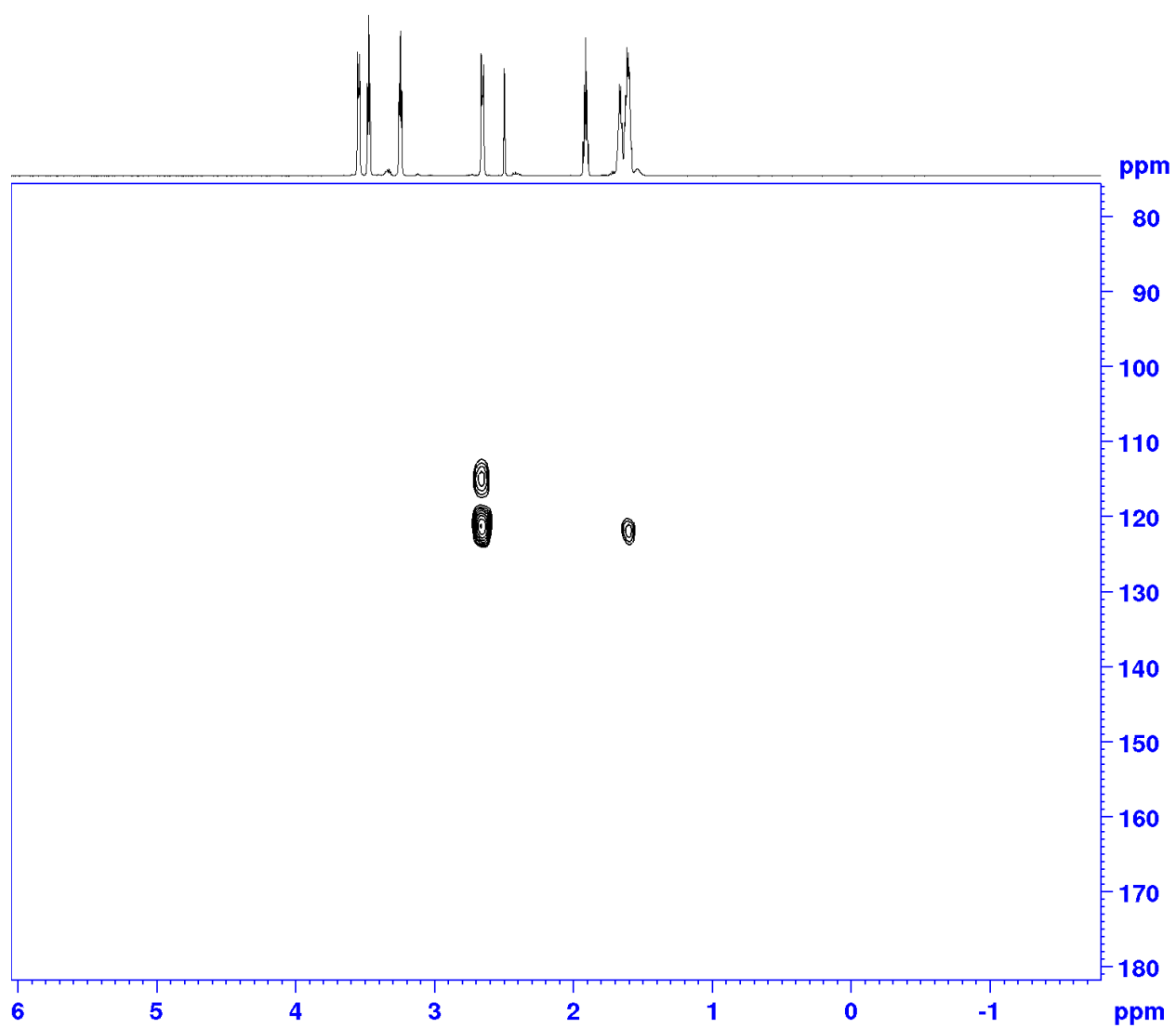
^{13}C spectrum

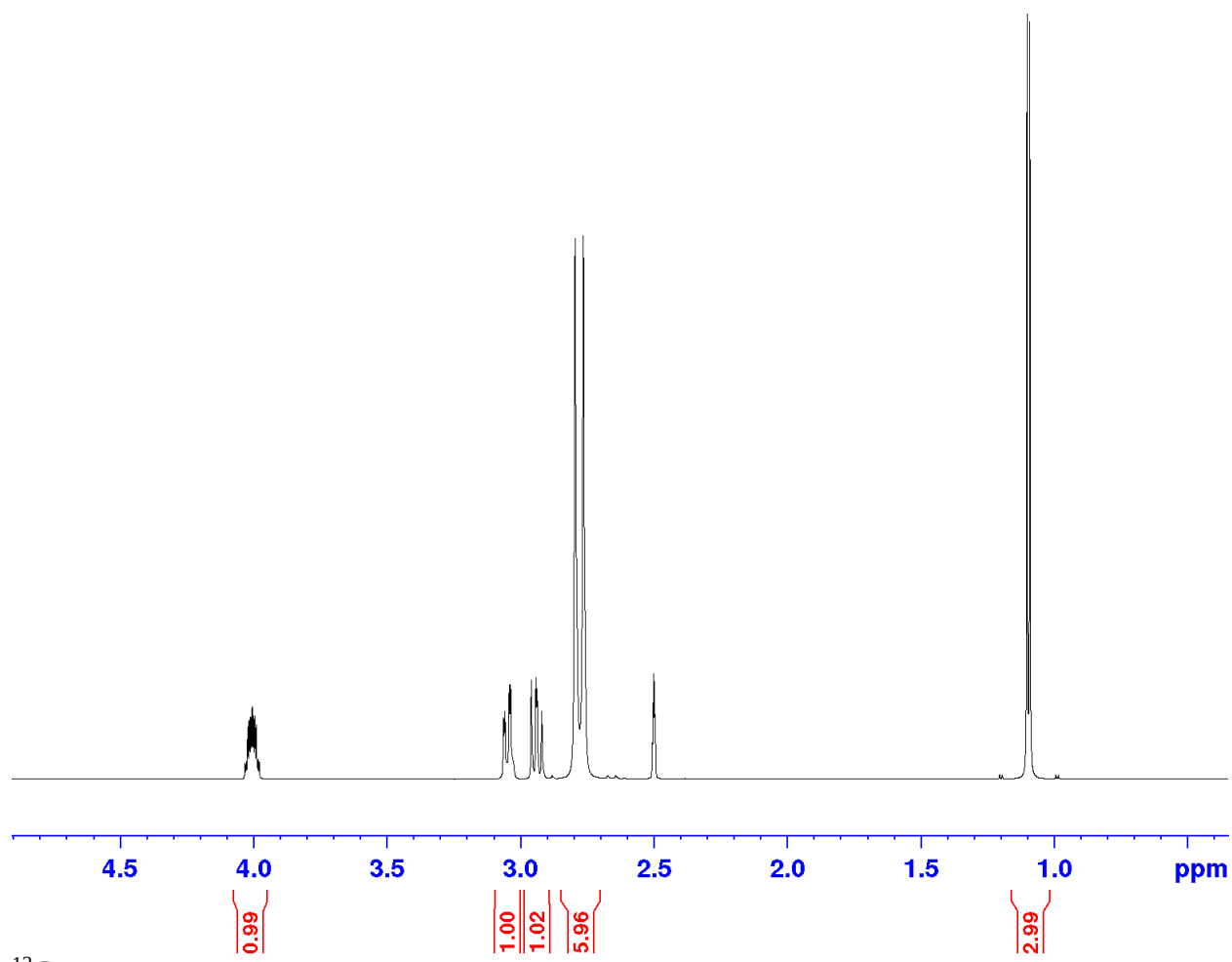




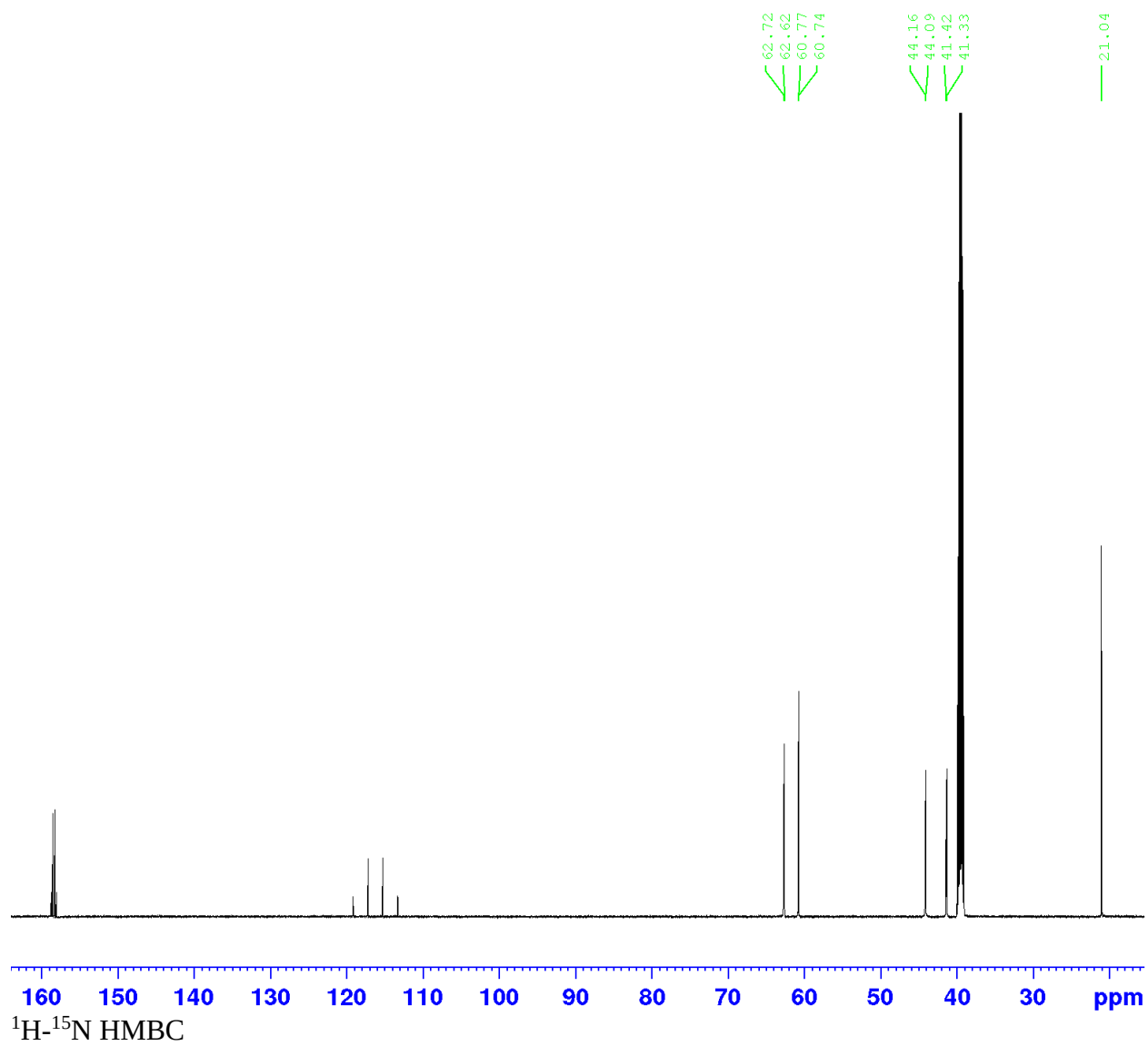
^1H spectrum

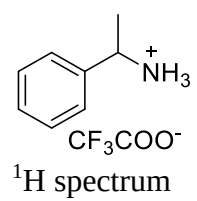
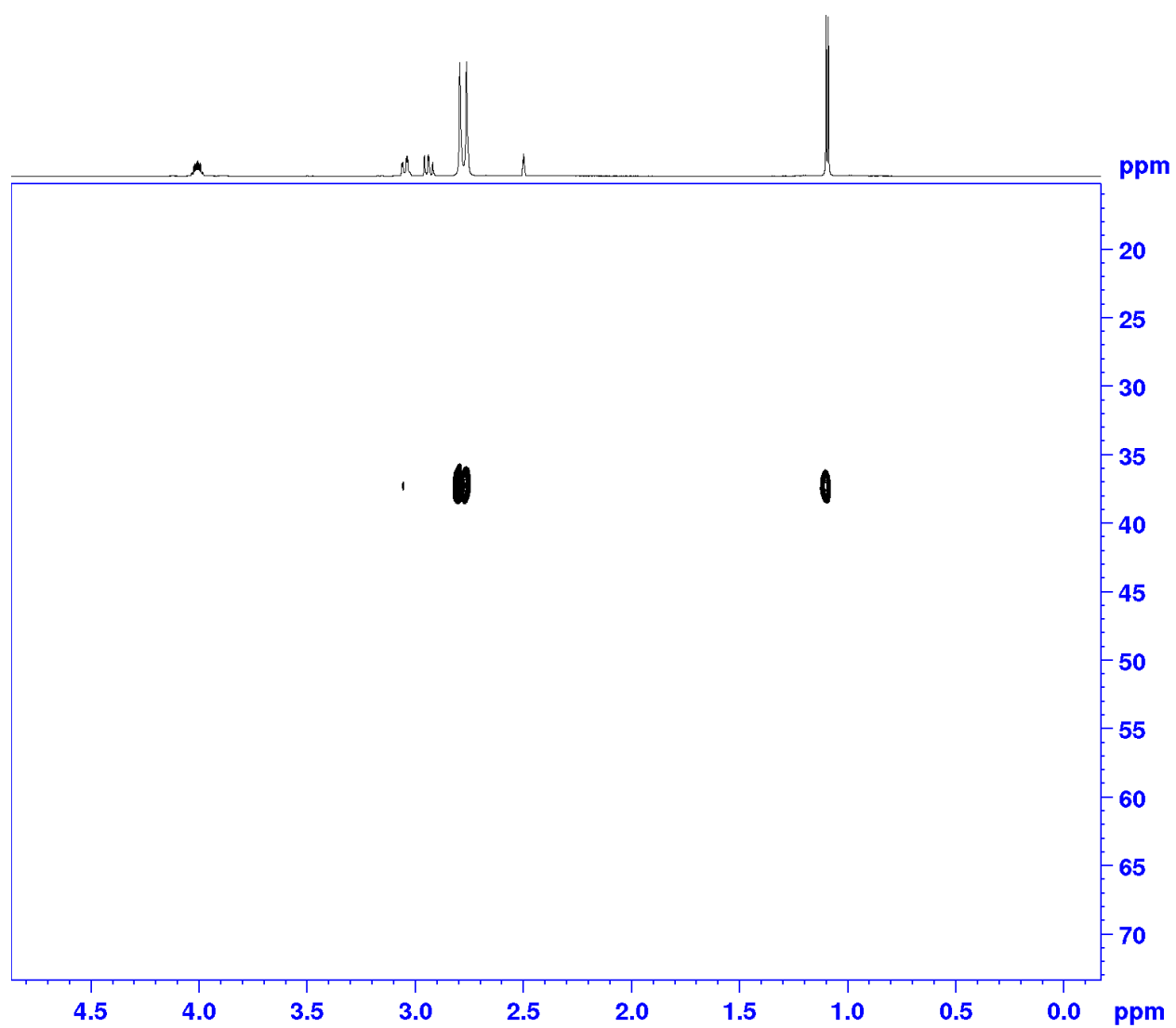


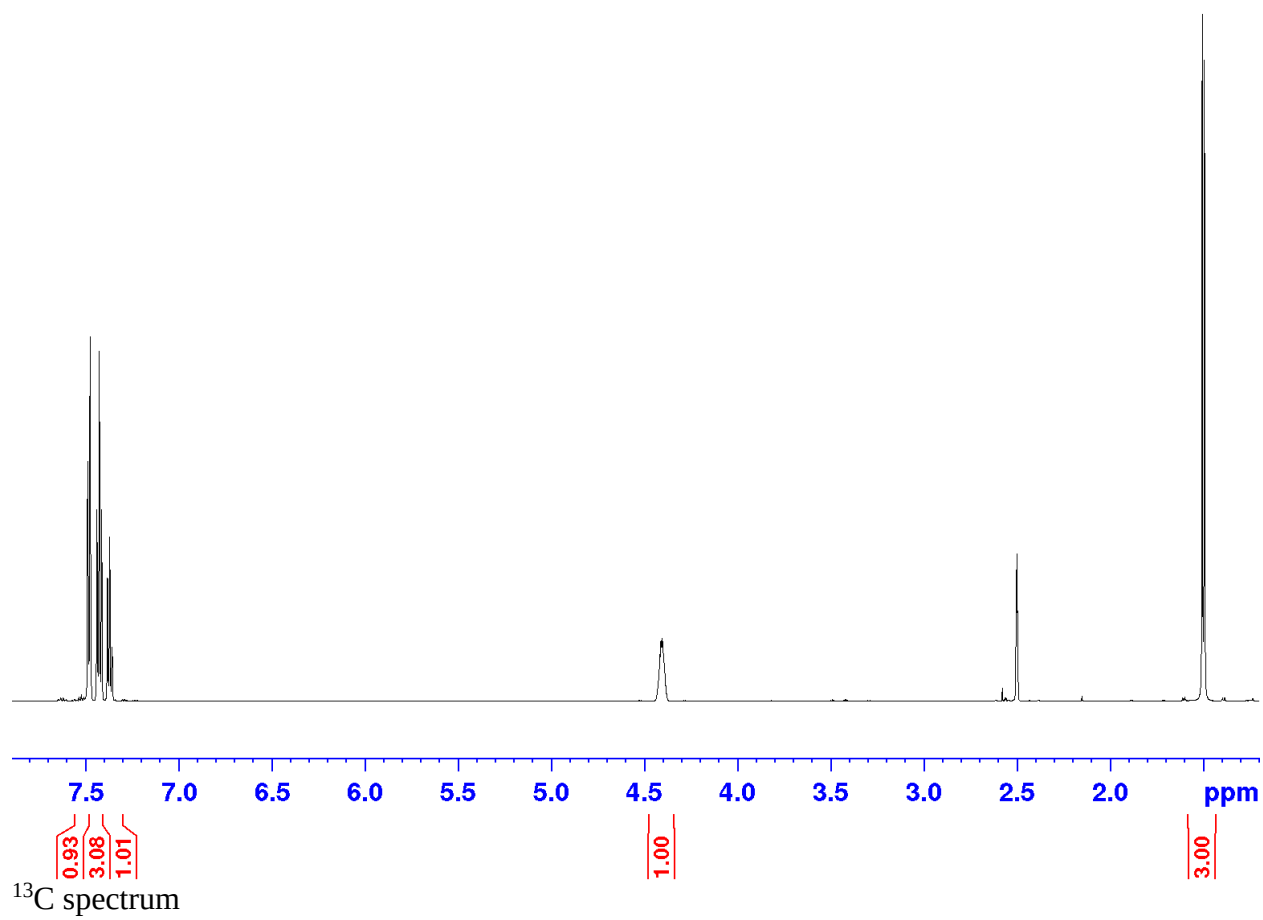


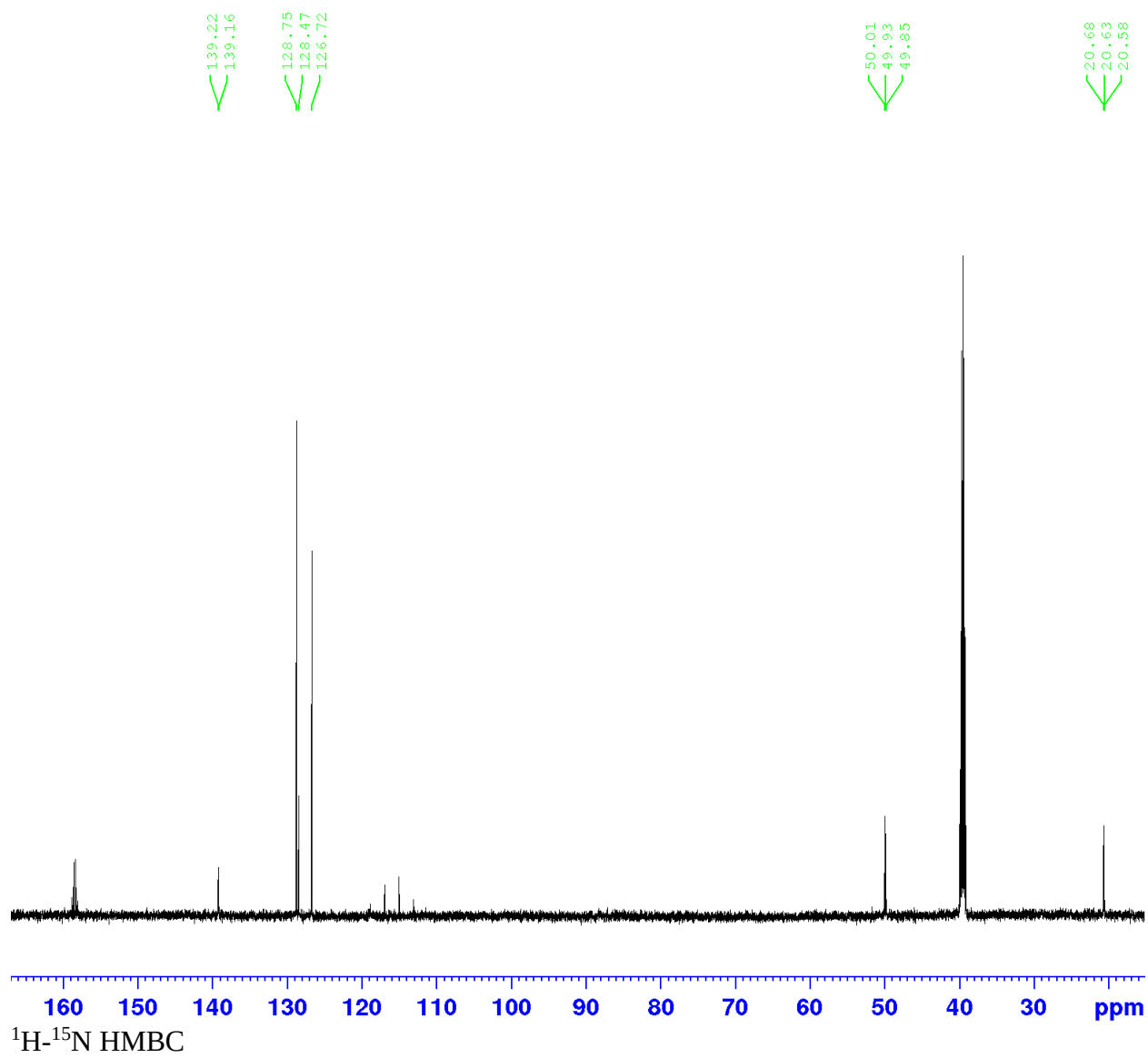


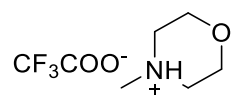
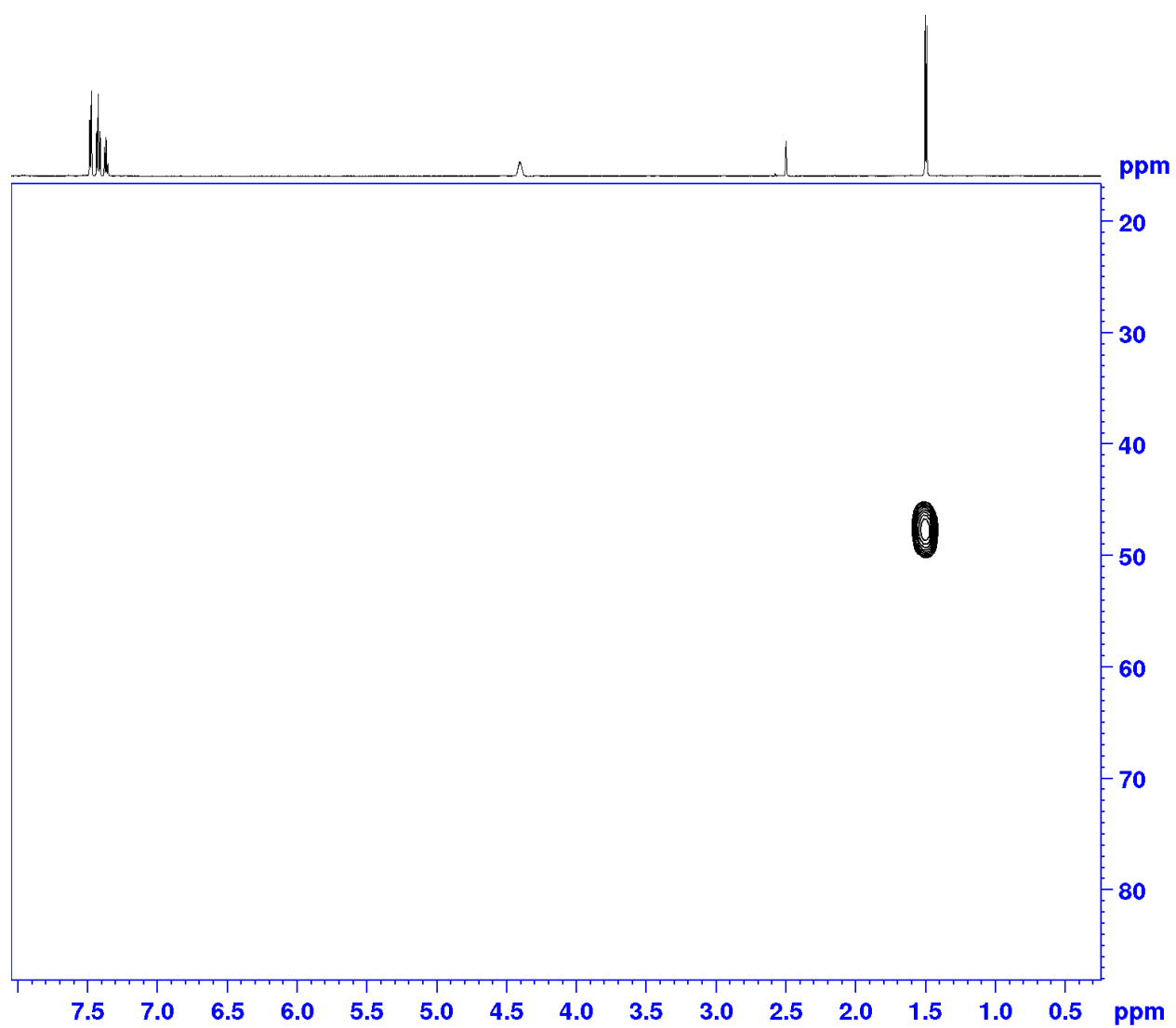
^{13}C spectrum



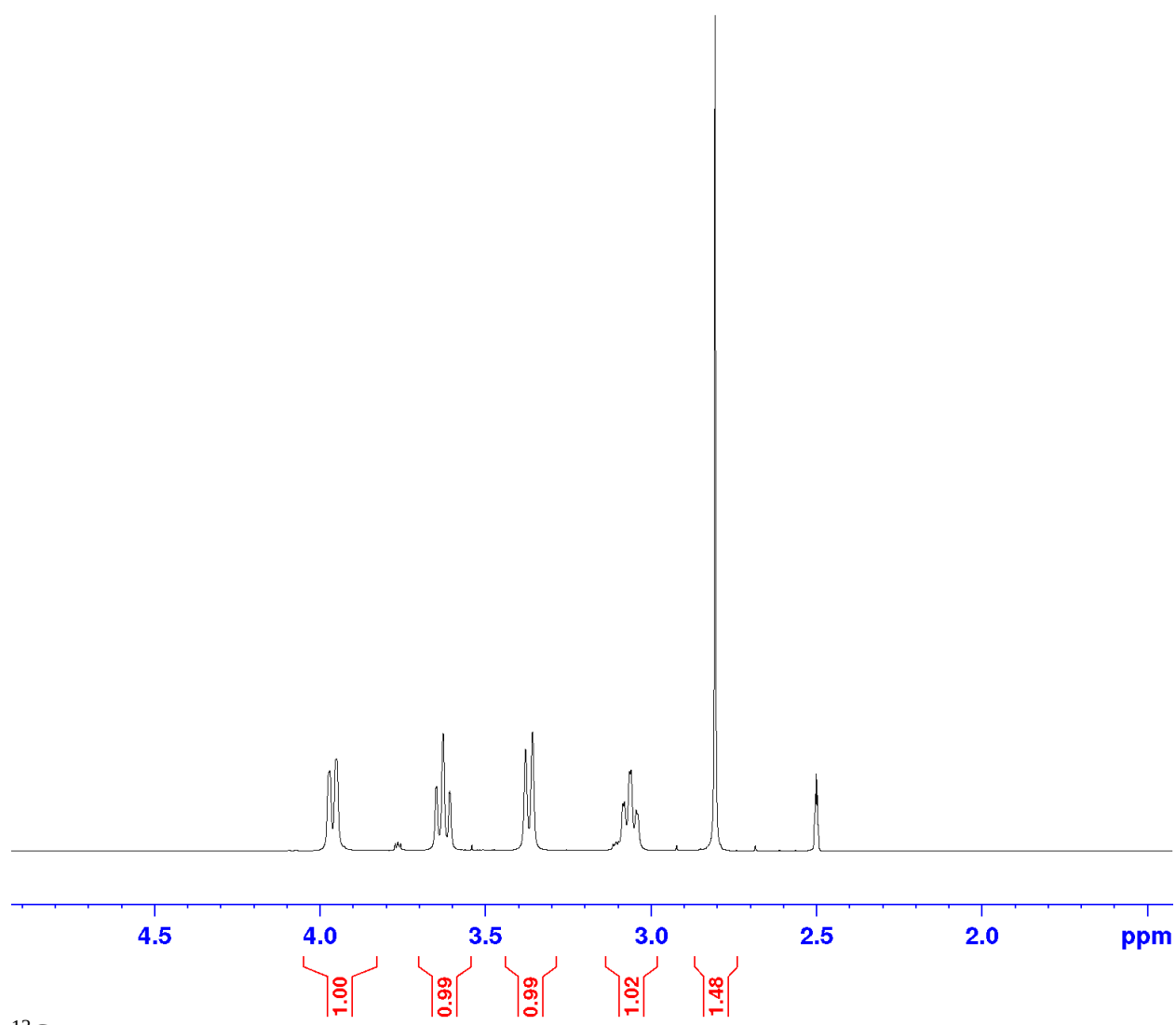




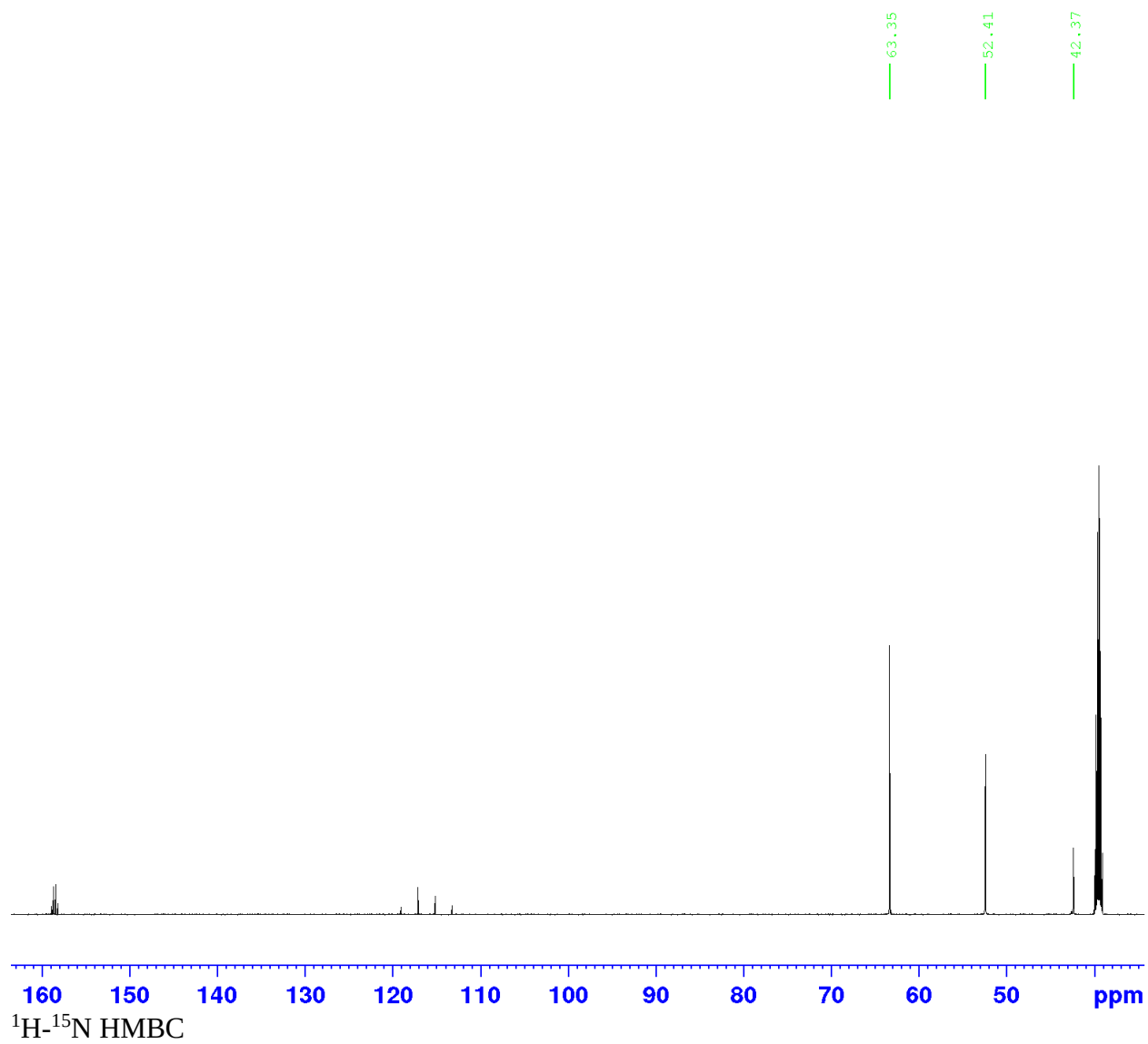


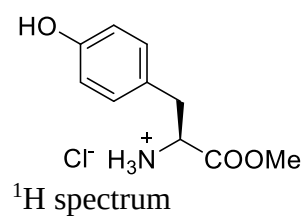
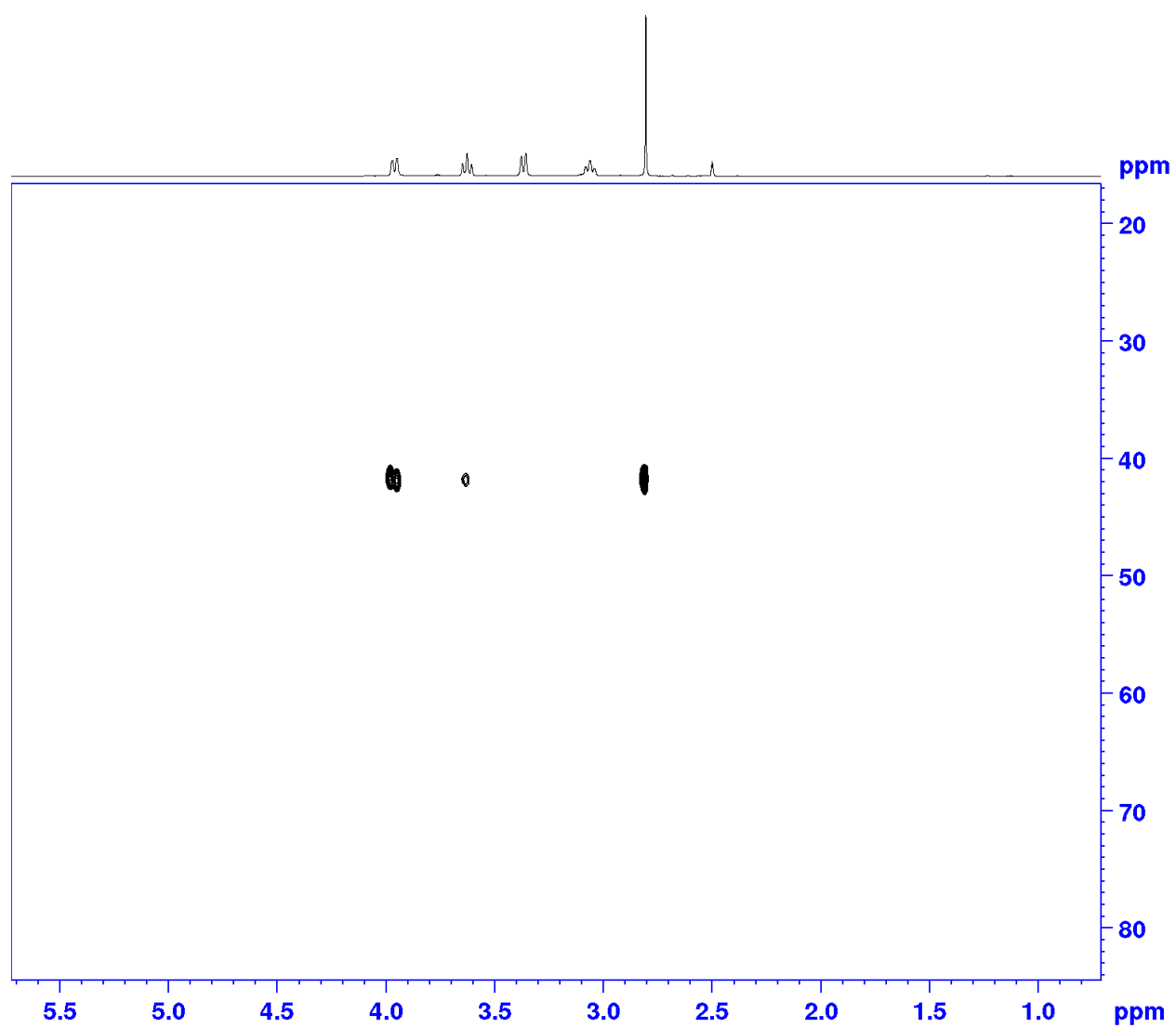


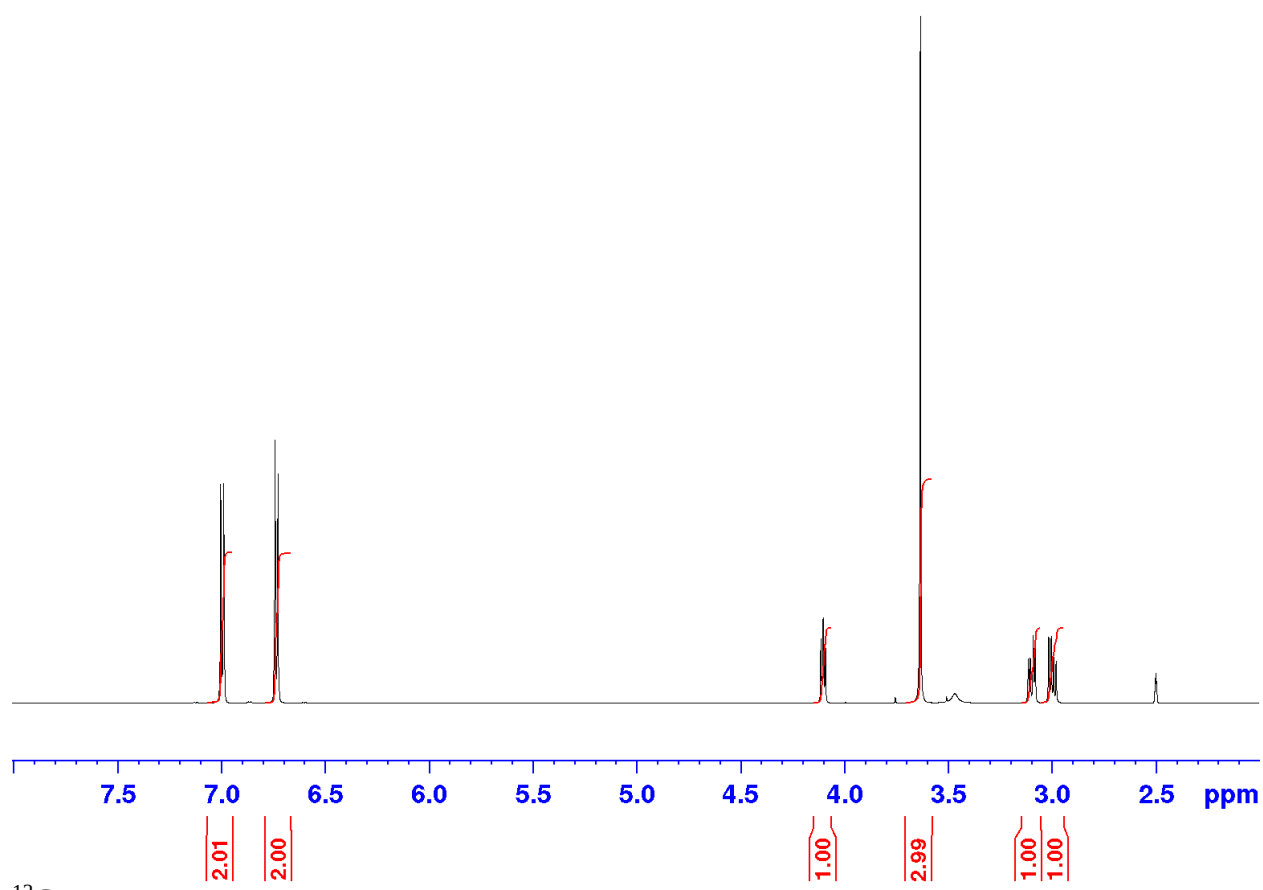
^1H spectrum



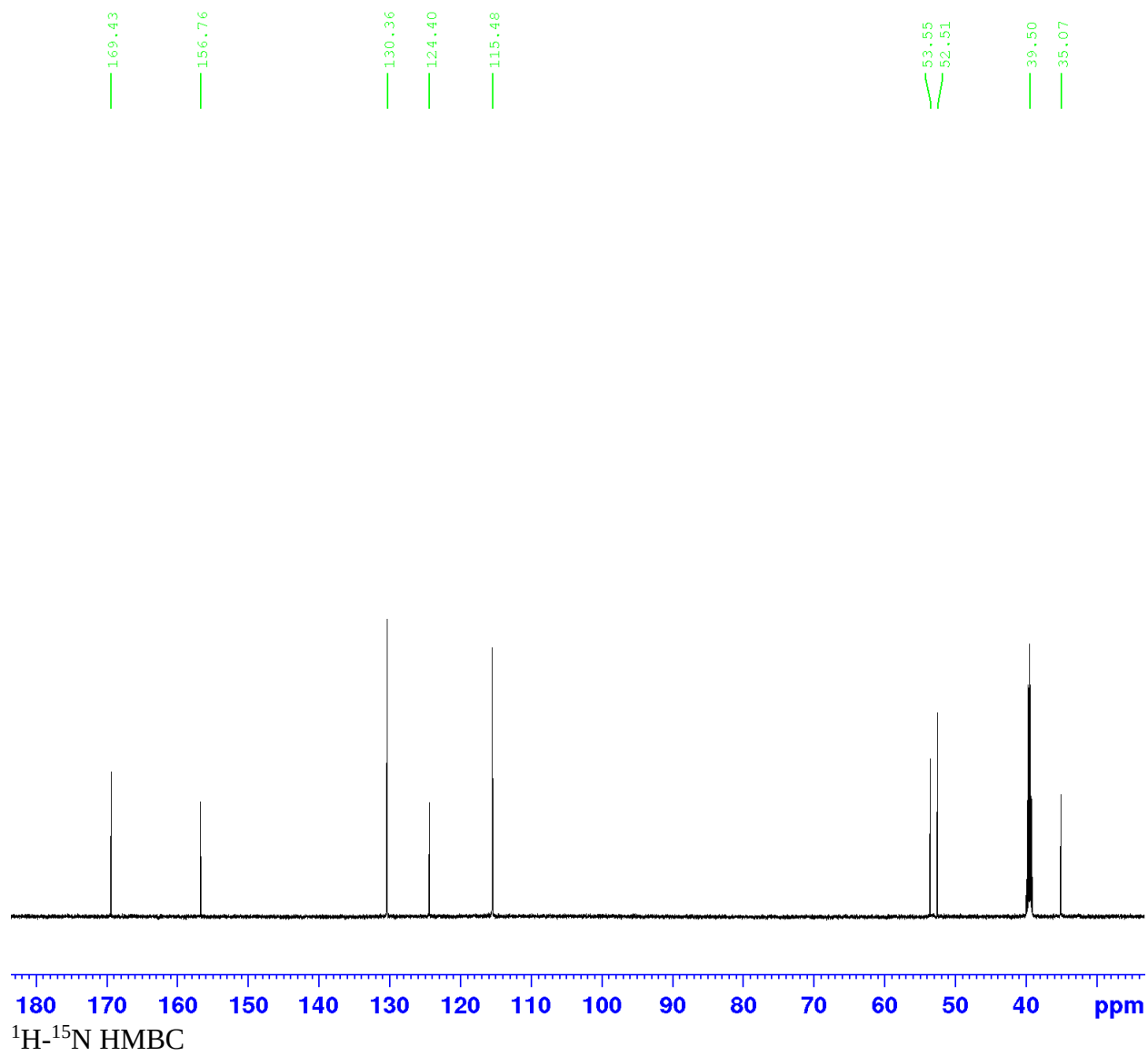
^{13}C spectrum

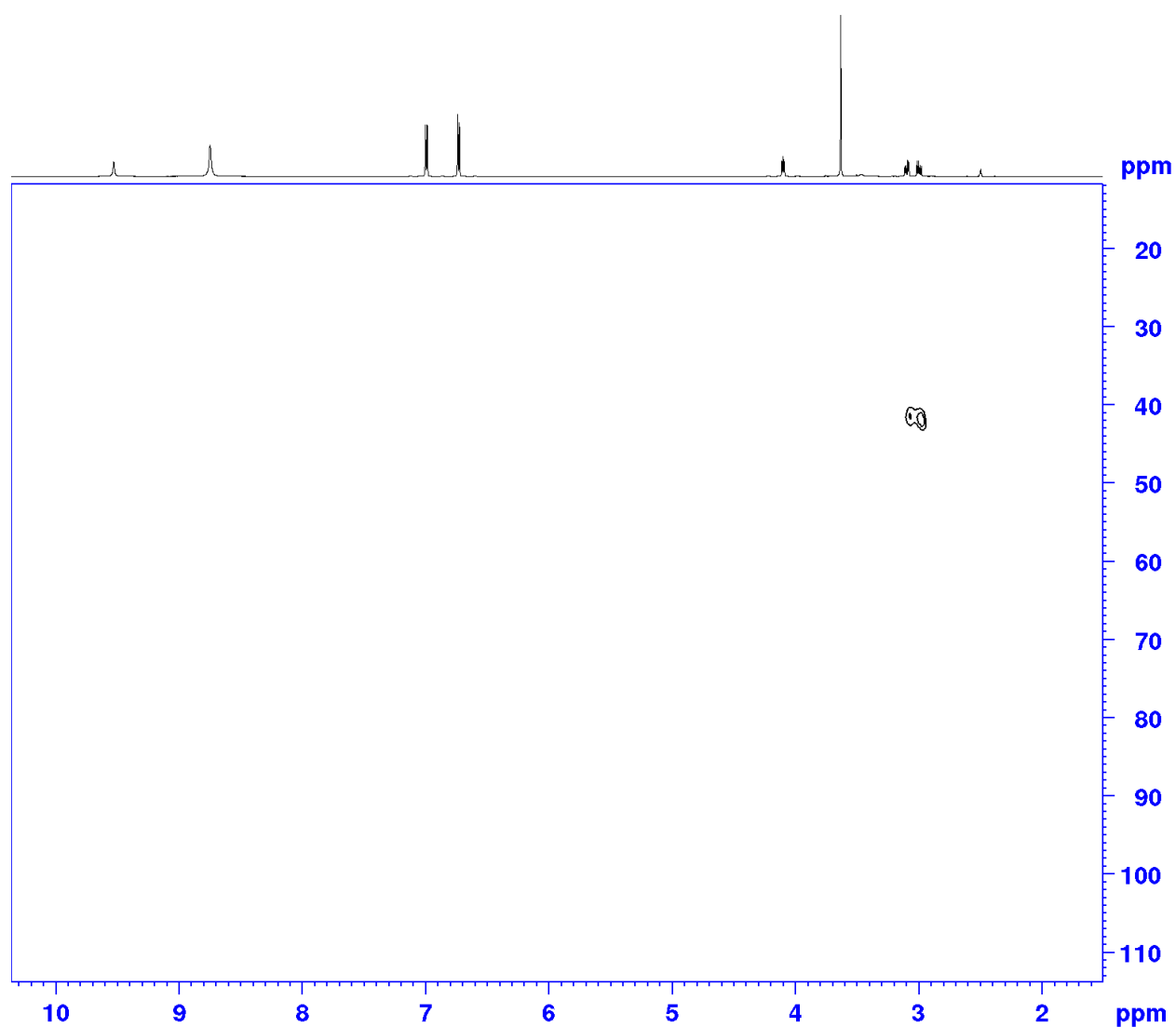






^{13}C spectrum



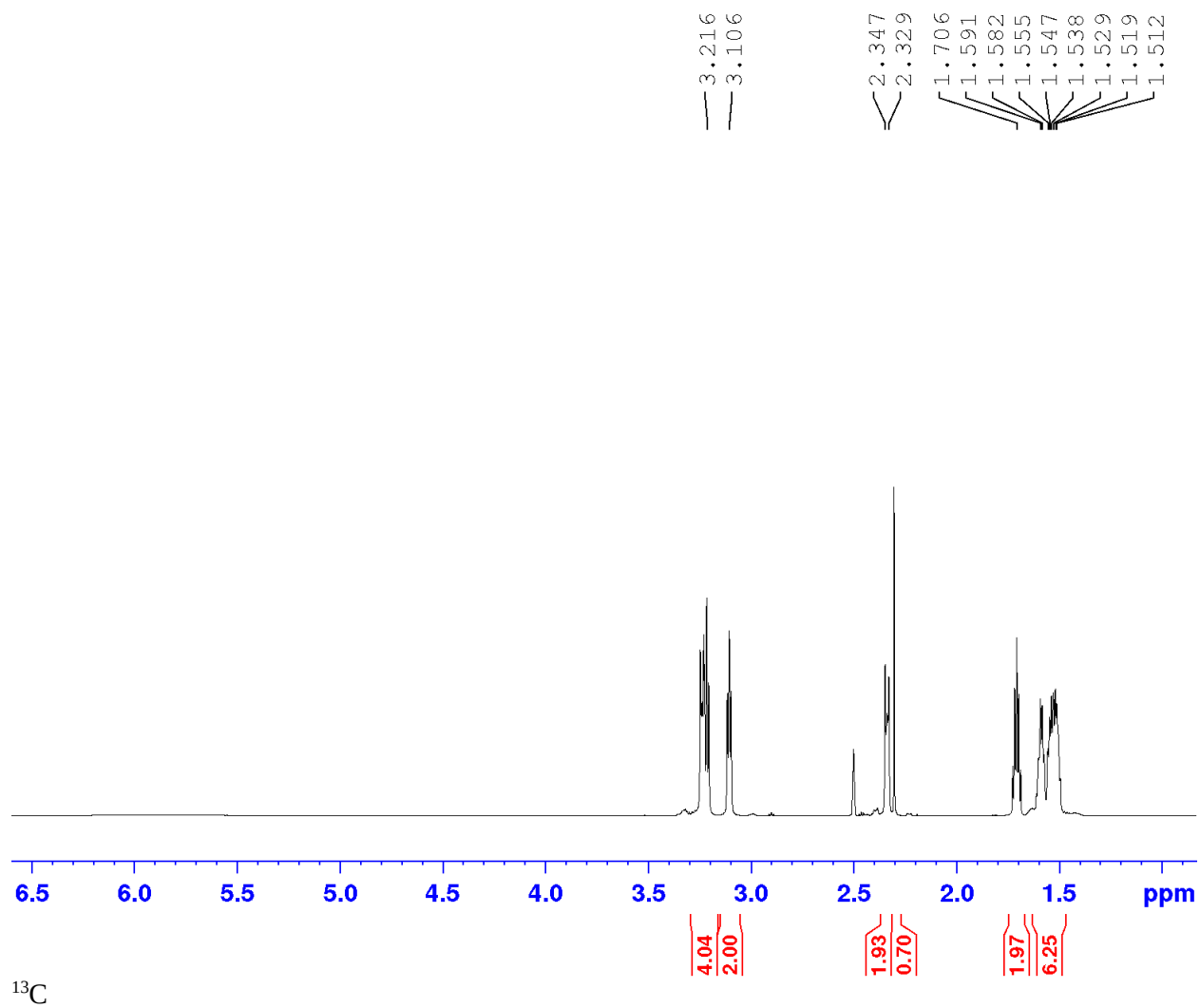


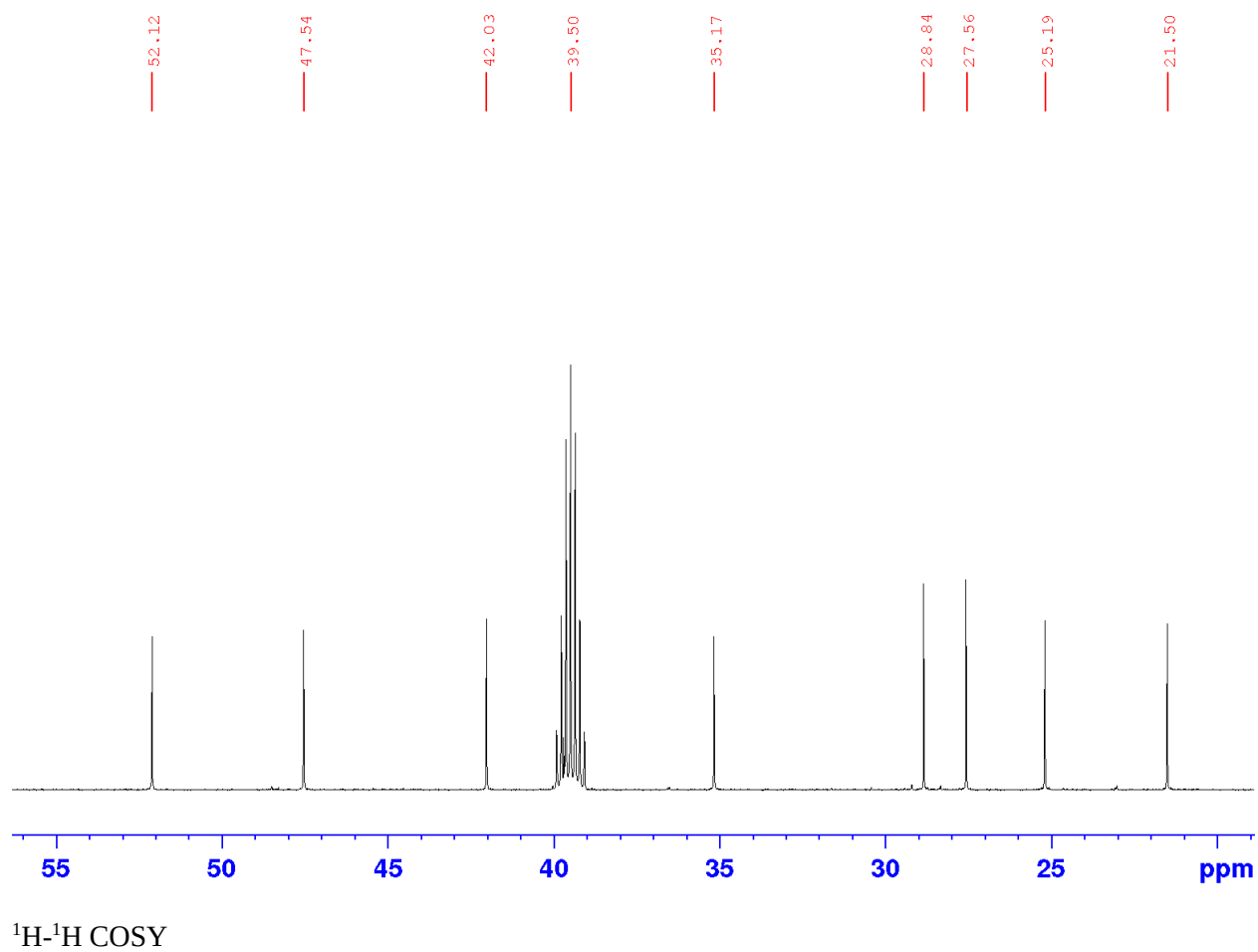
9. NMR Spectra of Partial Salt Samples

MsOH was added to free base solution to generate partial salt samples. Experimental partial salt ratios were determined by comparing ^1H integration of MsOH –Me peak (~ 2.35 ppm) with peaks of partial salt.

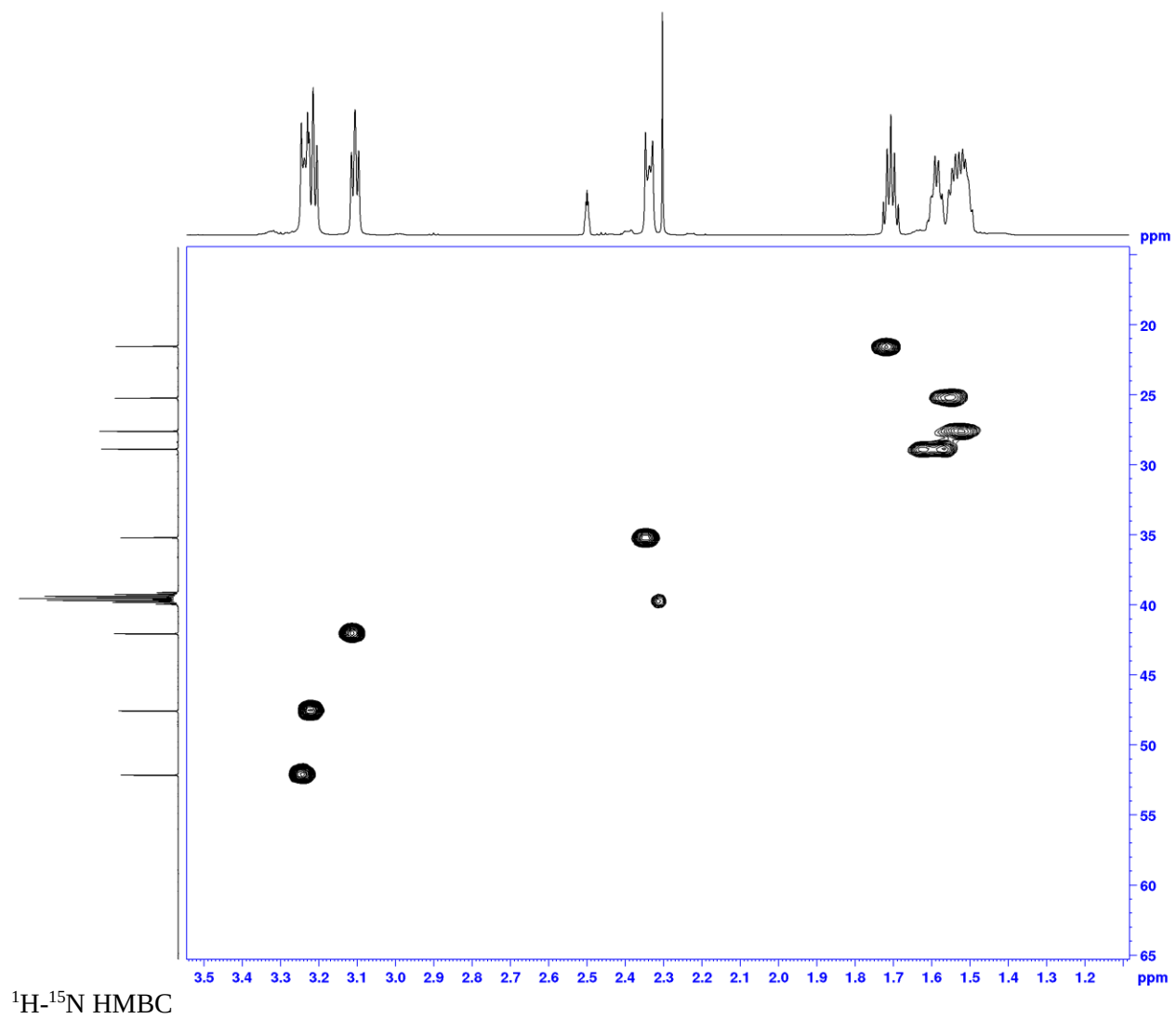
2,3,4,6,7,8,9,10-octahydropyrimido[1,2-a]azepine (2)

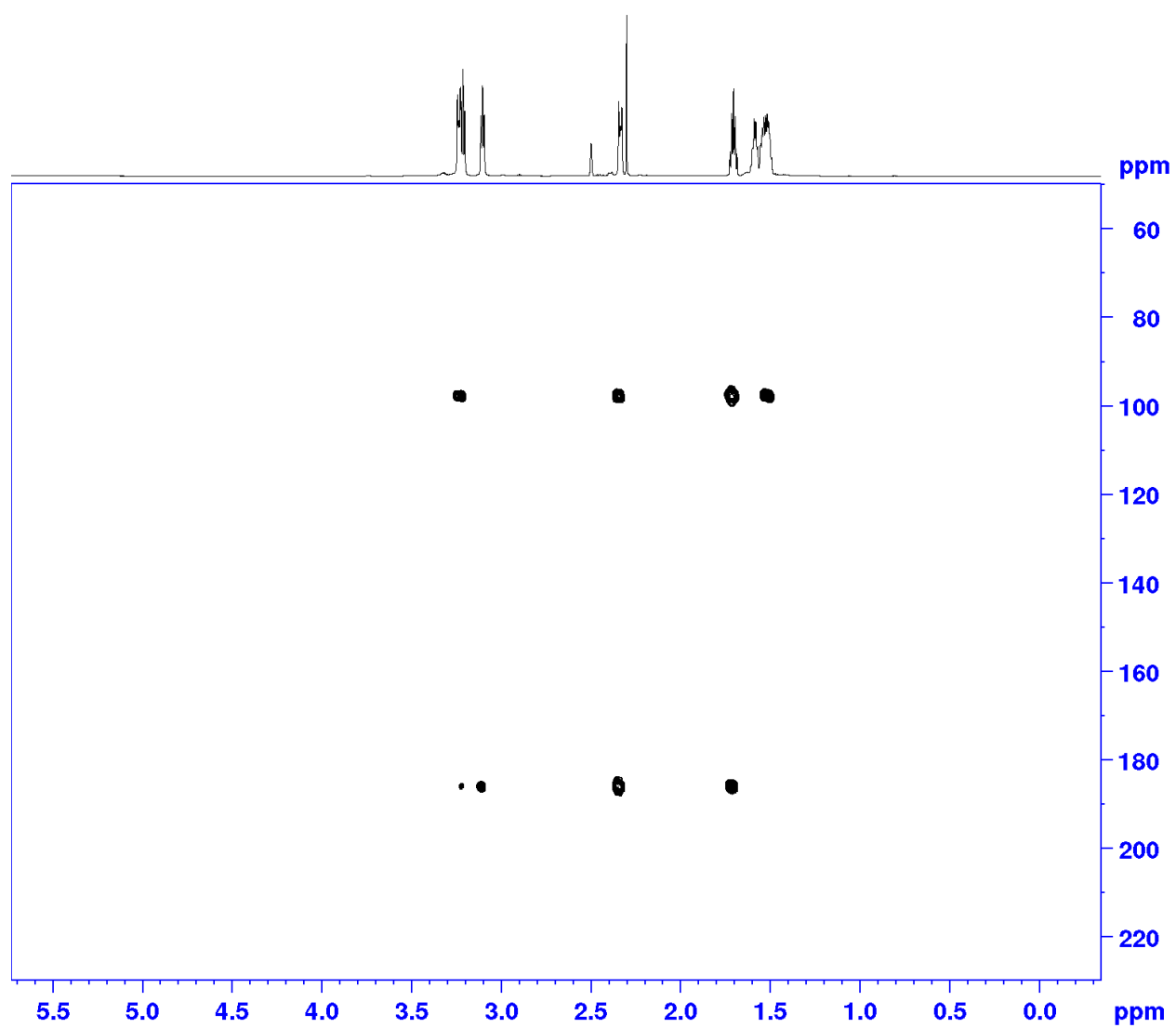
^1H





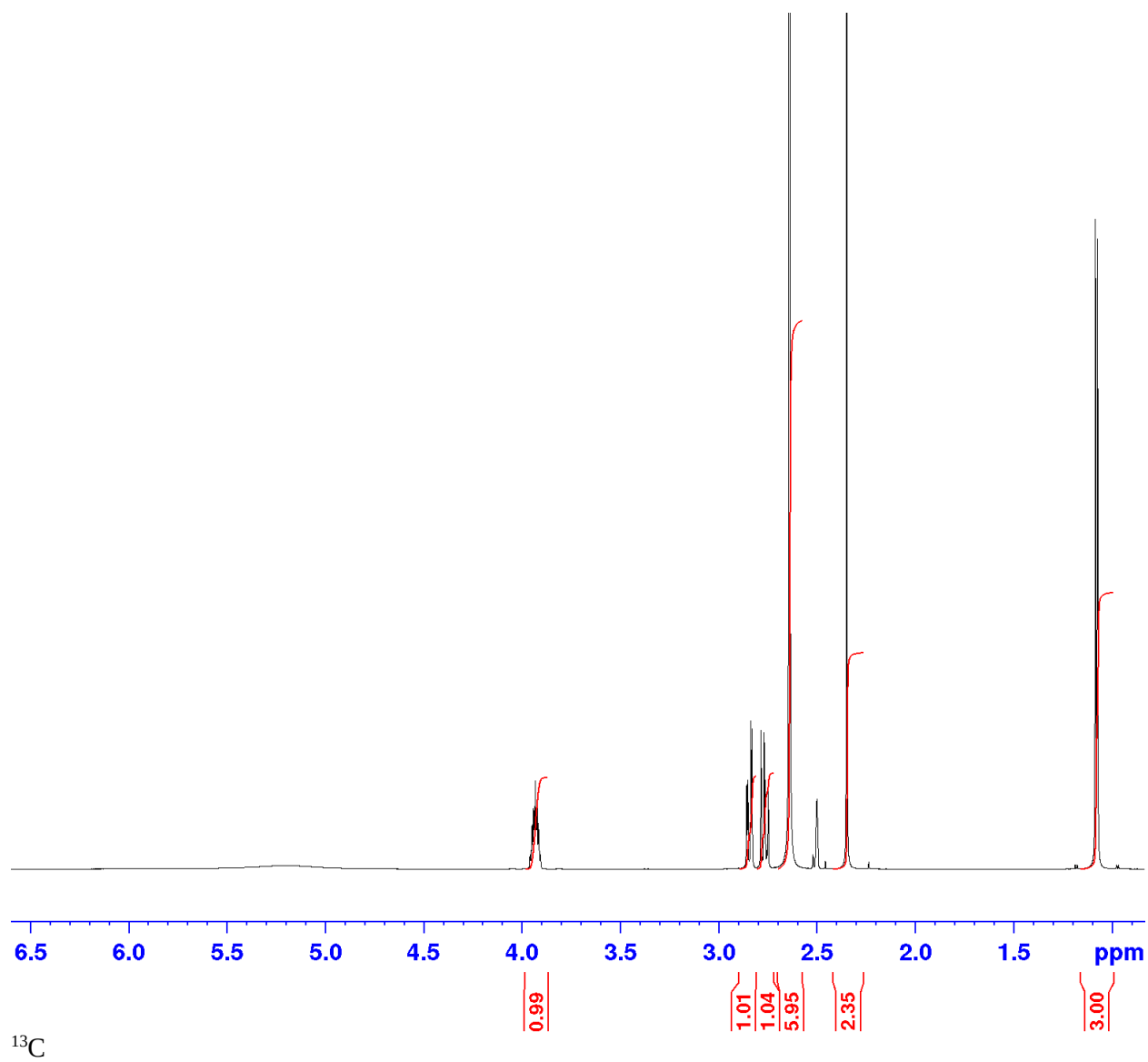


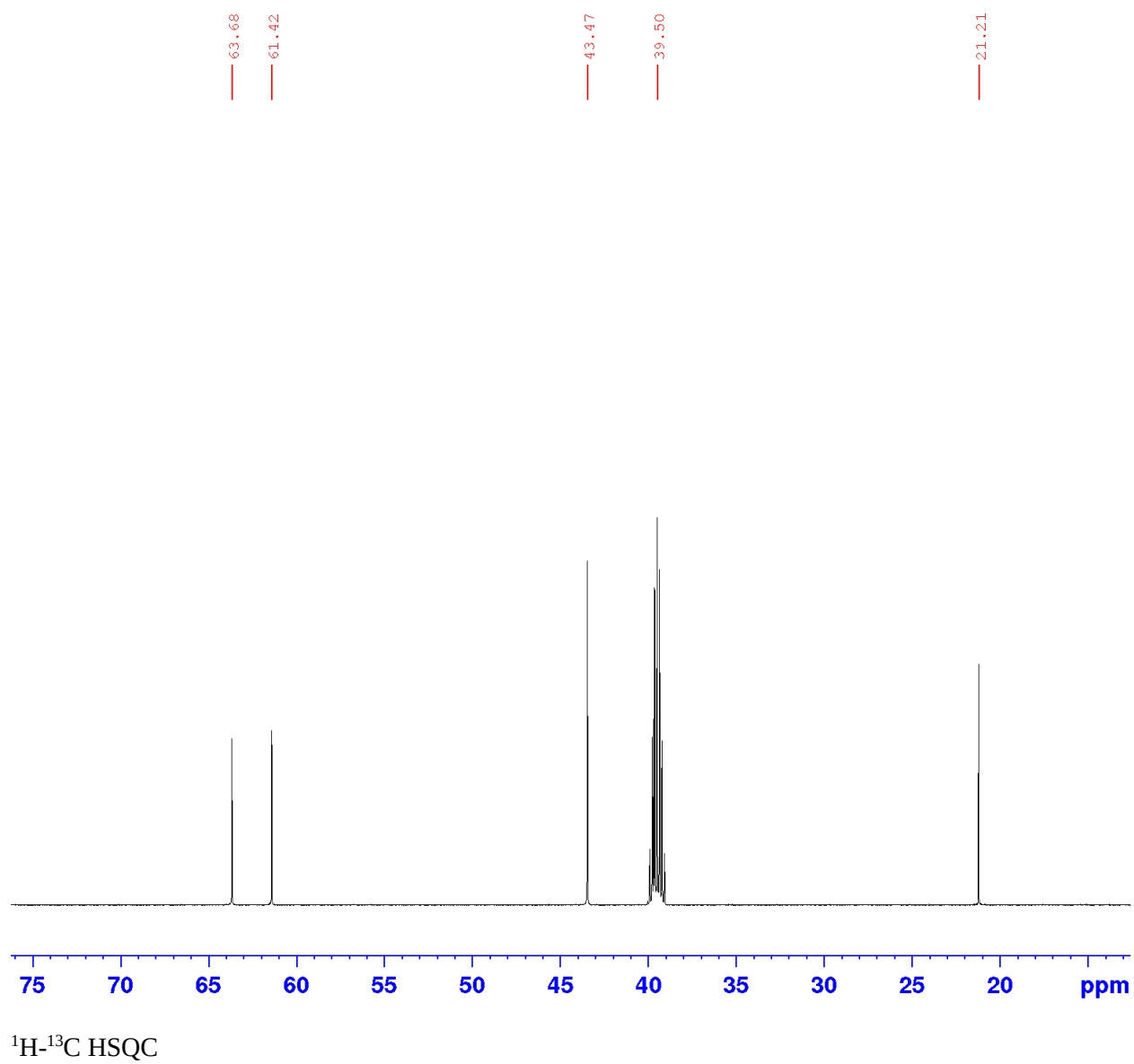


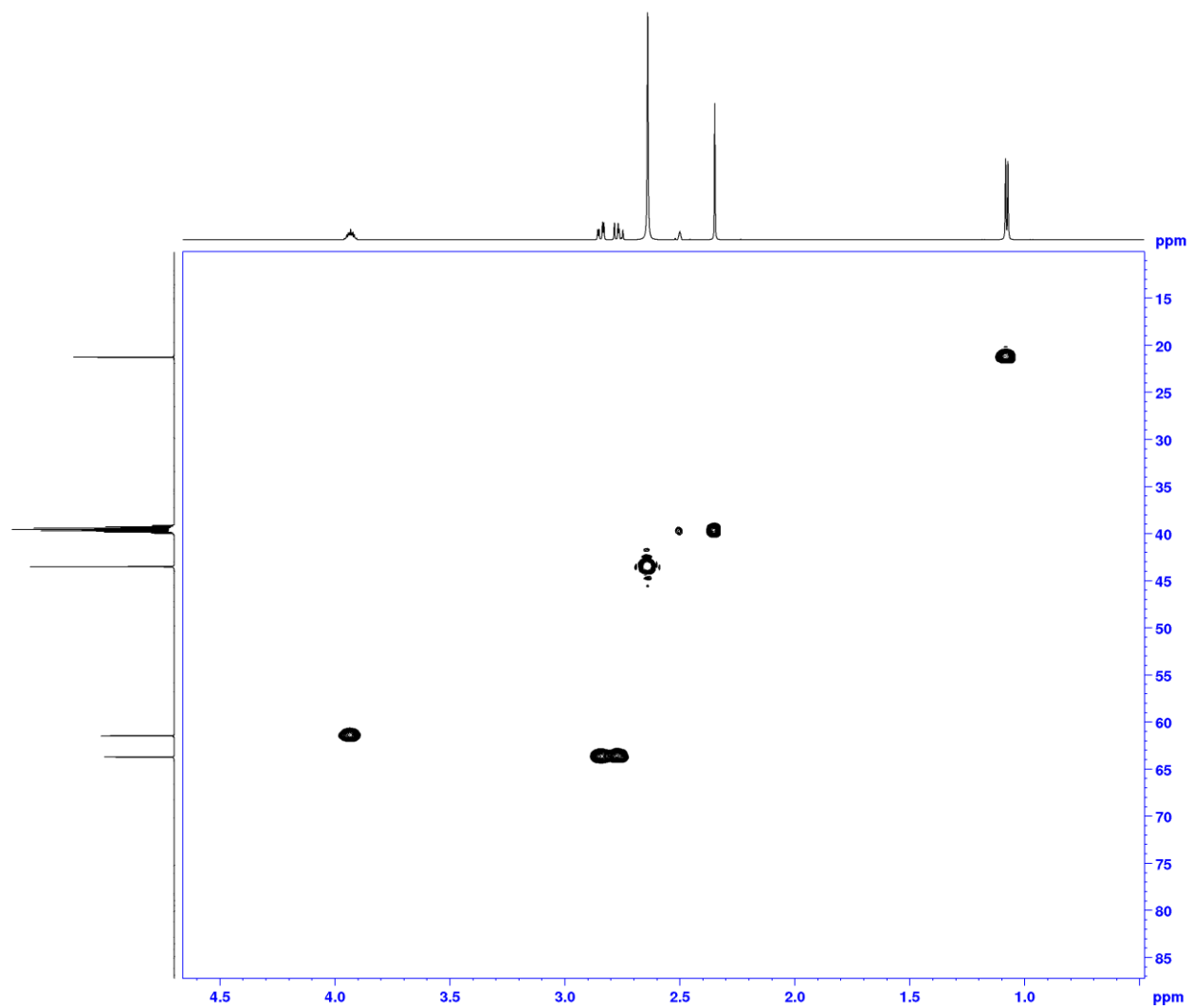


1-(dimethylamino)propan-2-ol (3)

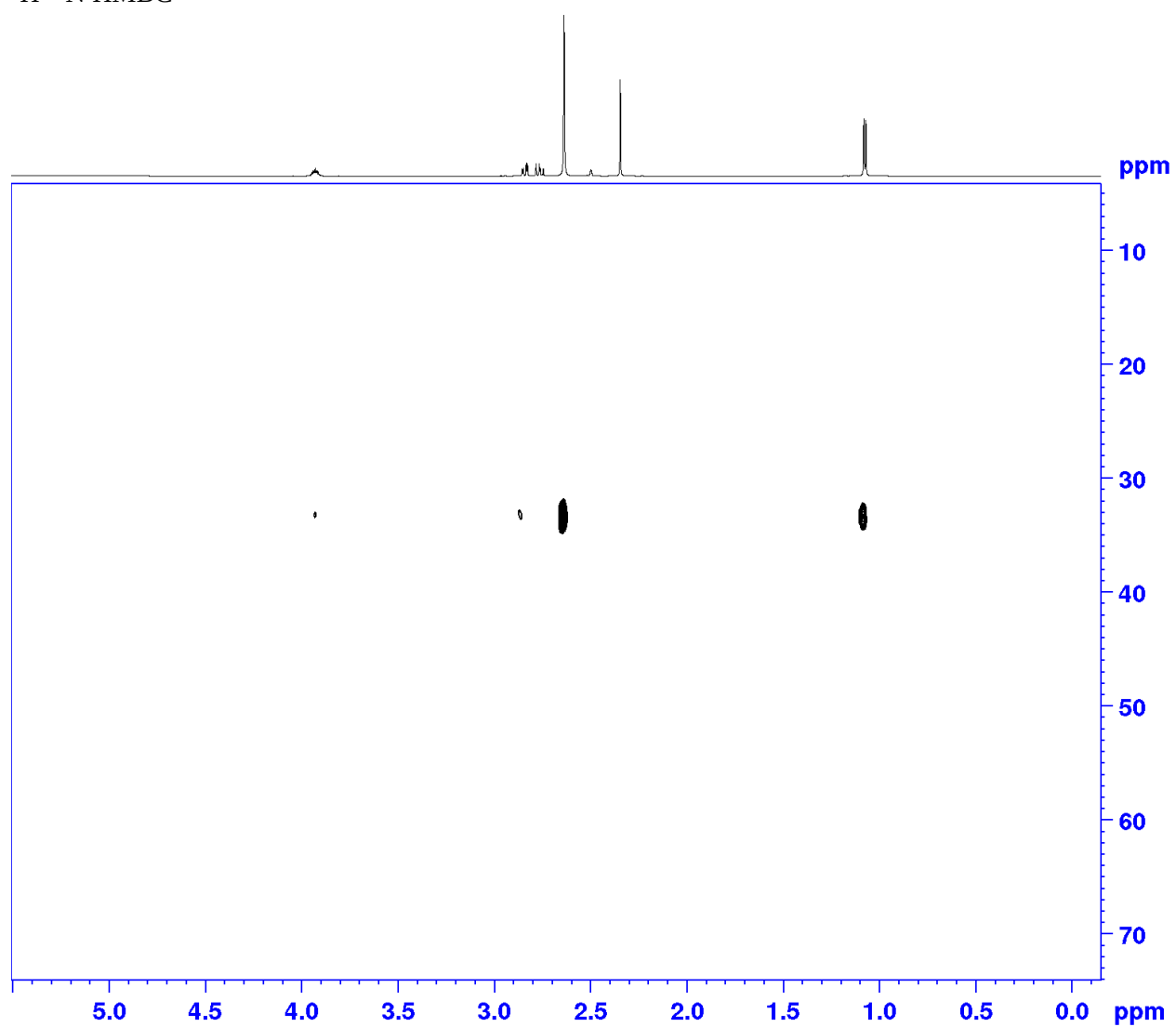
^1H





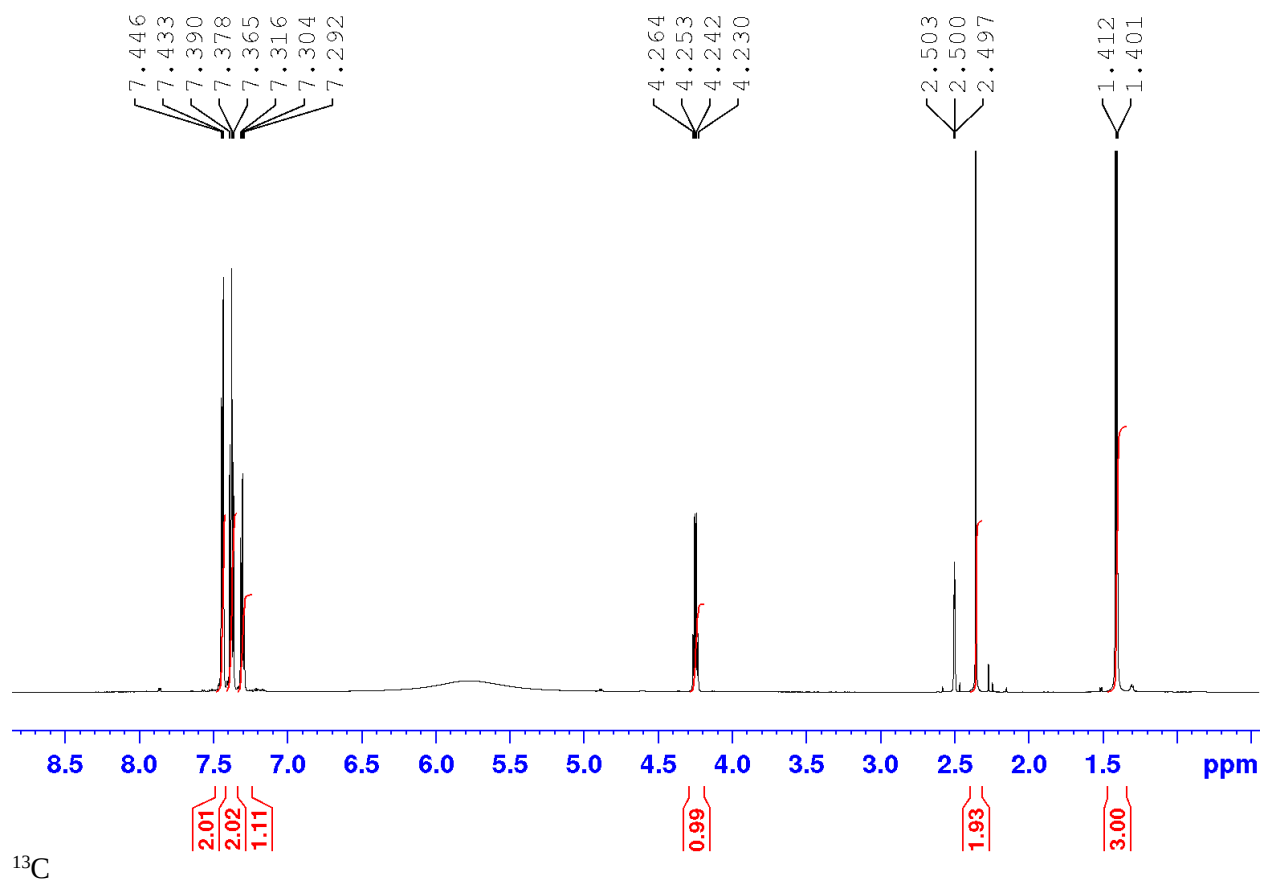


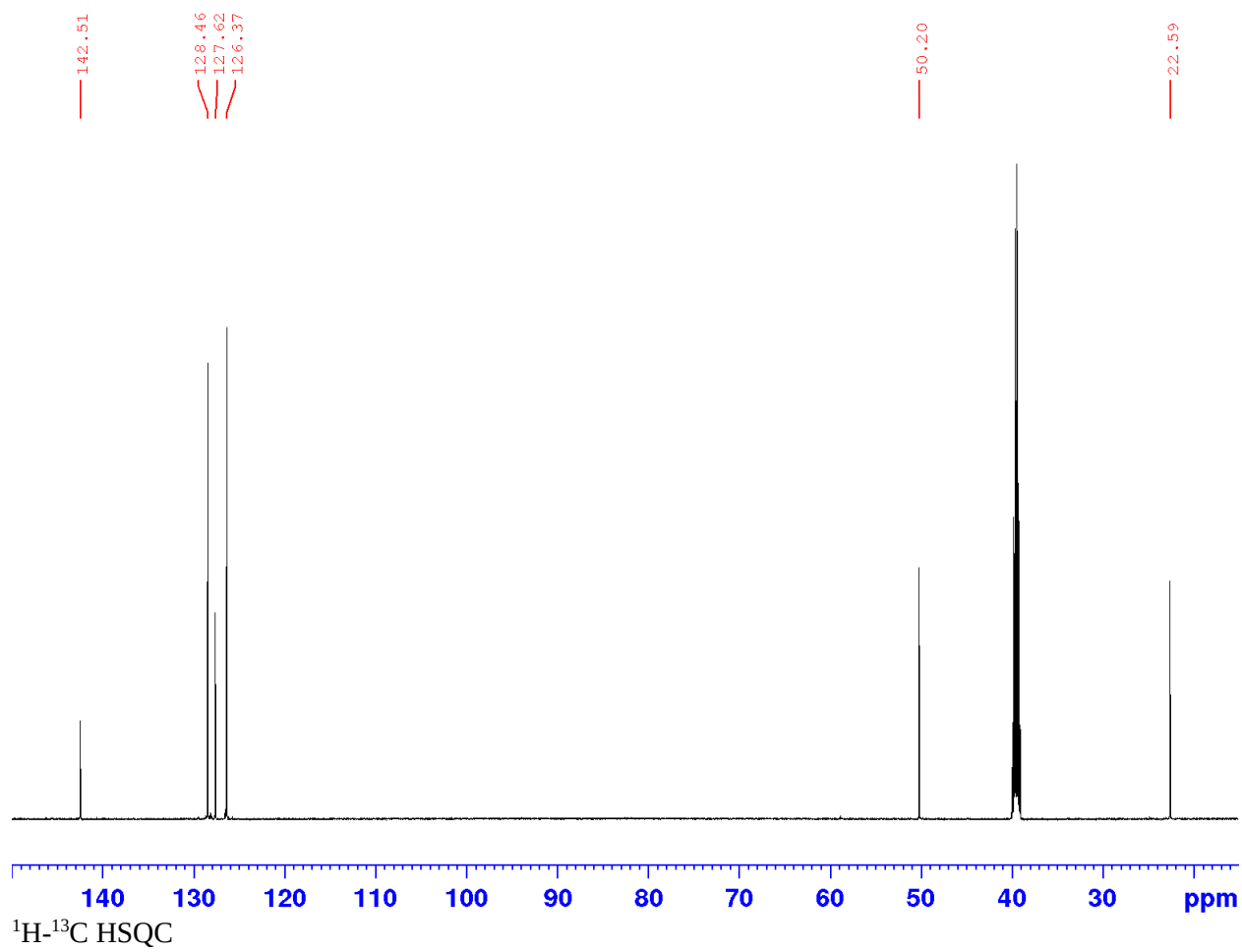
^1H - ^{15}N HMBC

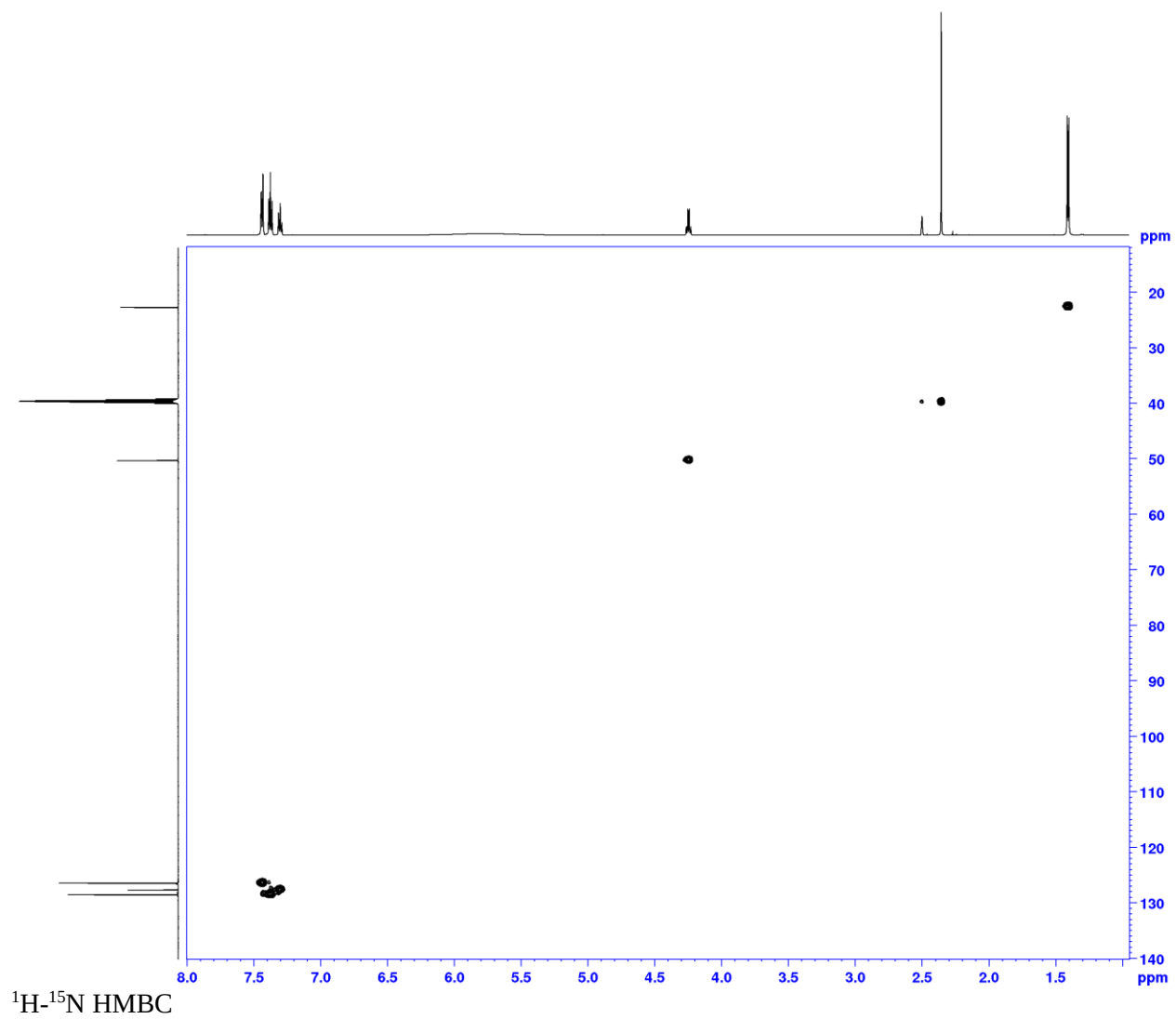


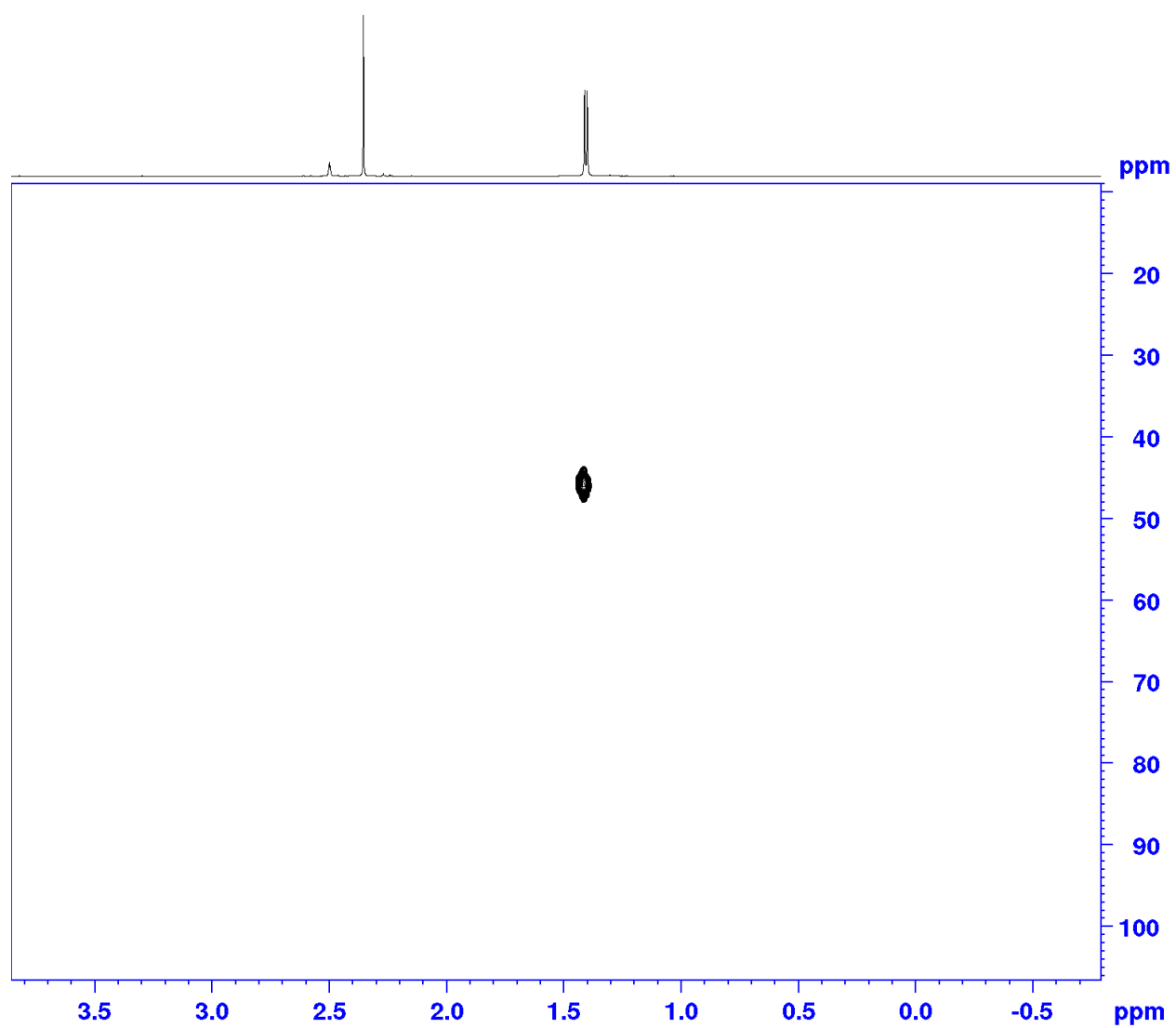
1-phenylethan-1-amine (**4**)

^1H



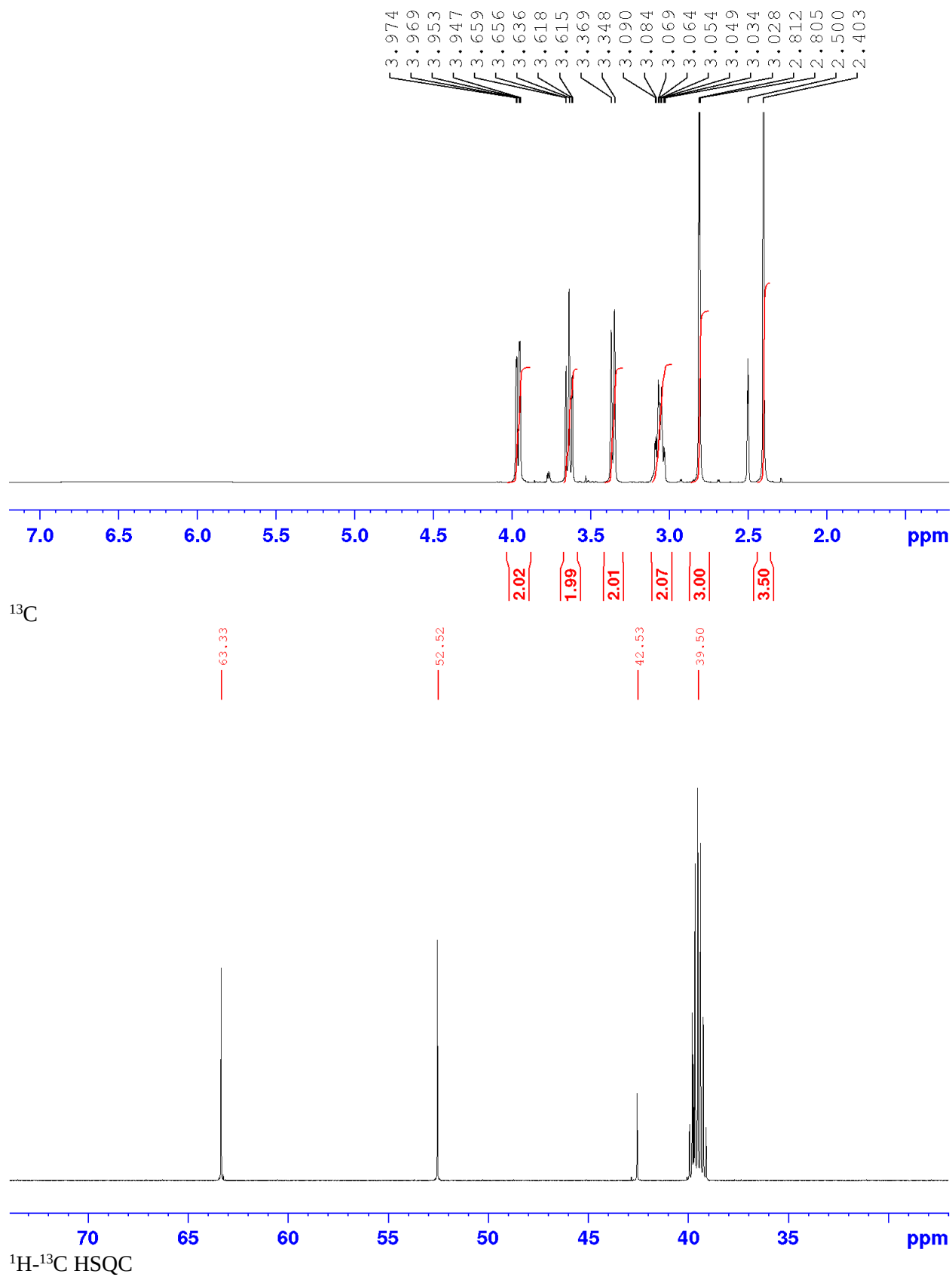


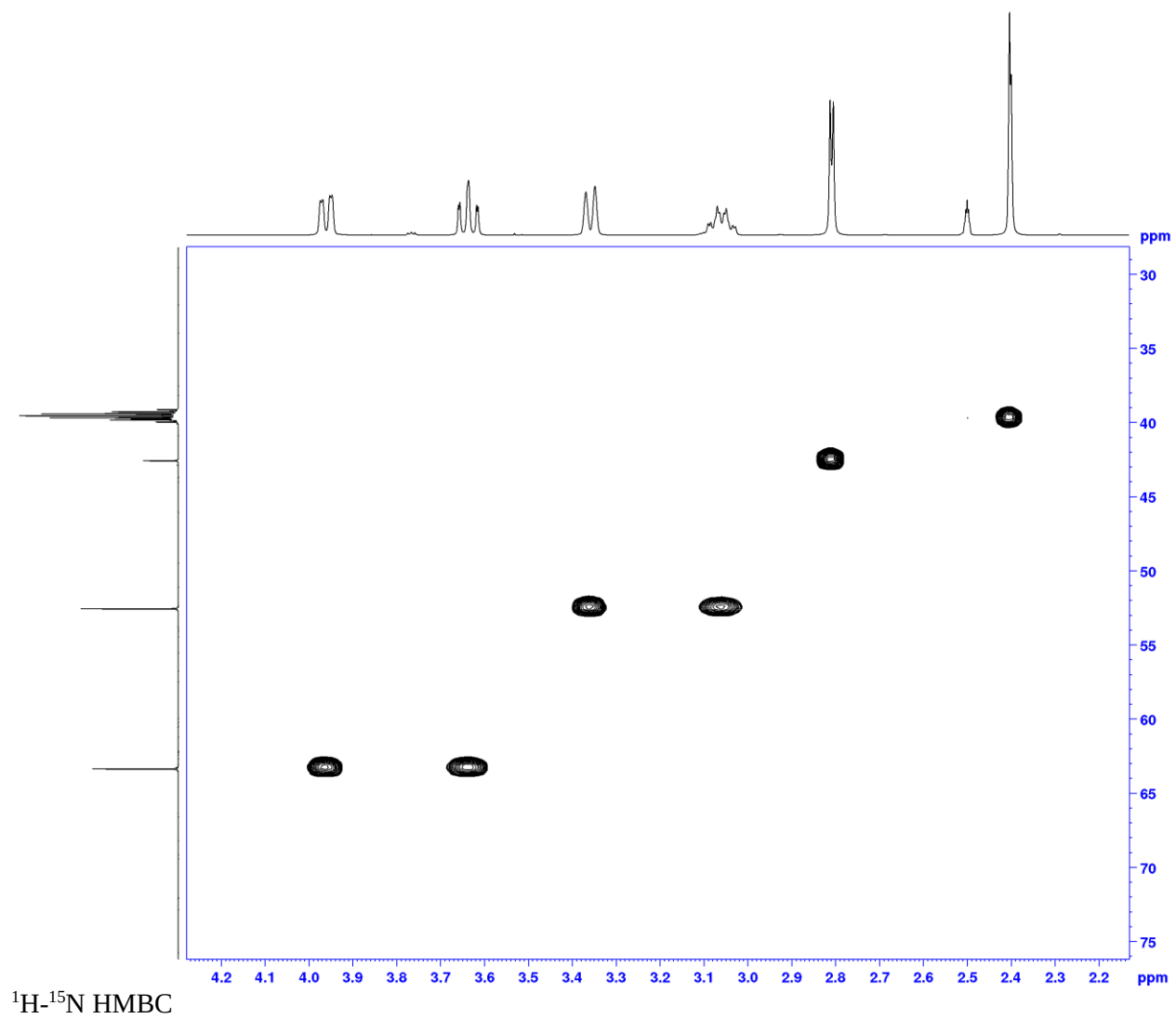


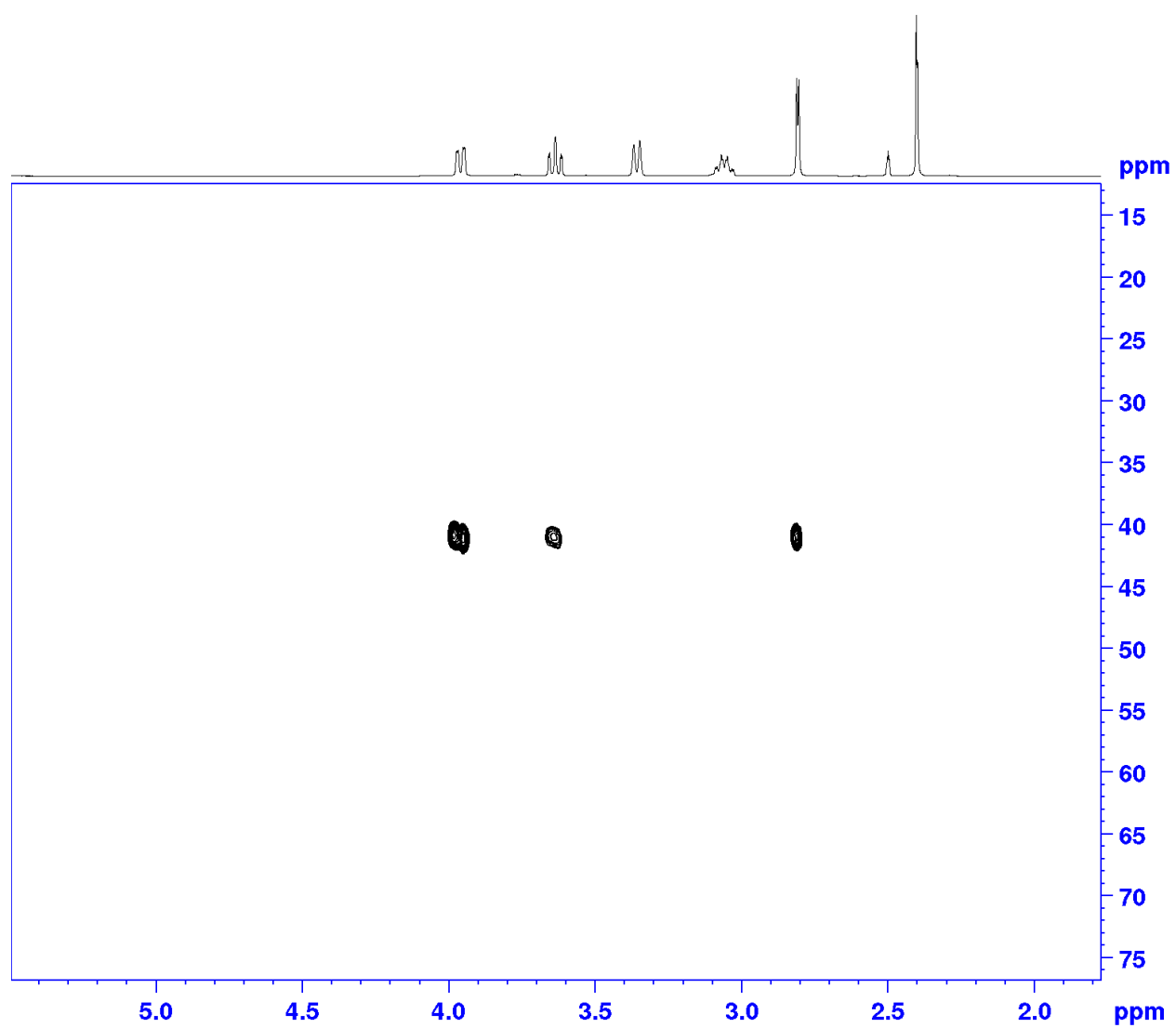


4-methylmorpholine (5)

^1H

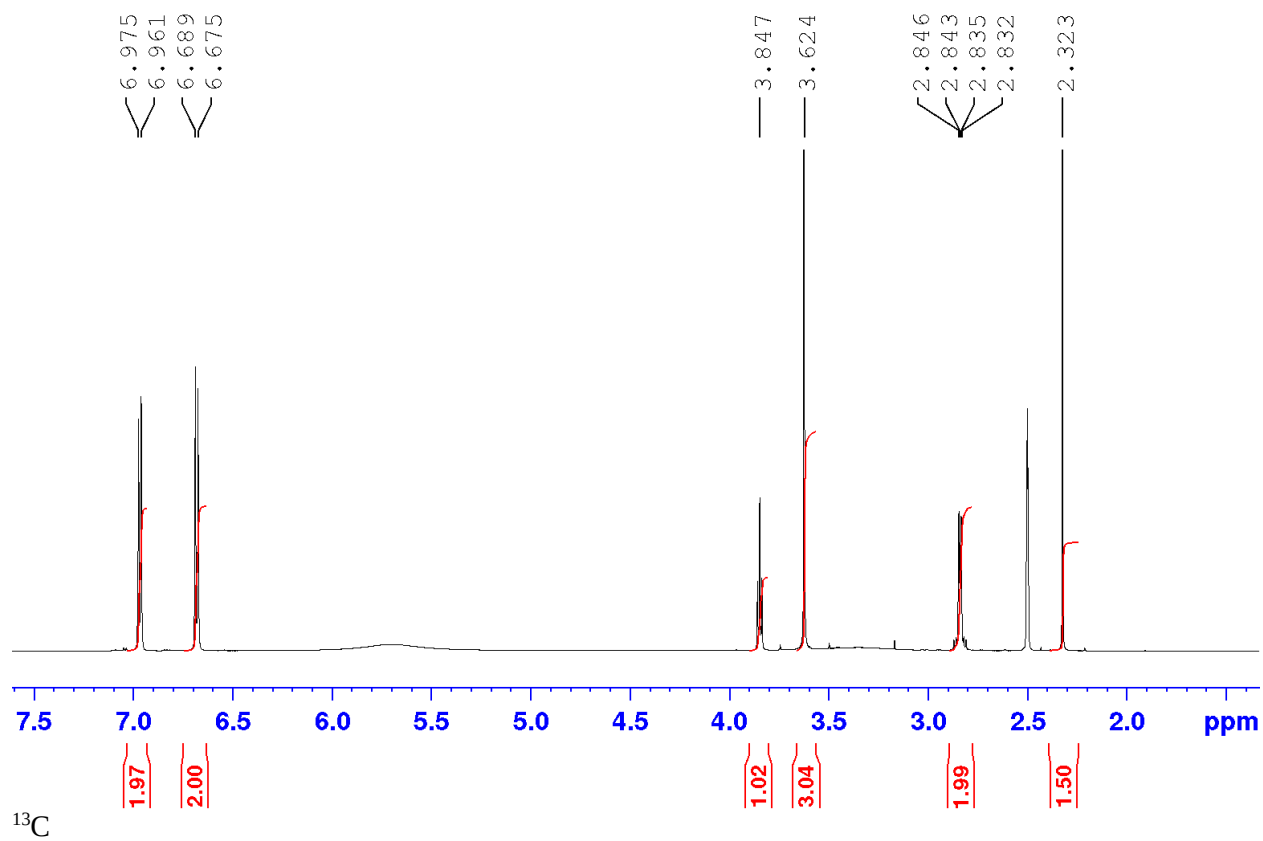


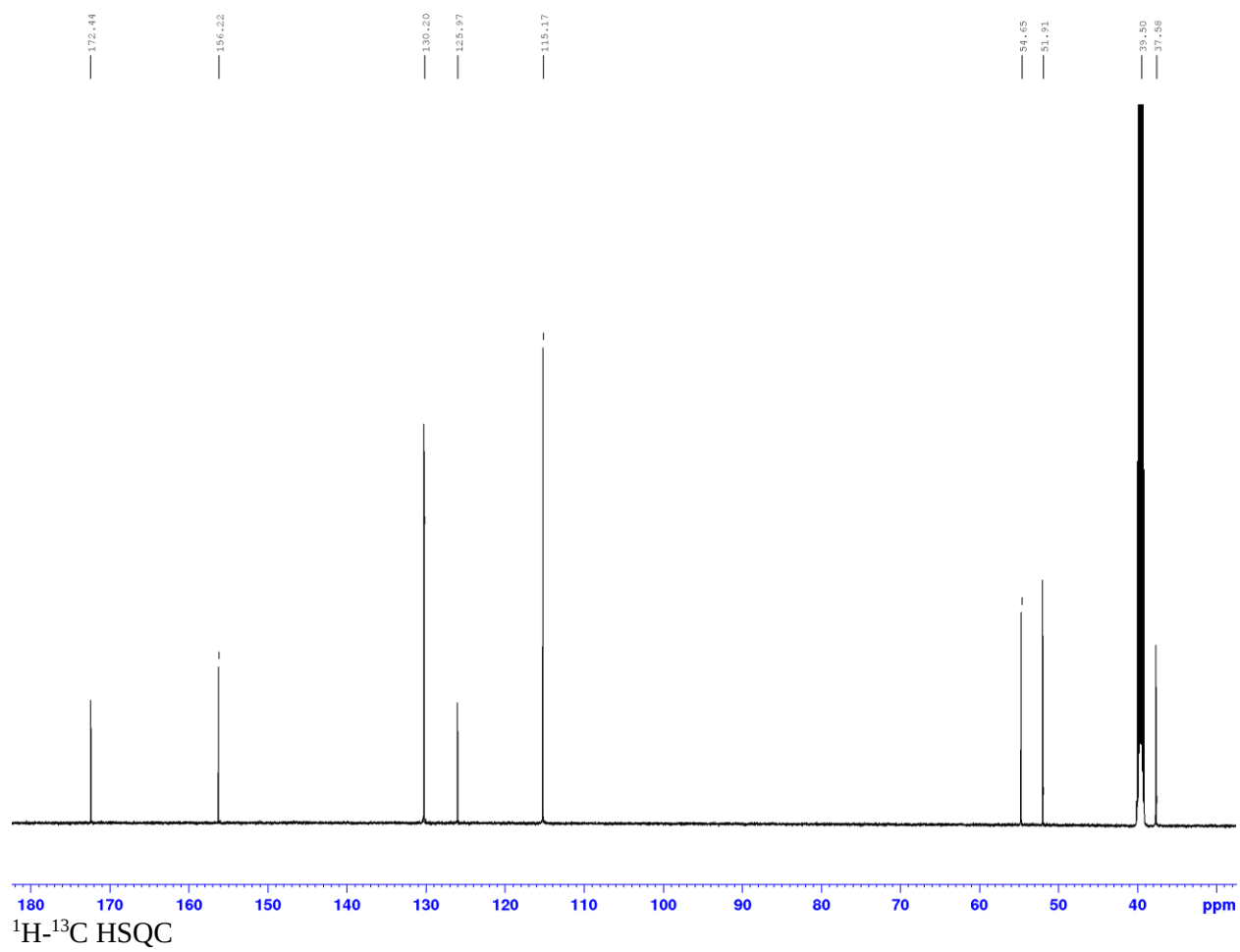


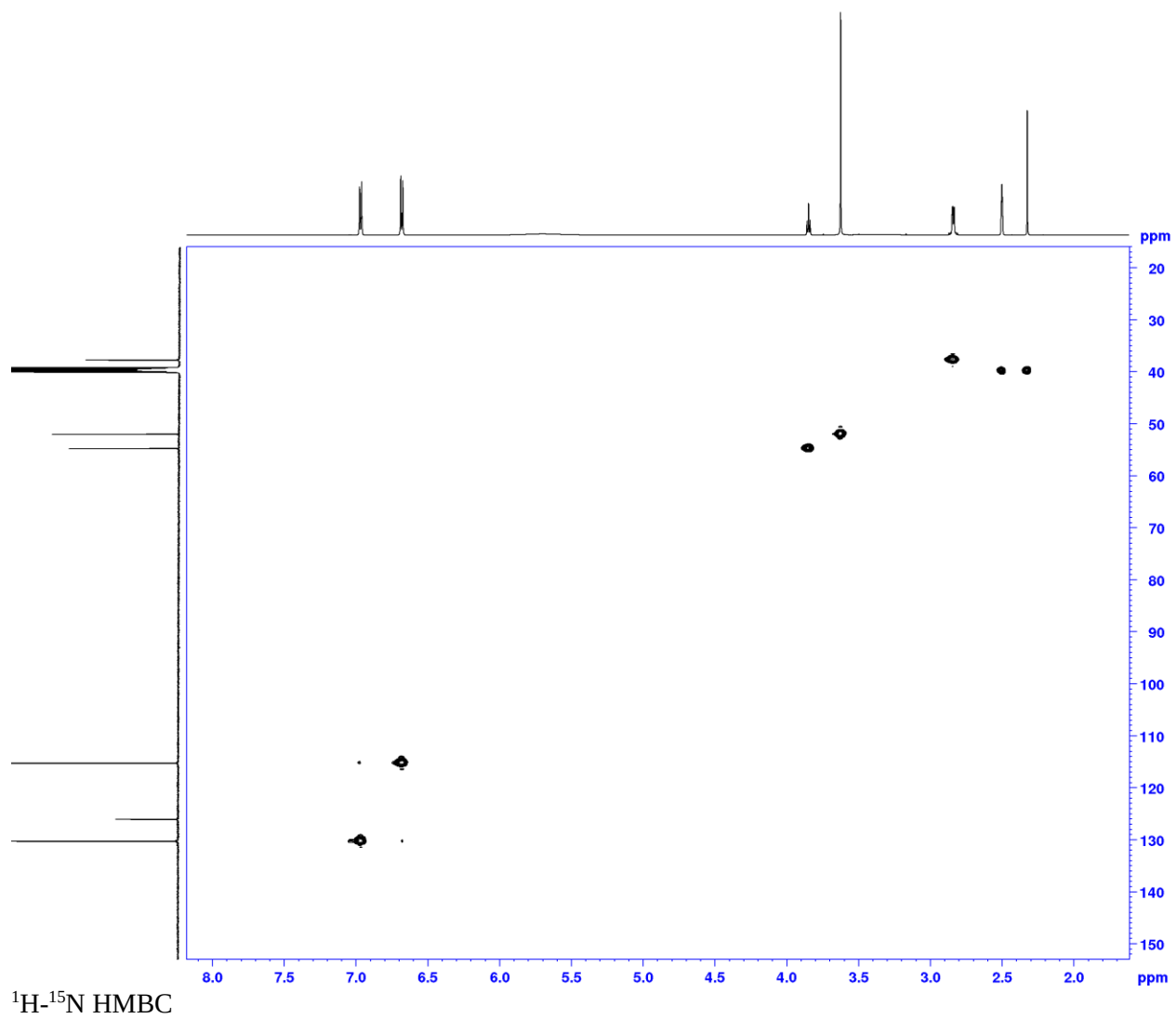


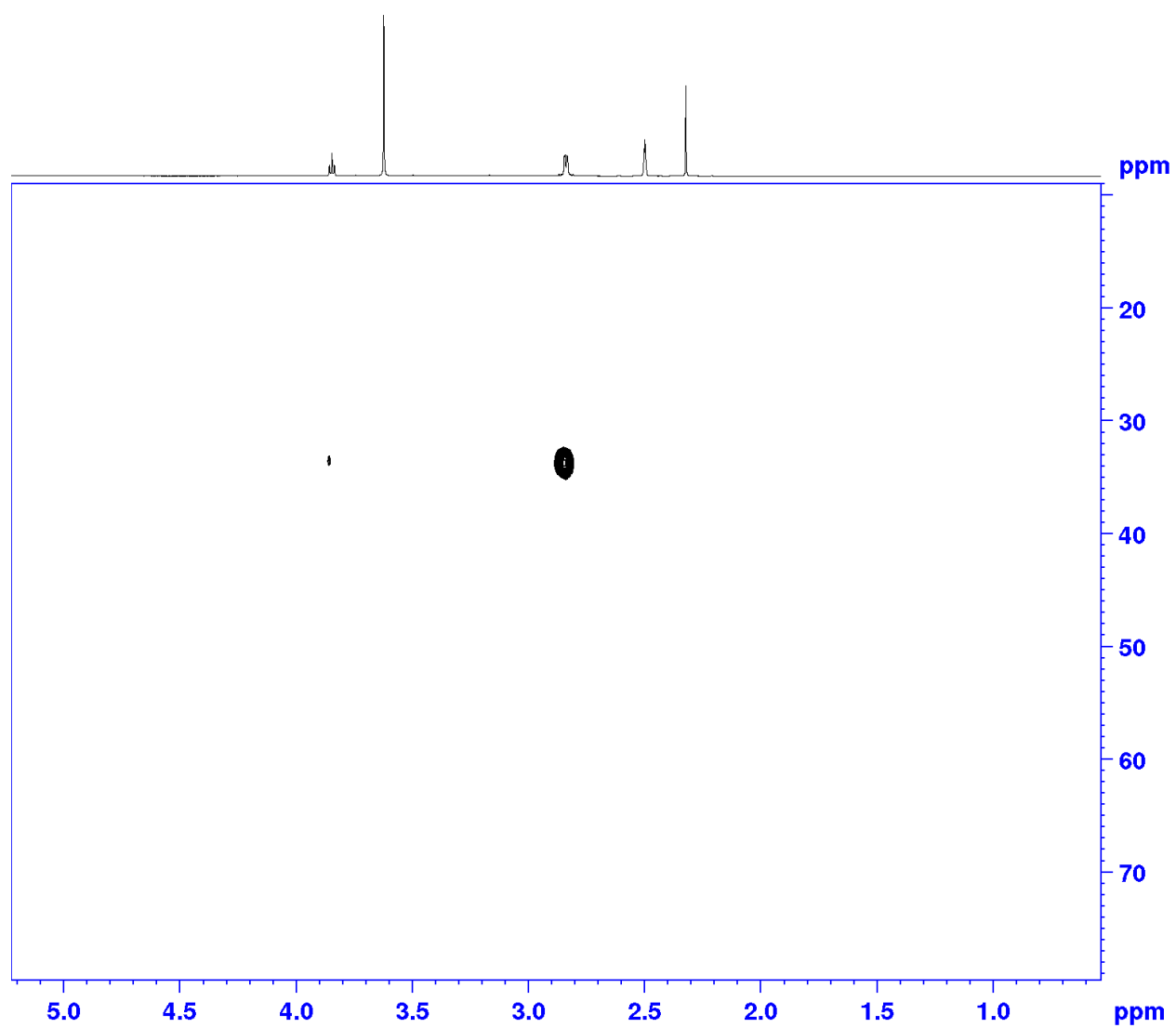
methyl L-tyrosinate (**6**)

^1H



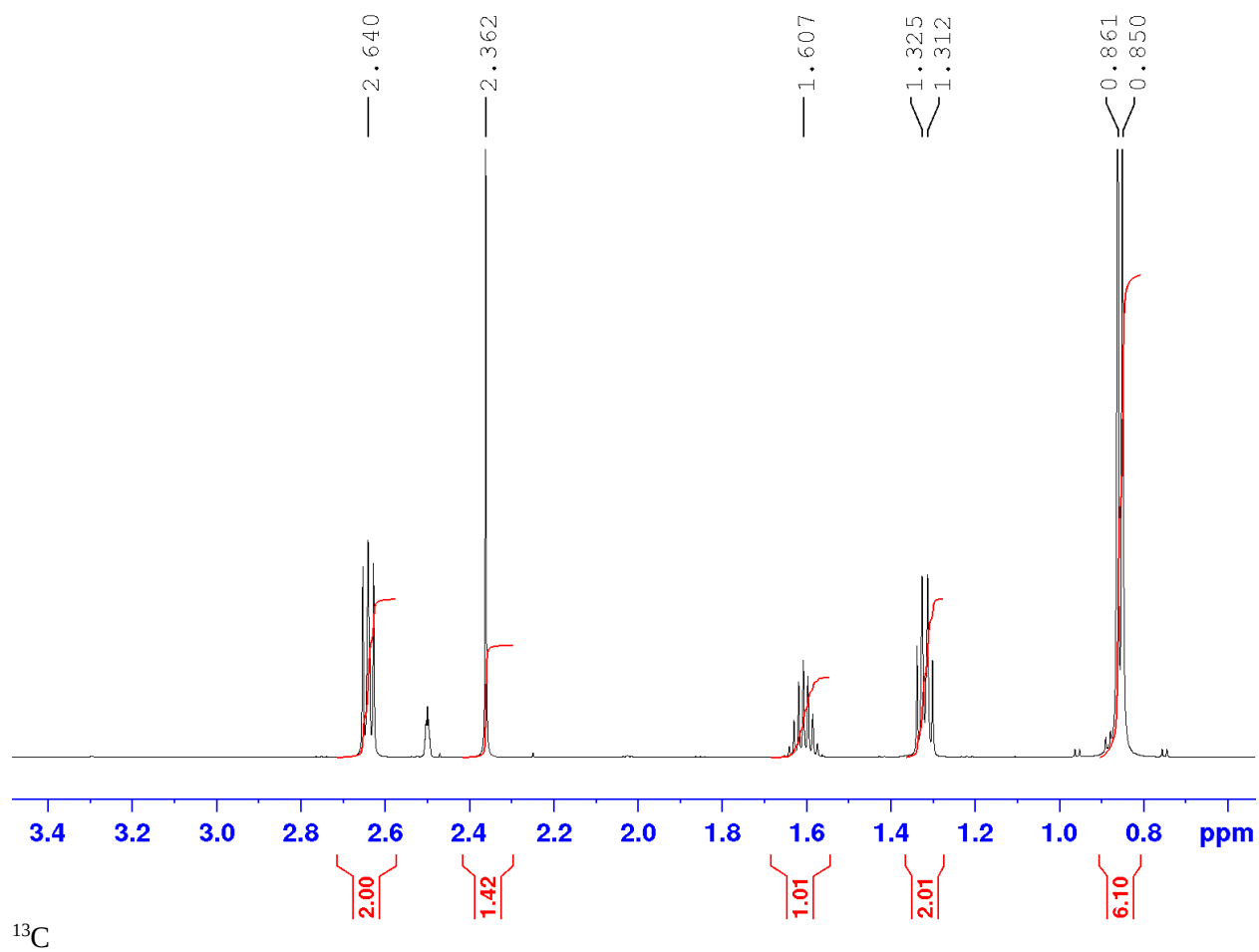


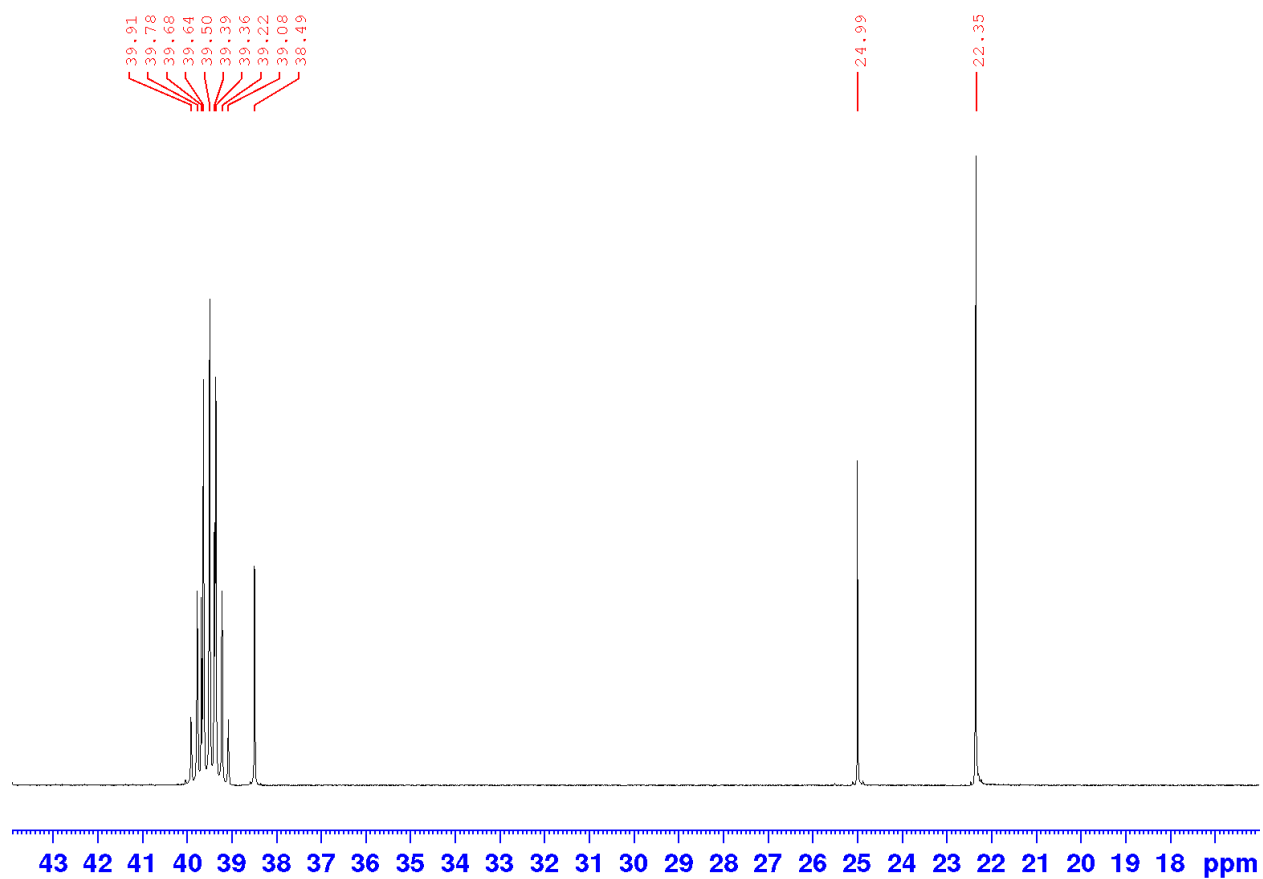




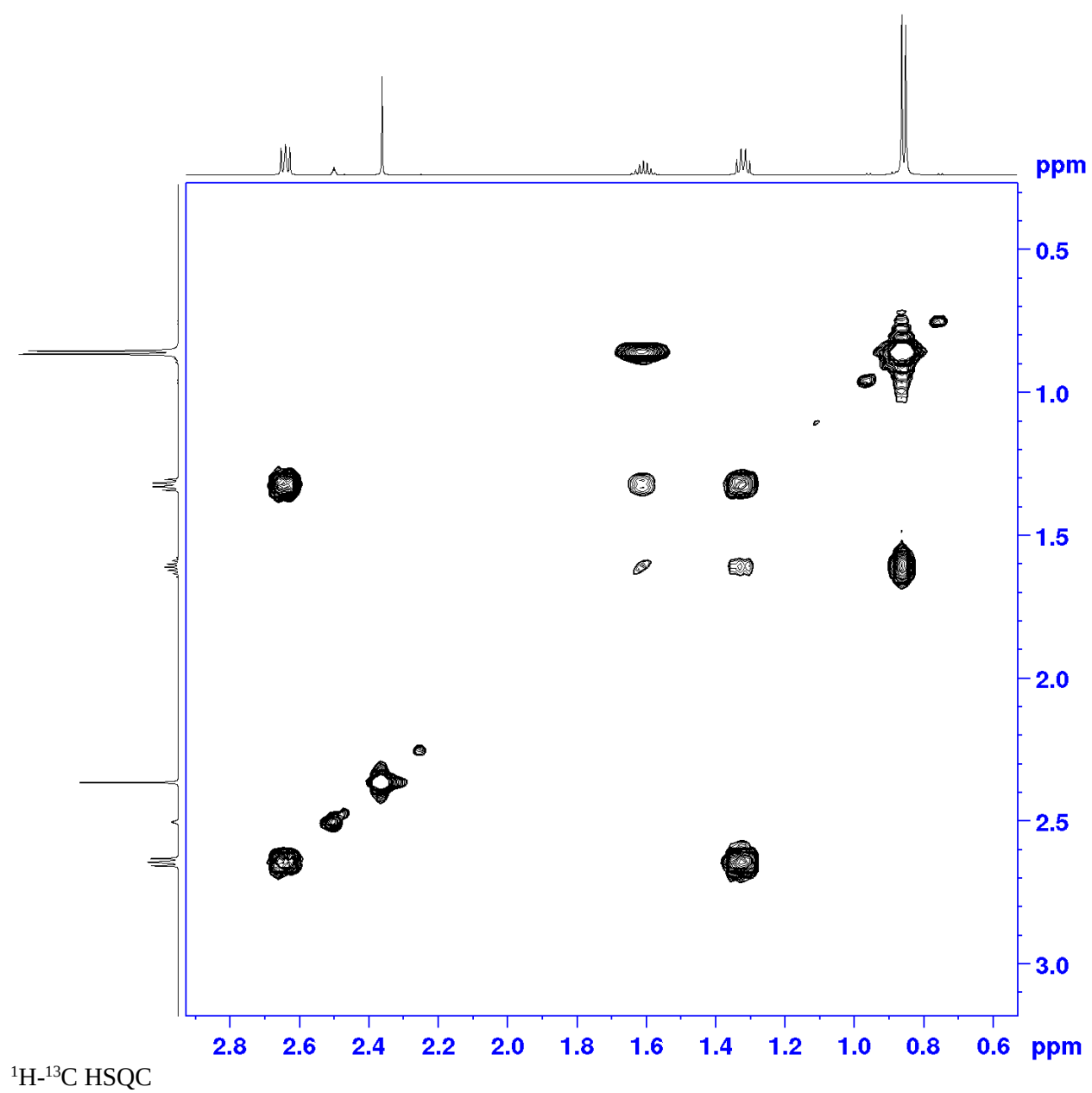
3-methylbutan-1-amine (7)

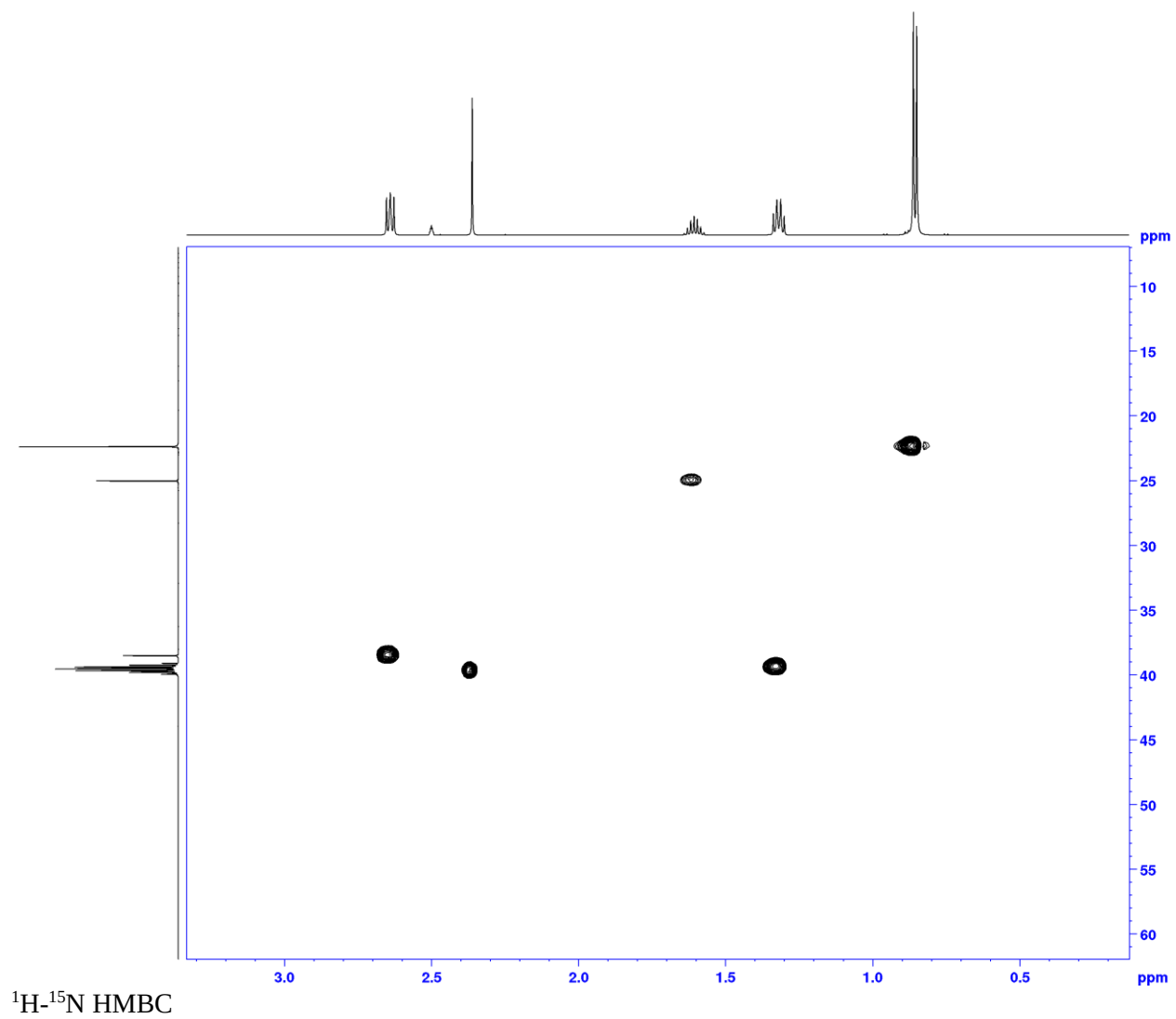
^1H

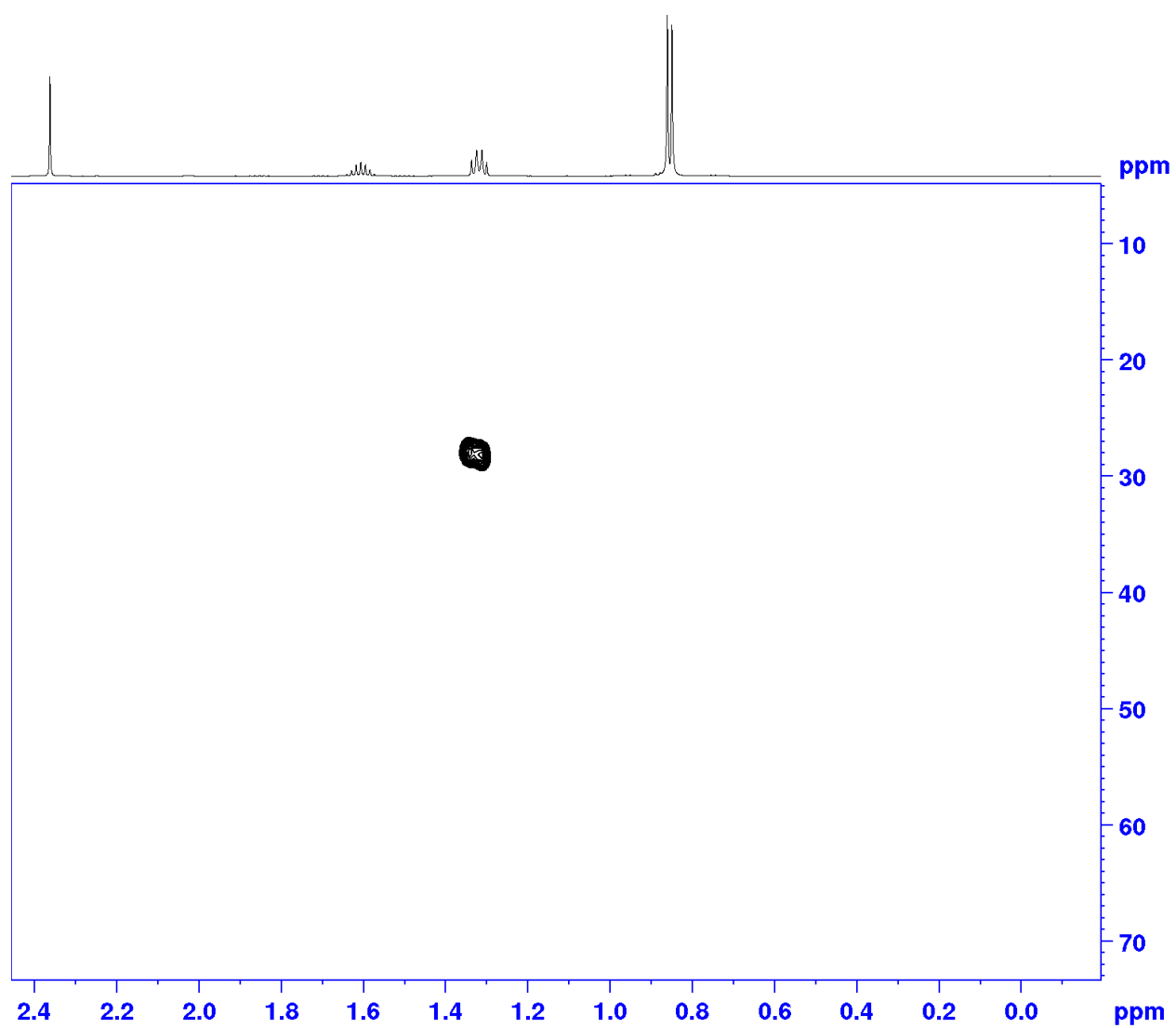




^1H - ^1H COSY

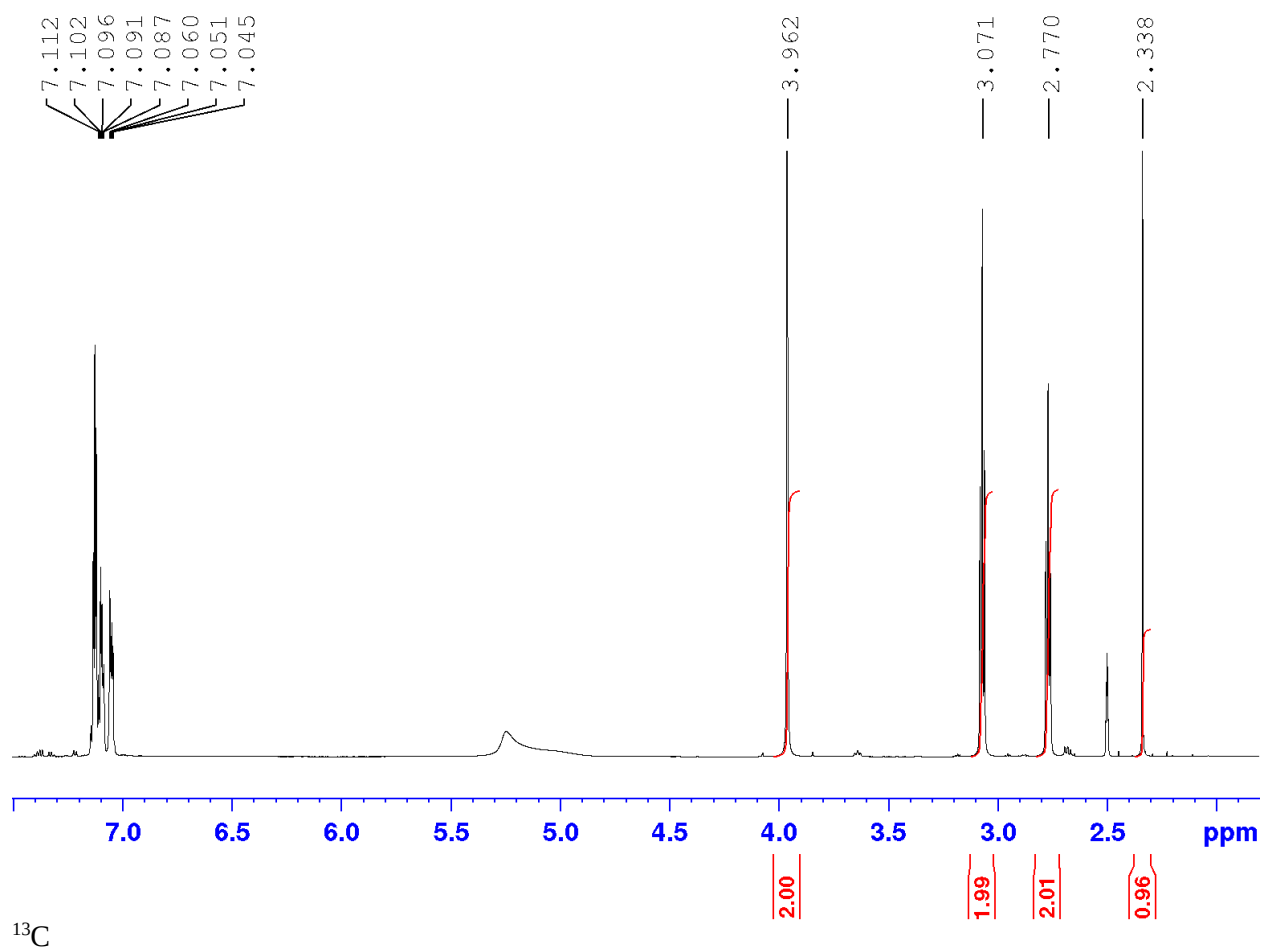


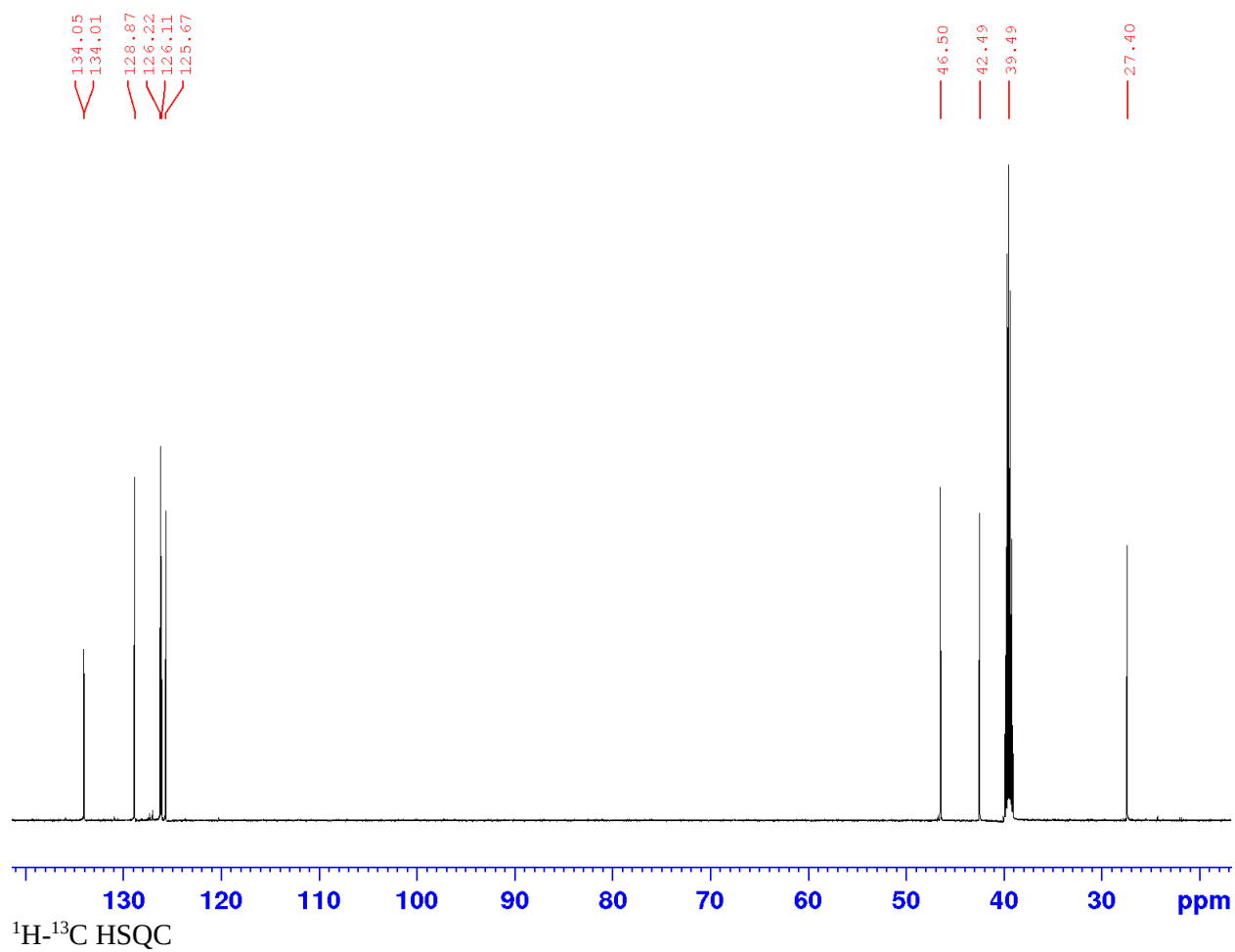


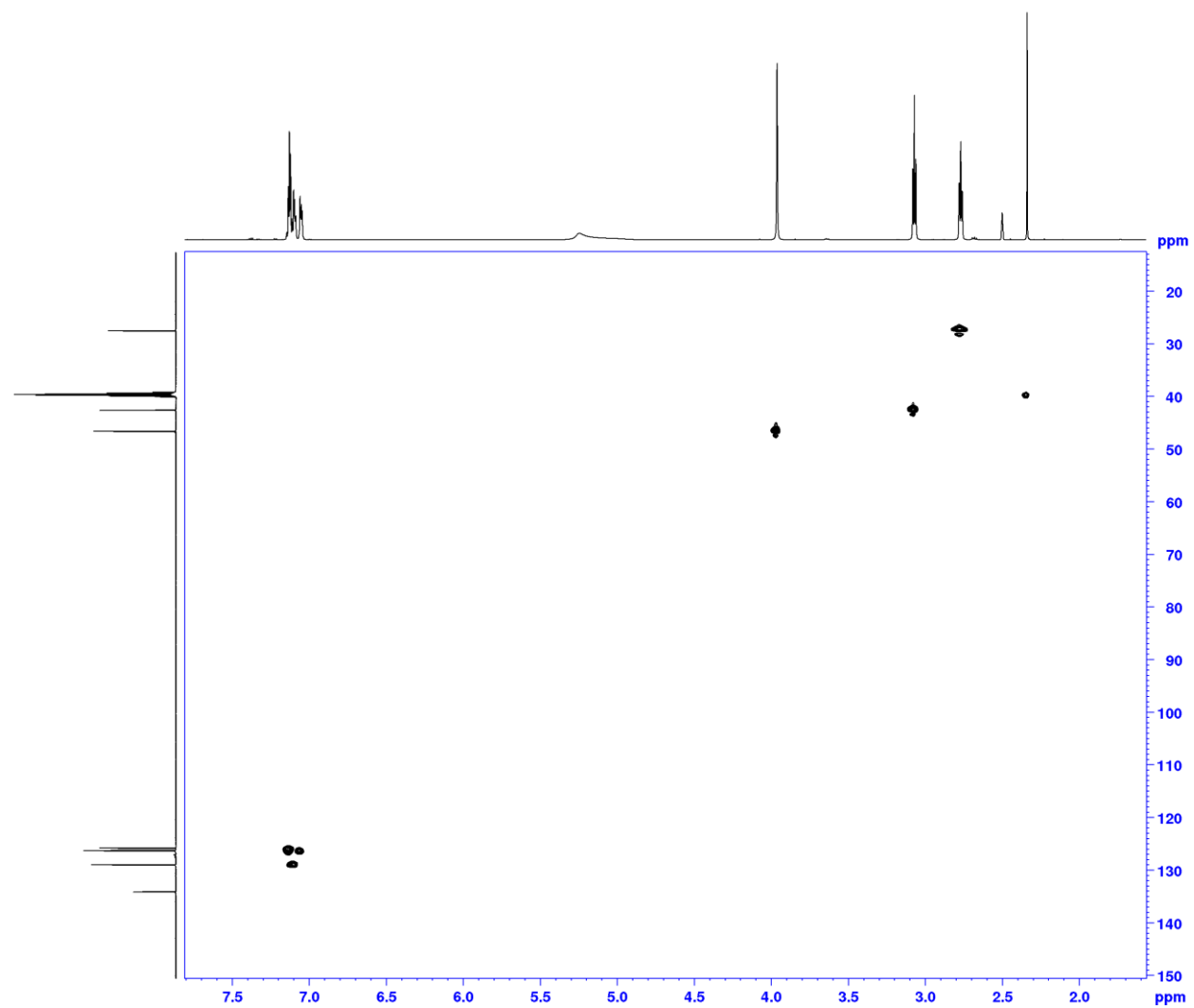


1,2,3,4-tetrahydroisoquinoline (**8**)

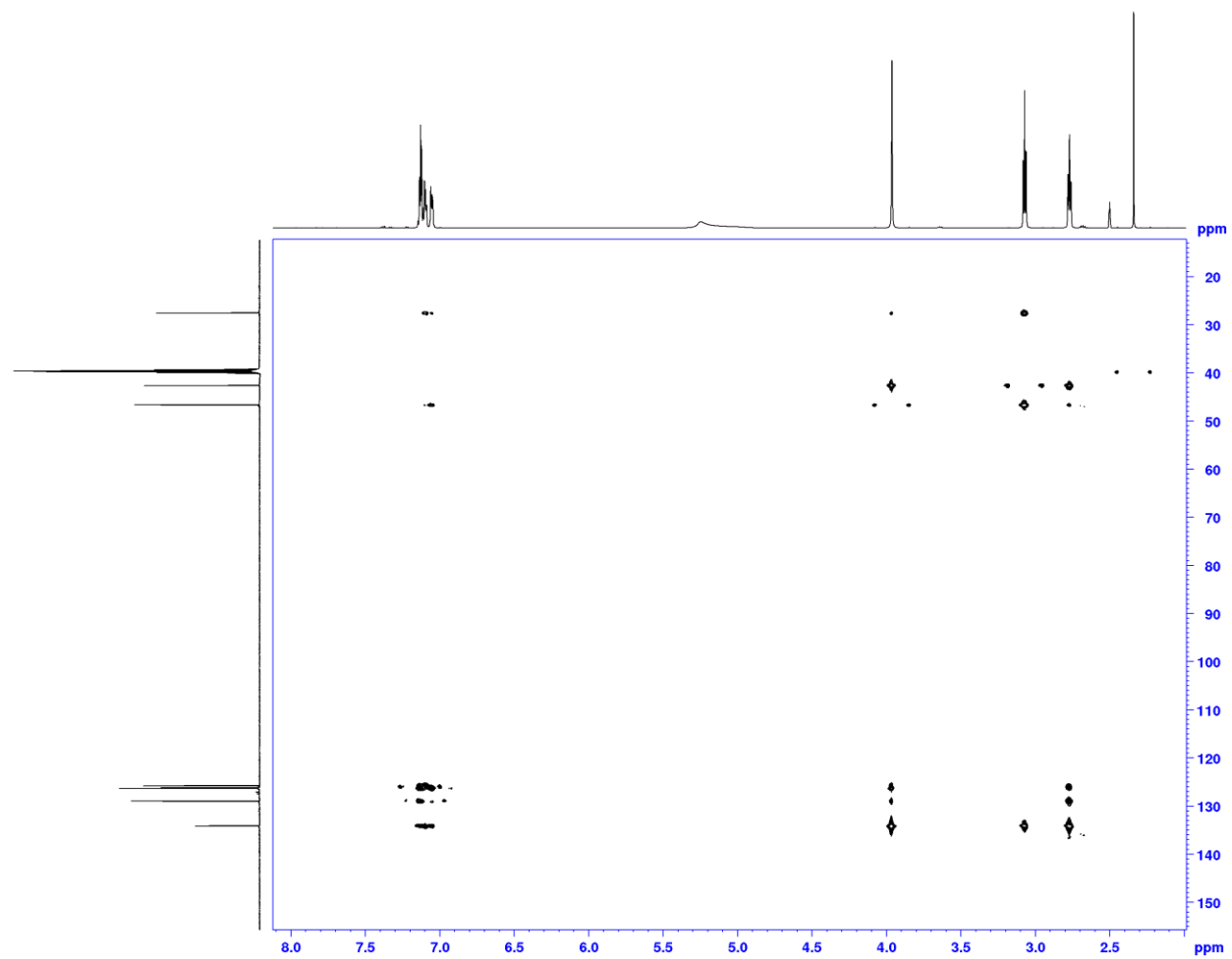
^1H



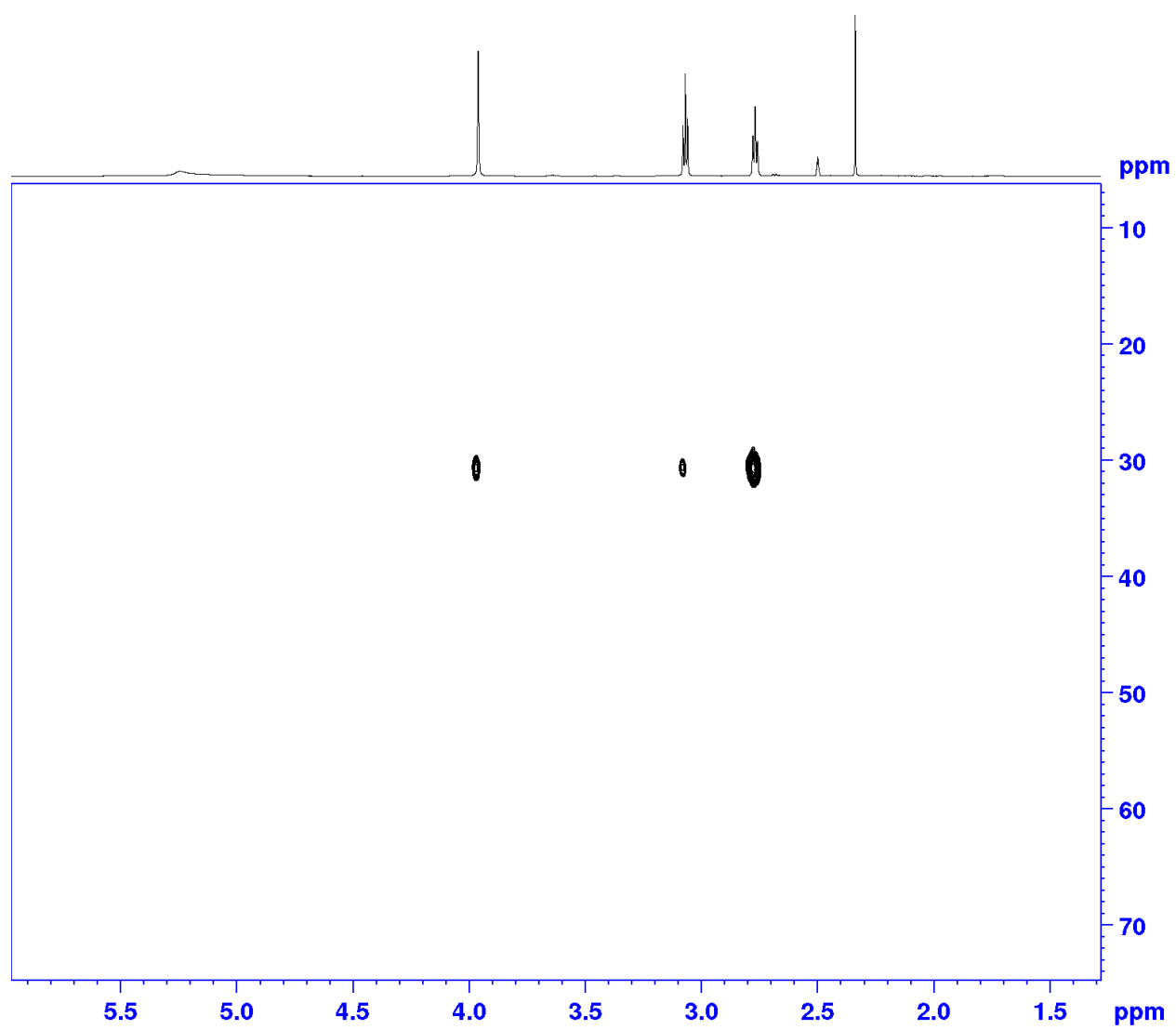




^1H - ^{13}C HMBC

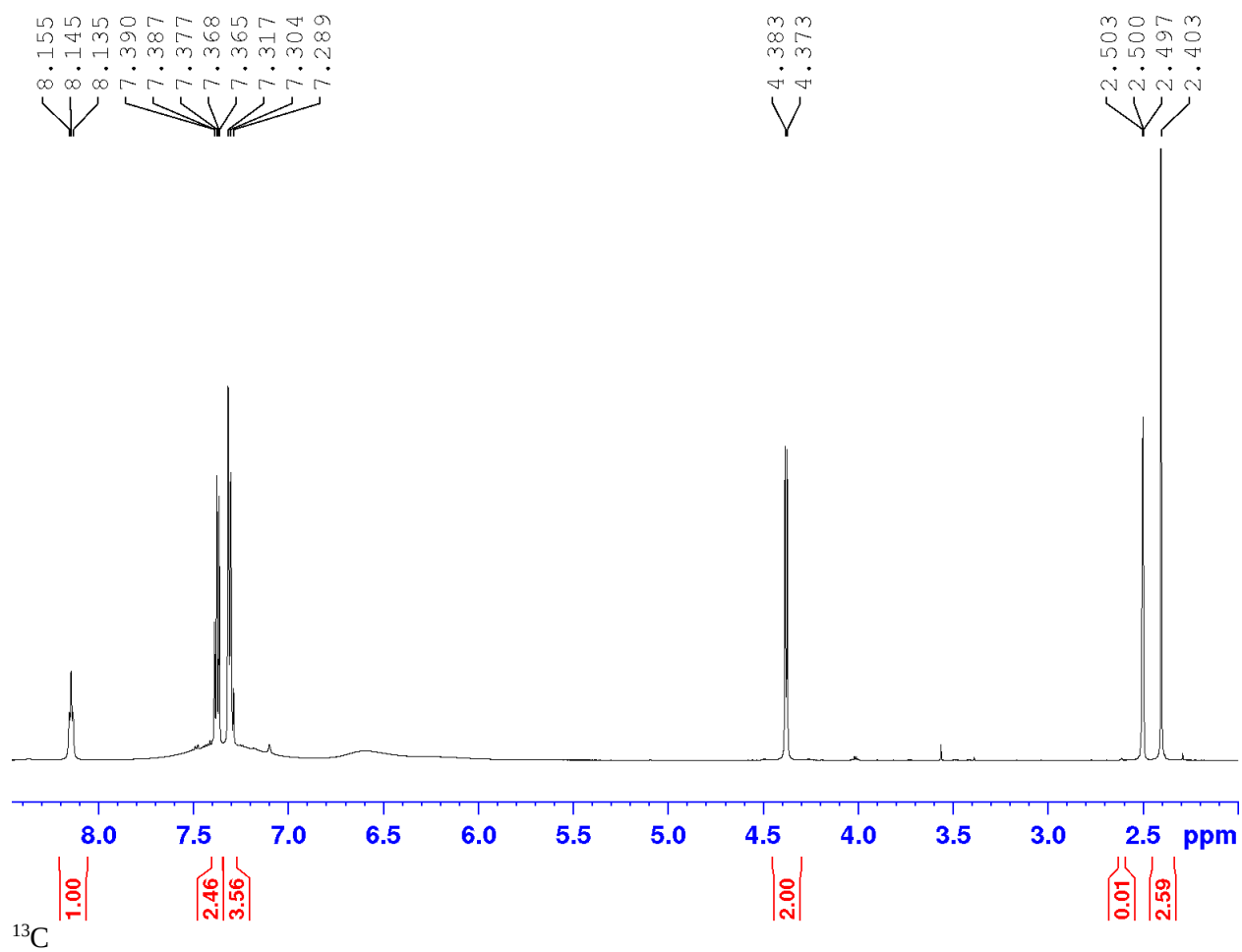


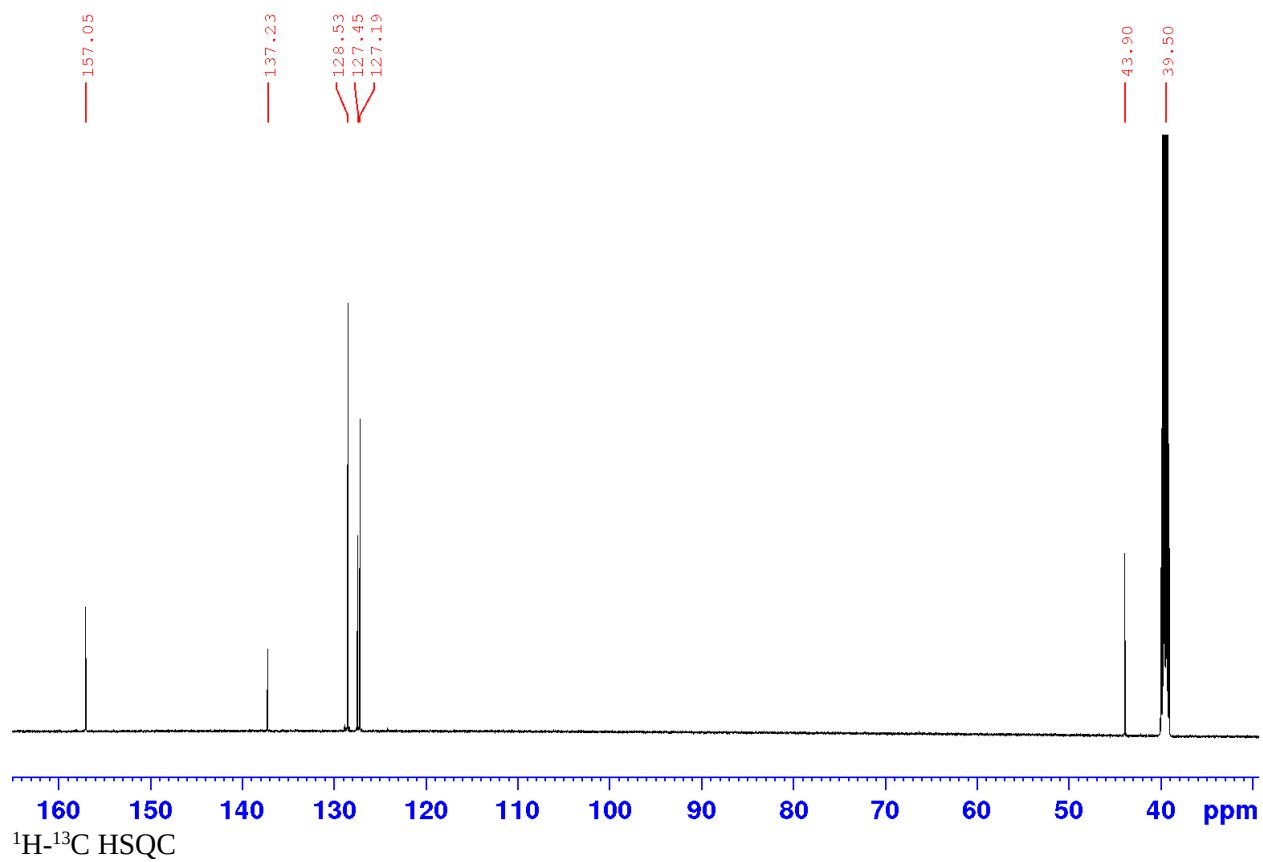
^1H - ^{15}N HMBC

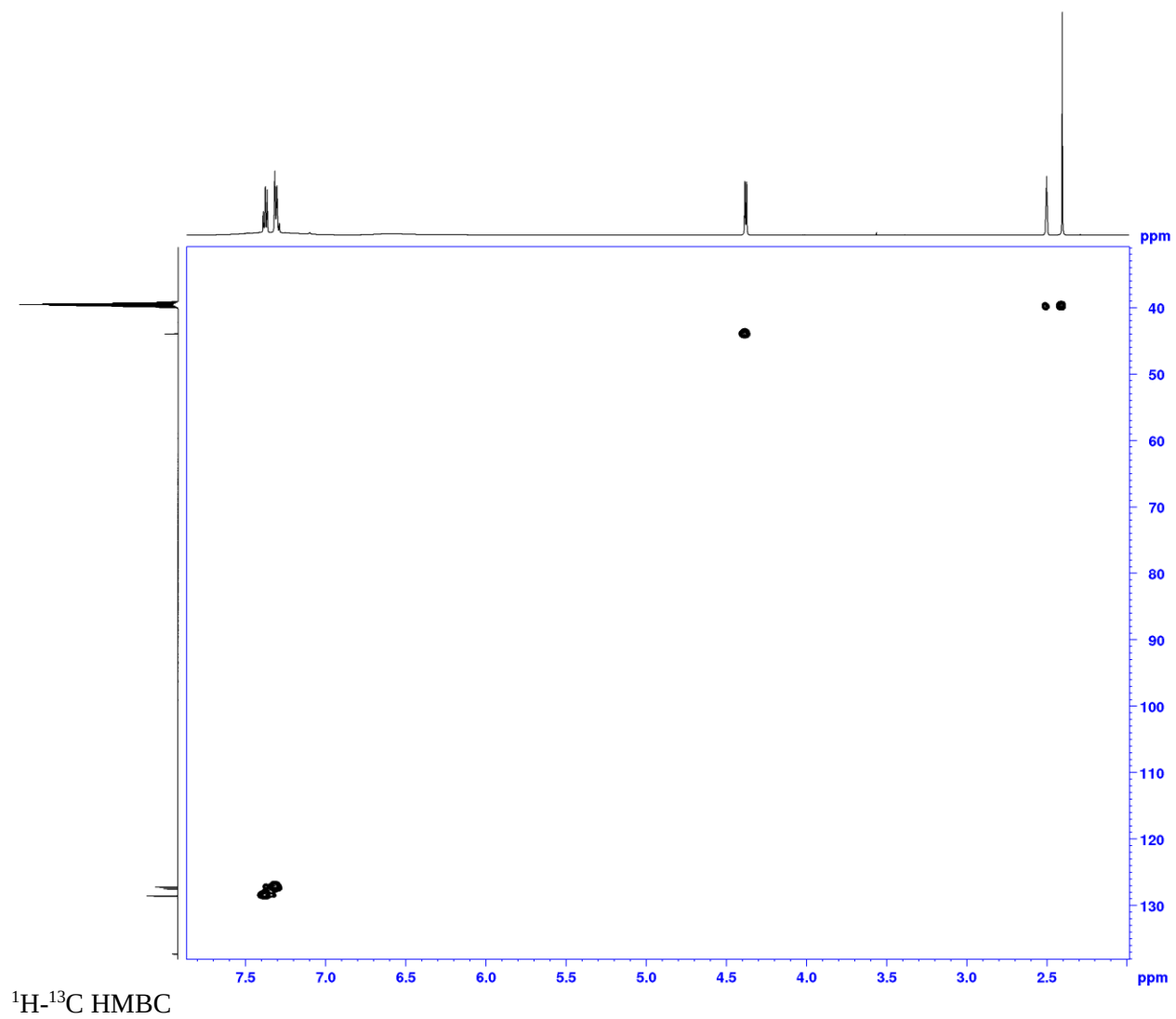


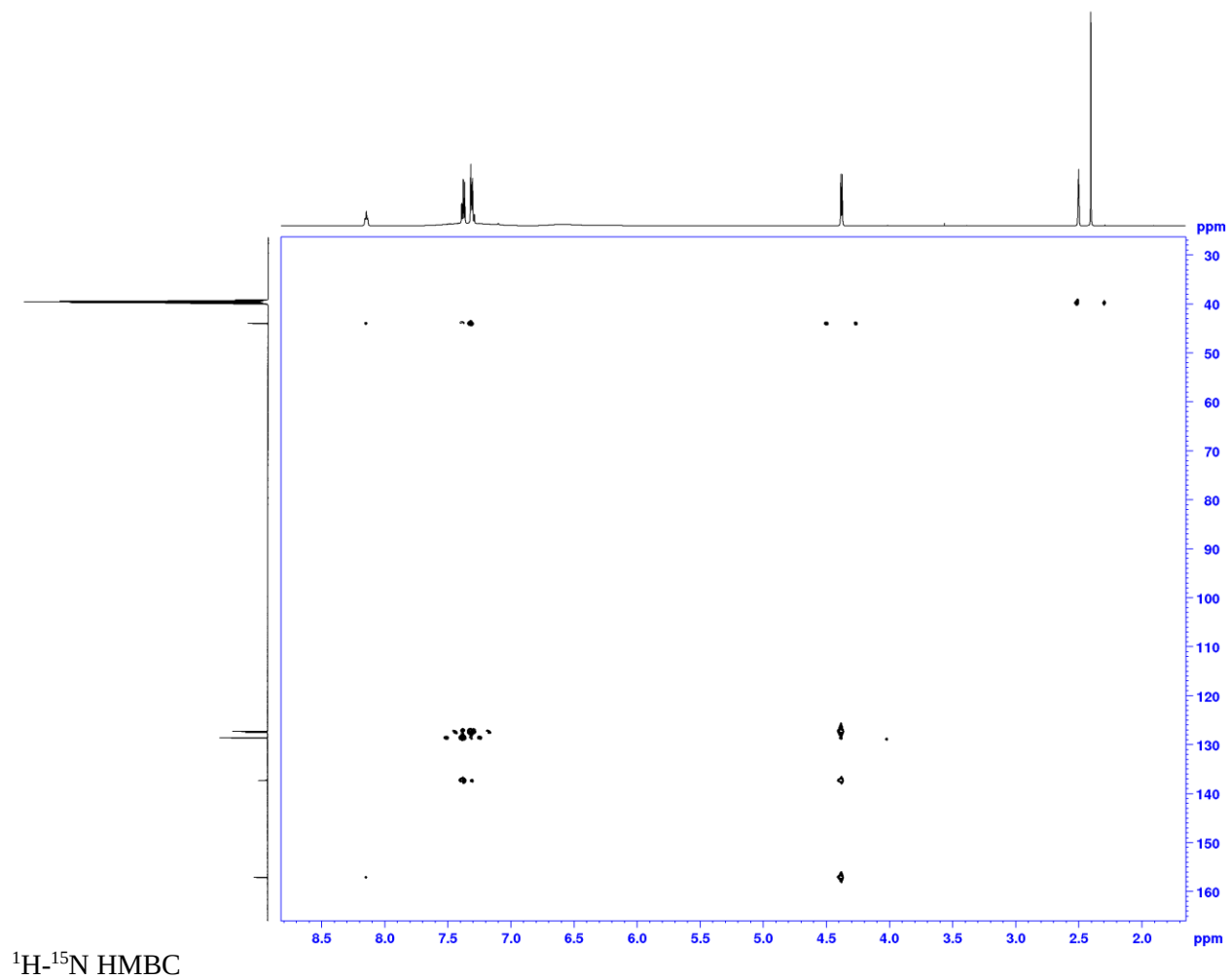
1-benzylguanidine (9)

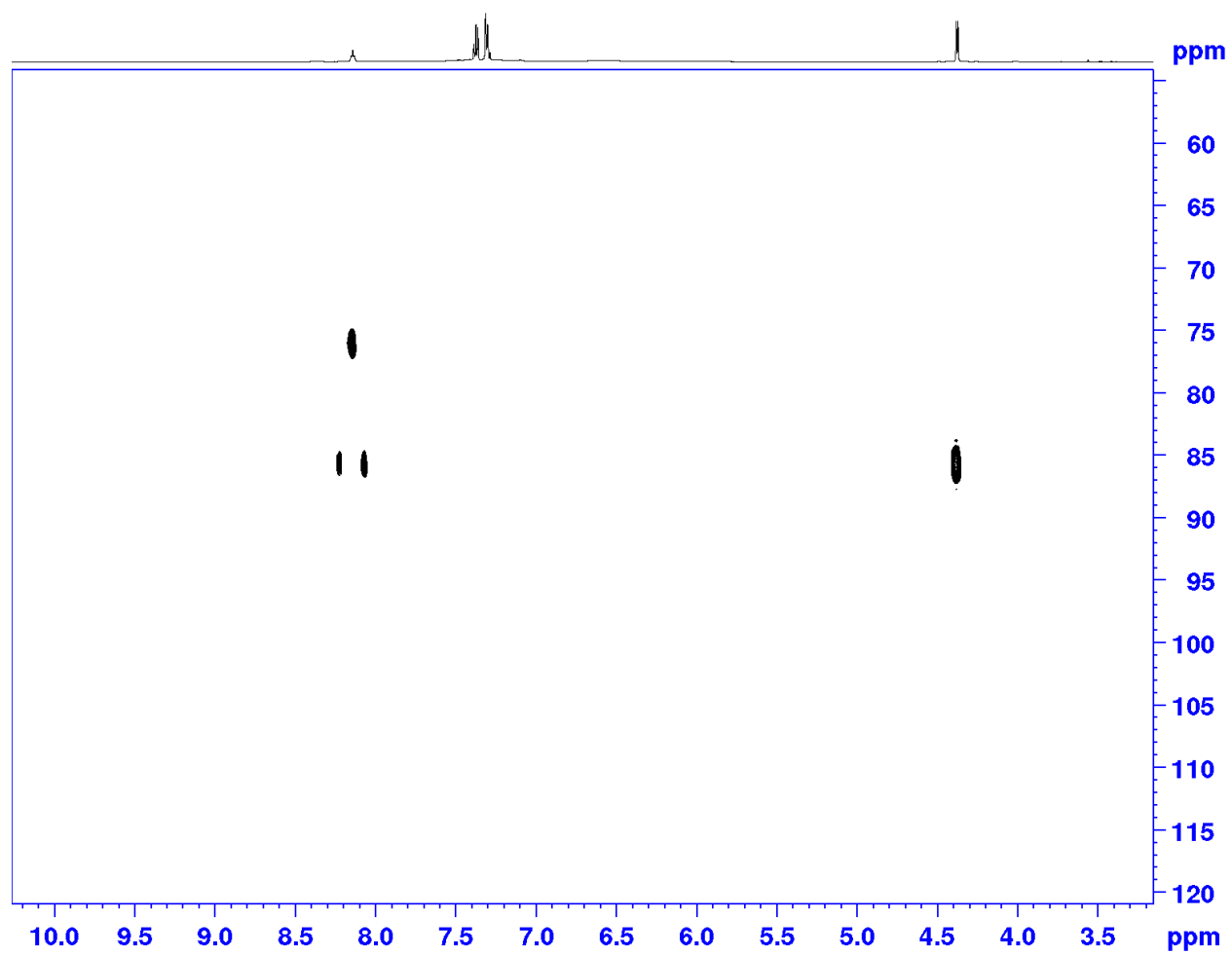
¹H





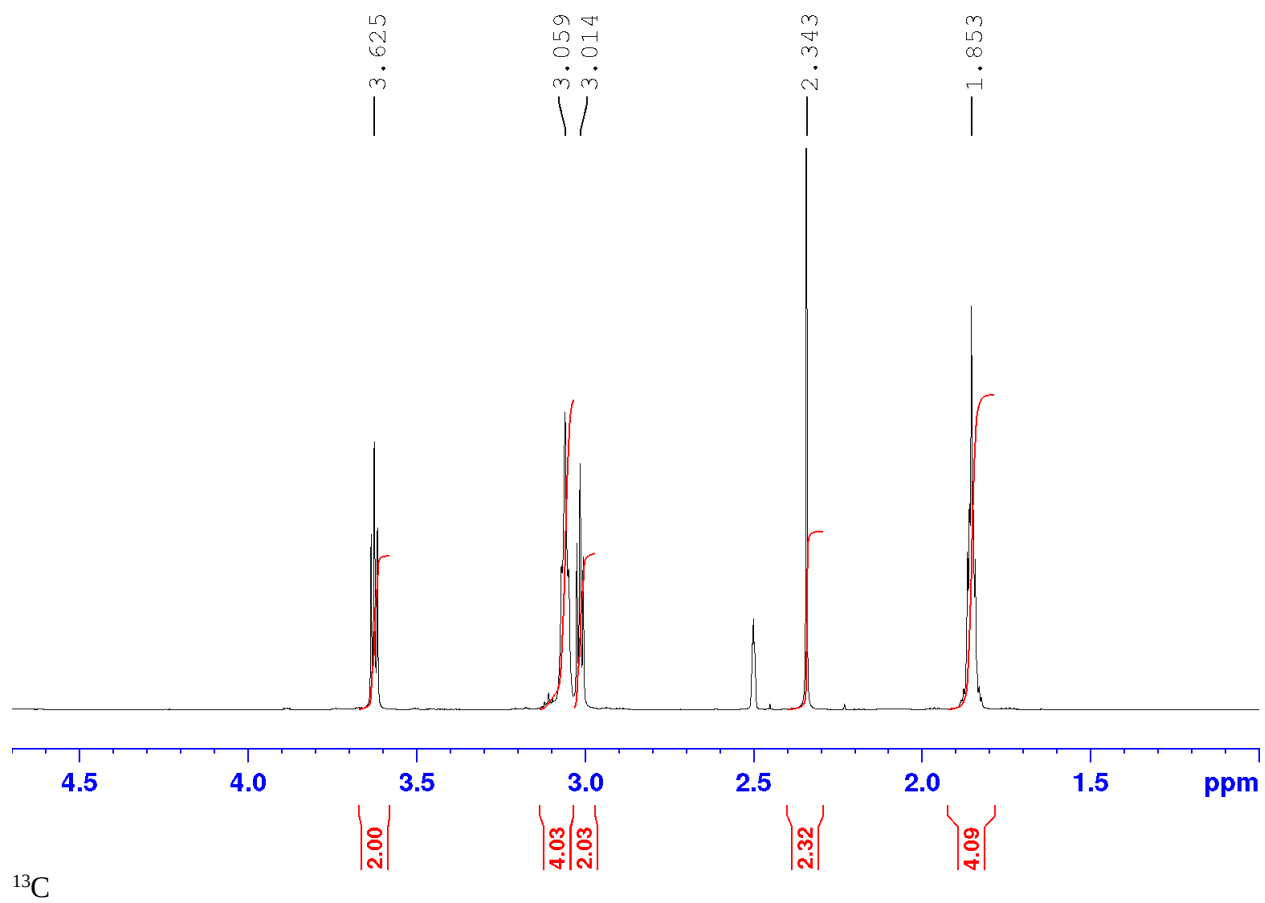


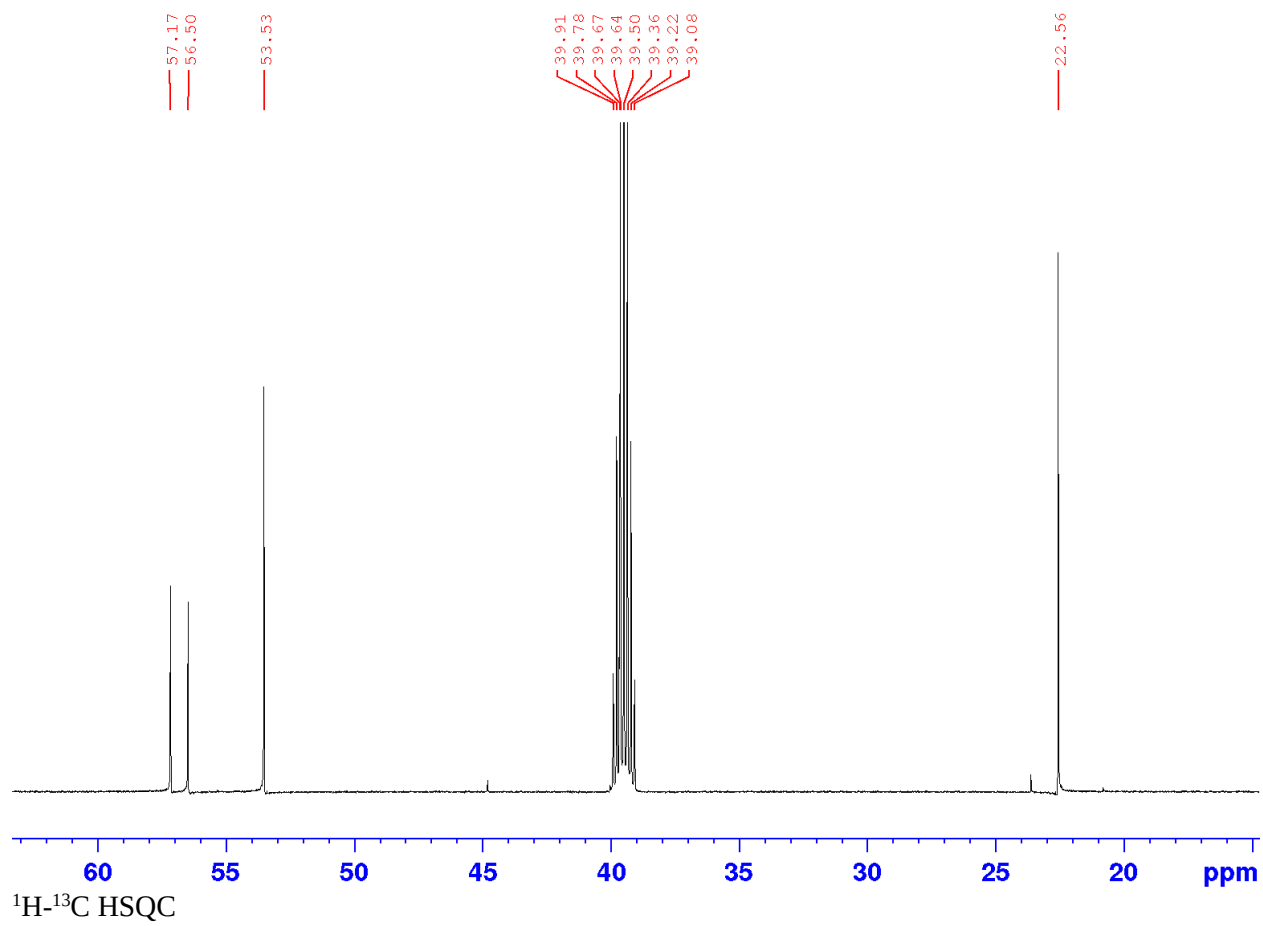


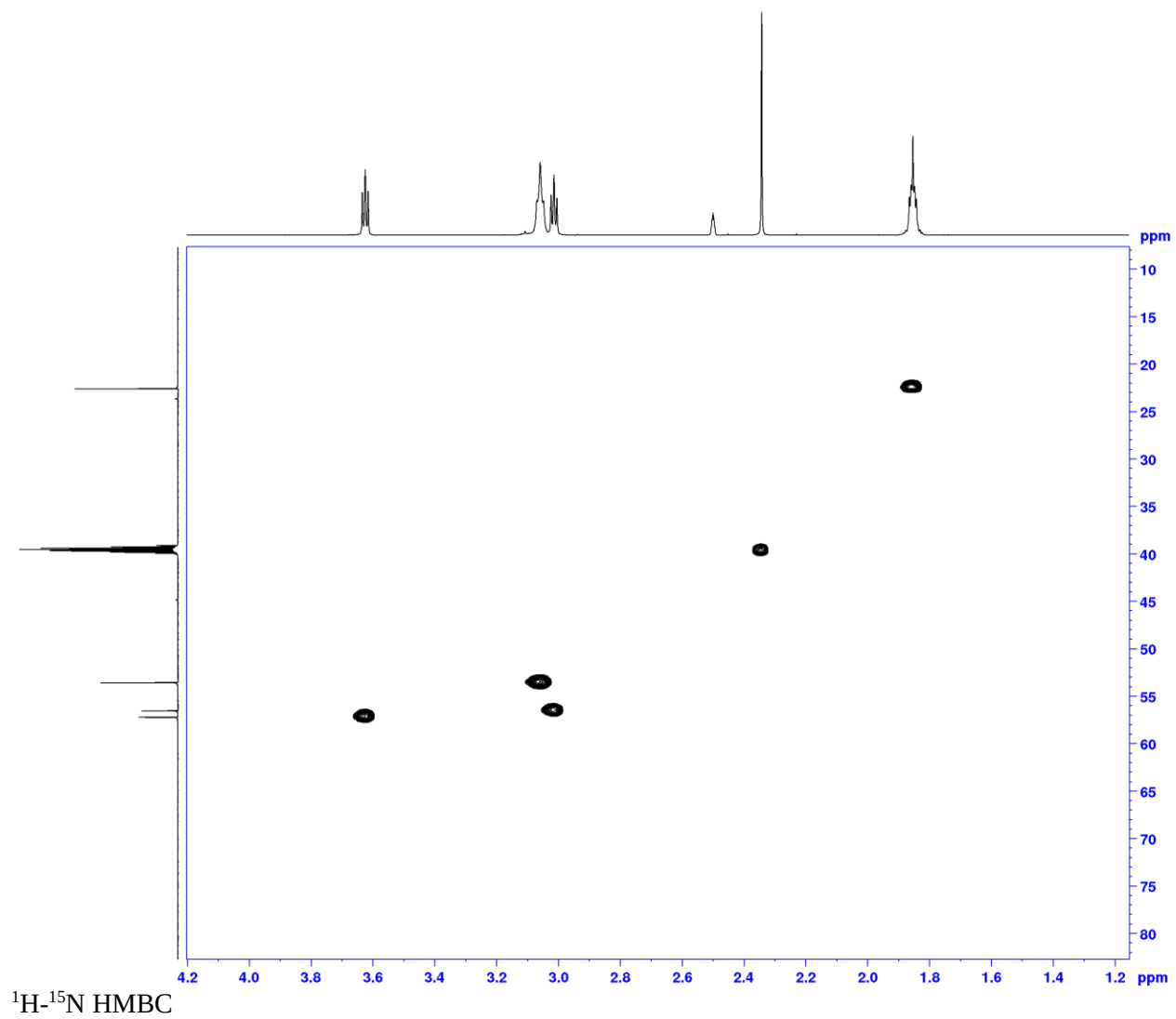


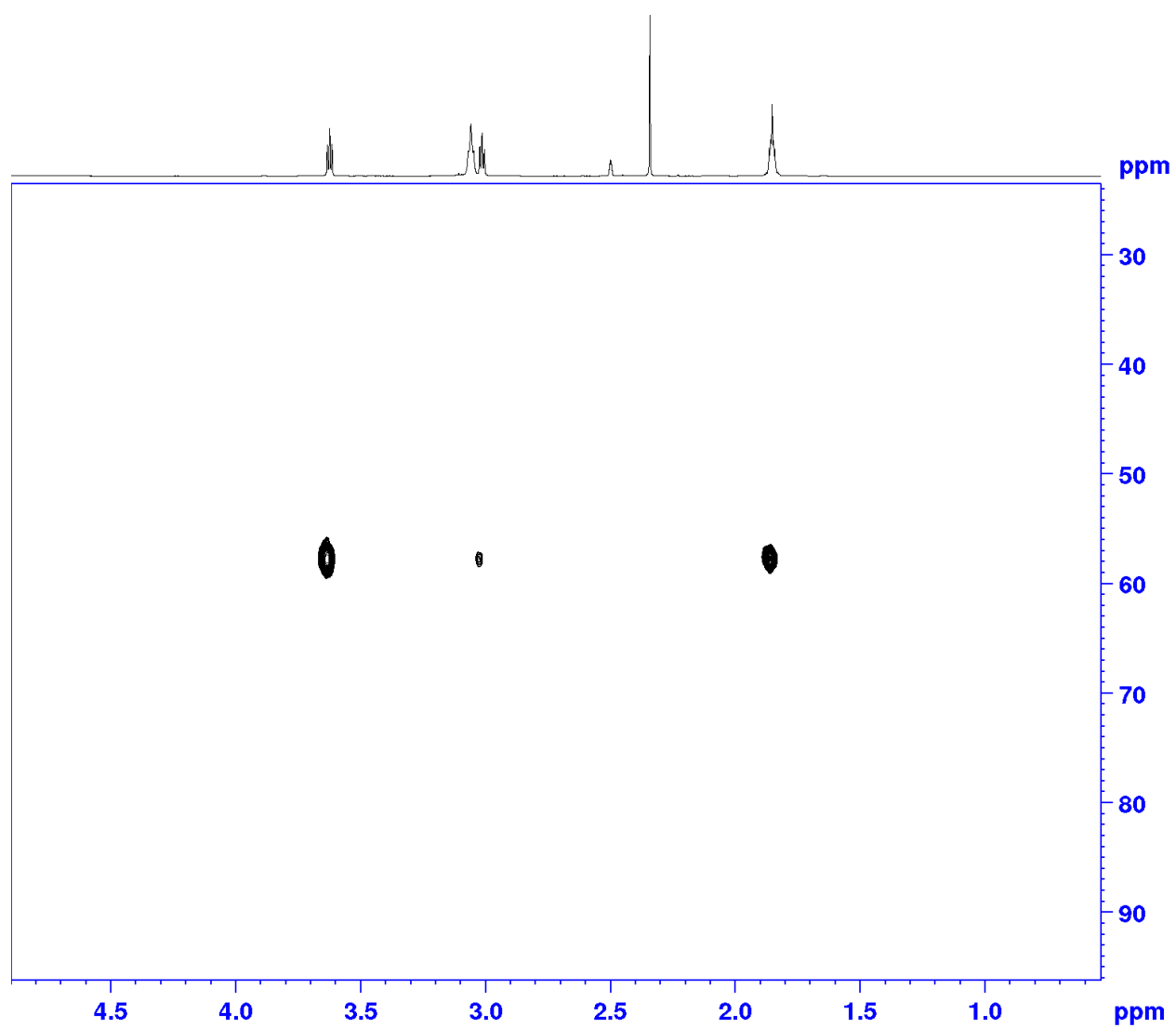
2-(pyrrolidin-1-yl)ethan-1-ol (**10**)

^1H



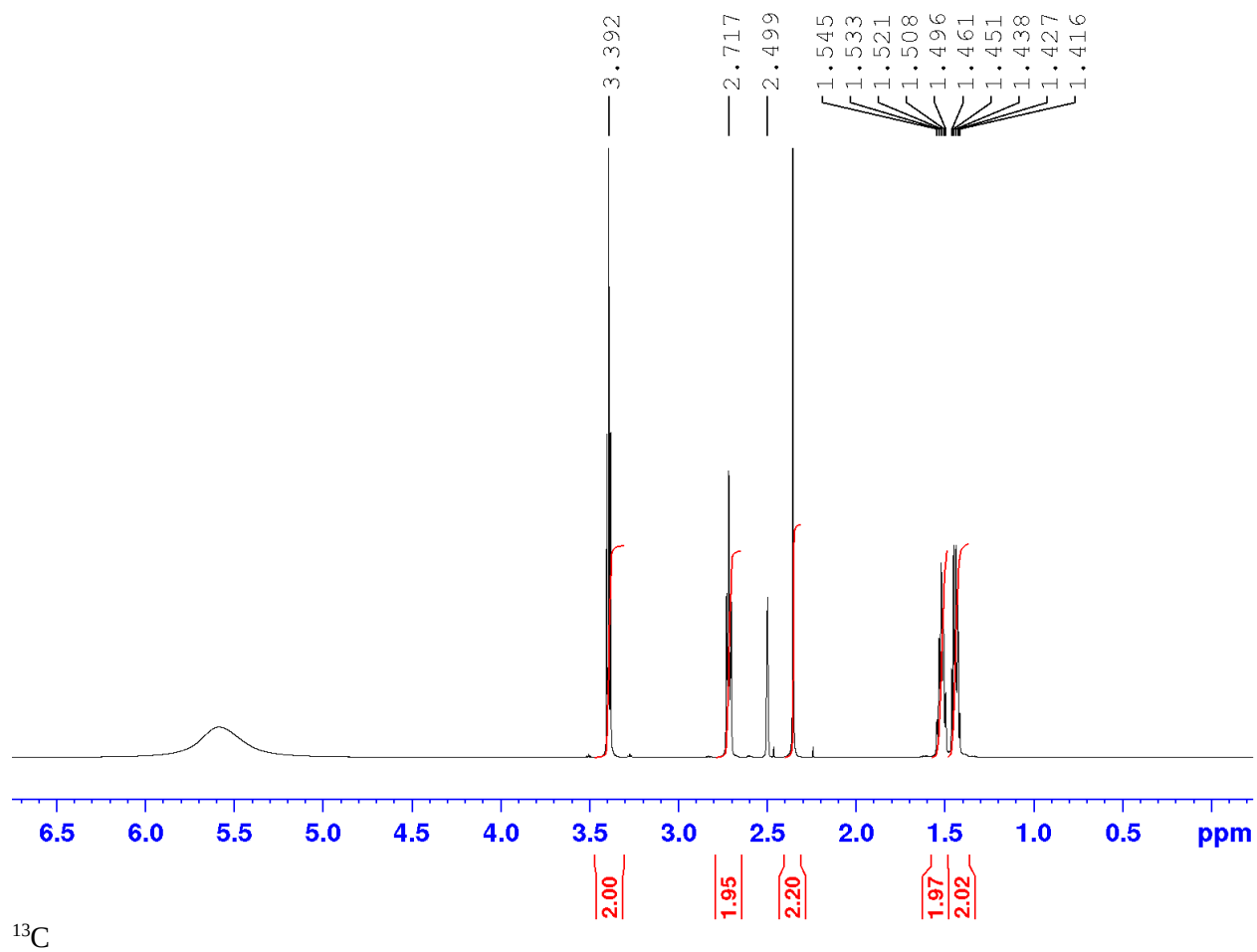


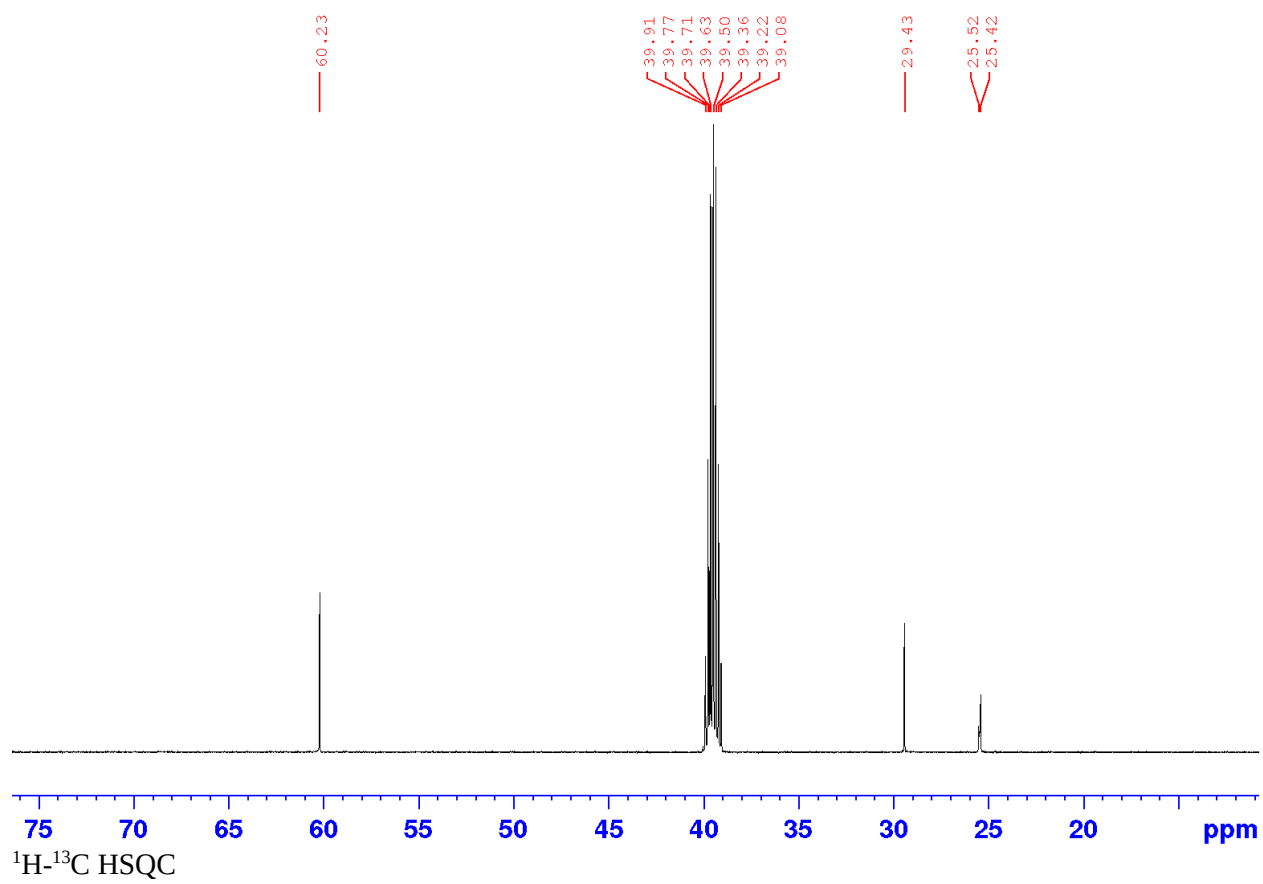


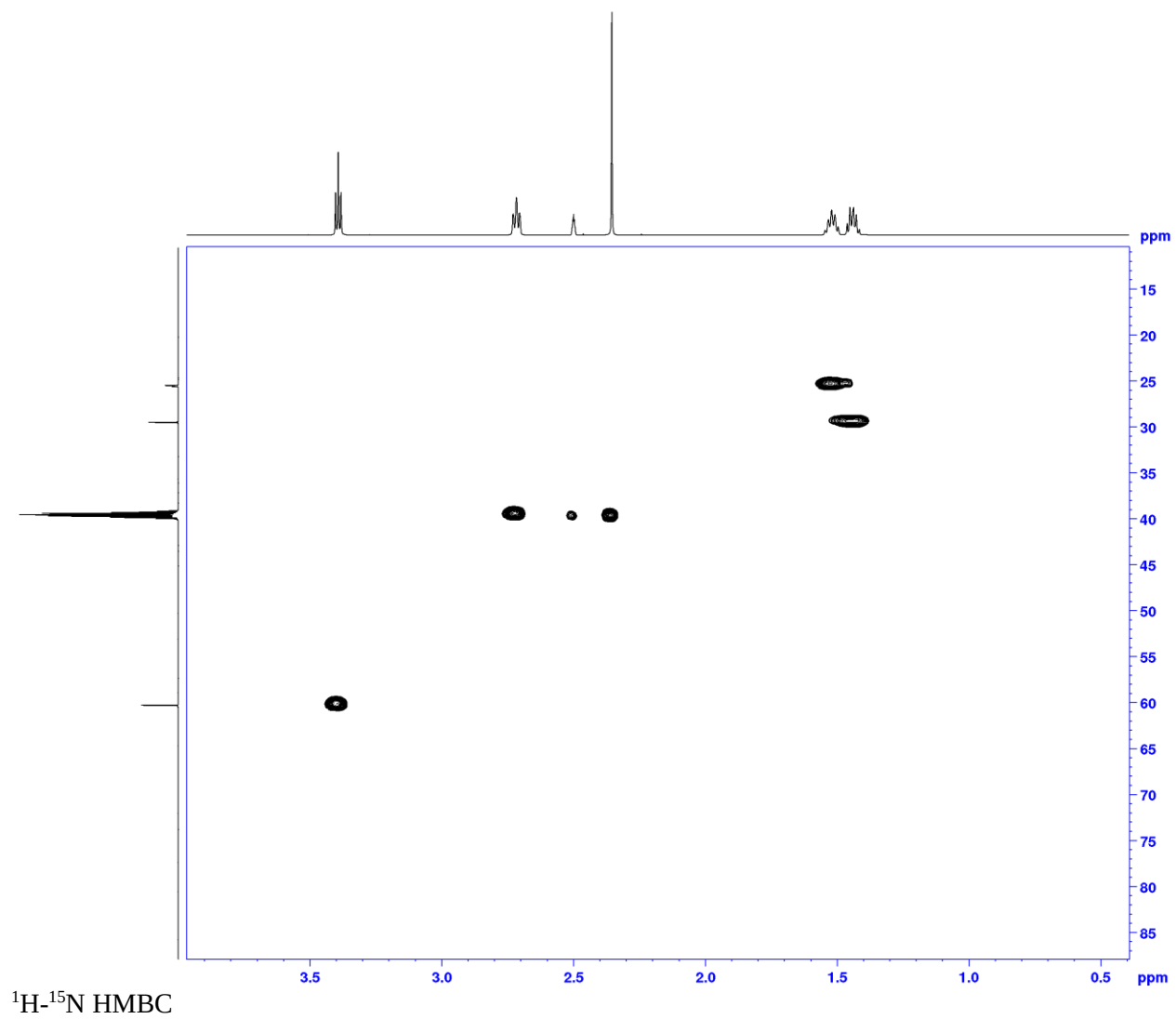


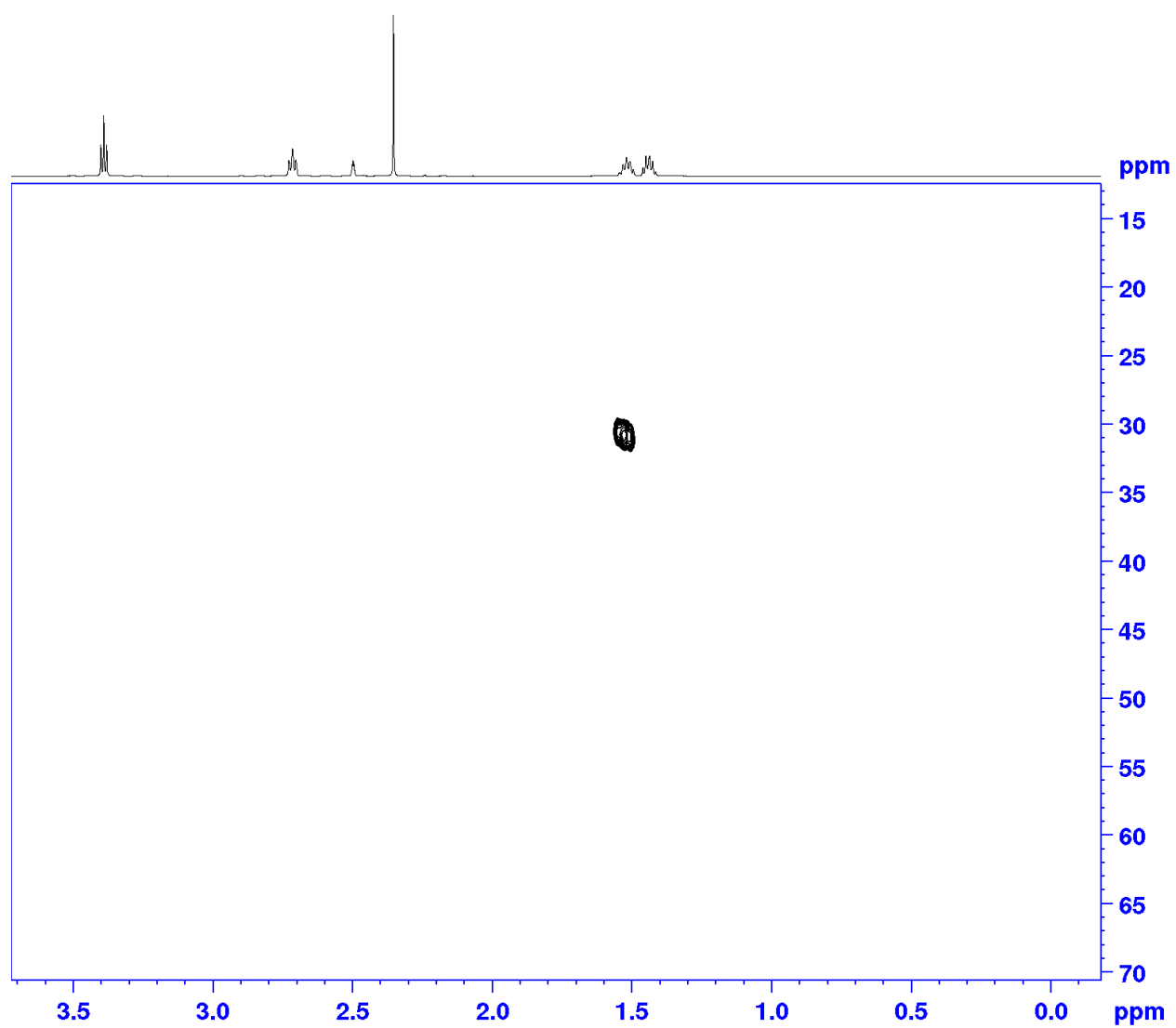
4-aminobutan-1-ol (**11**)

^1H



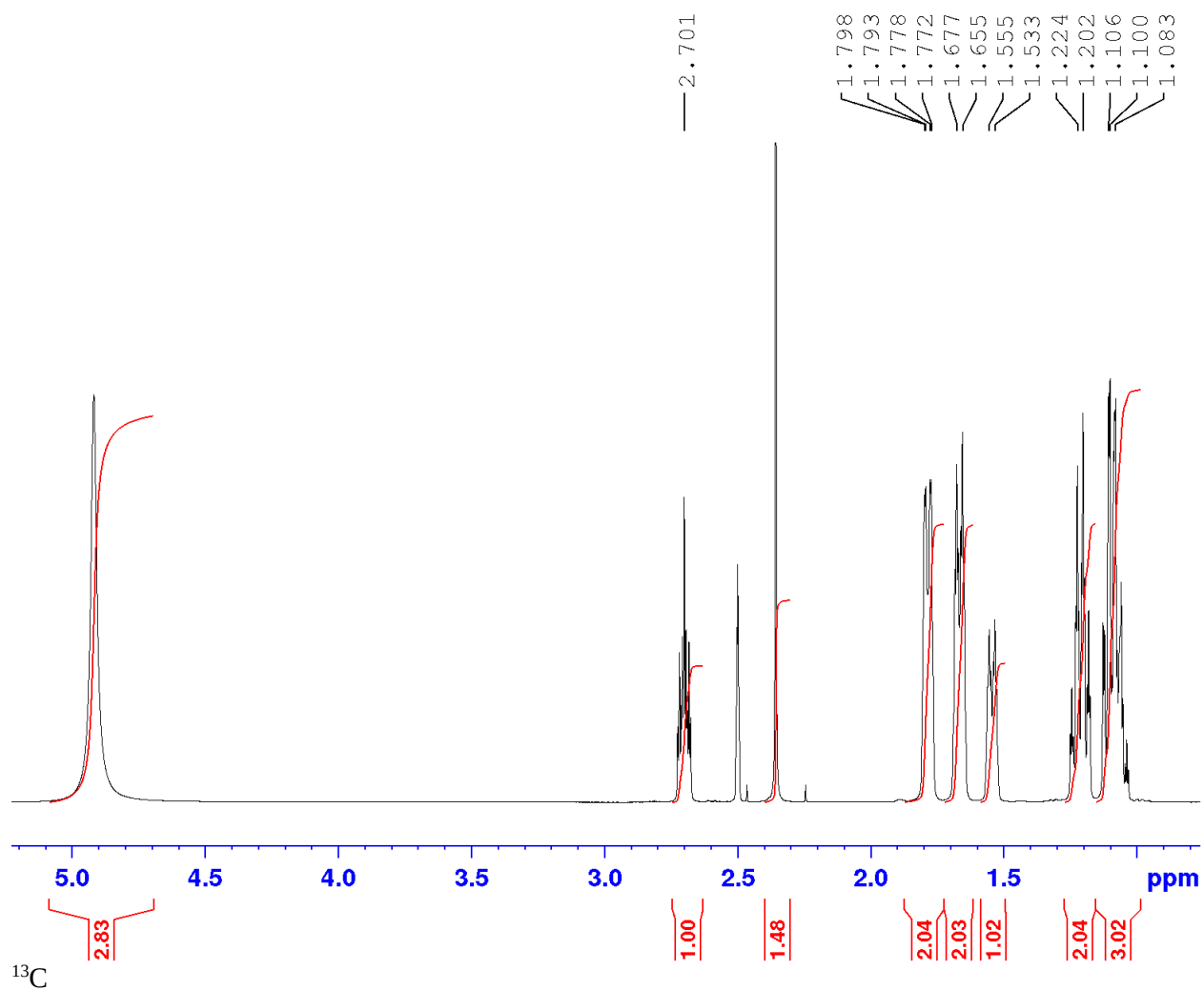


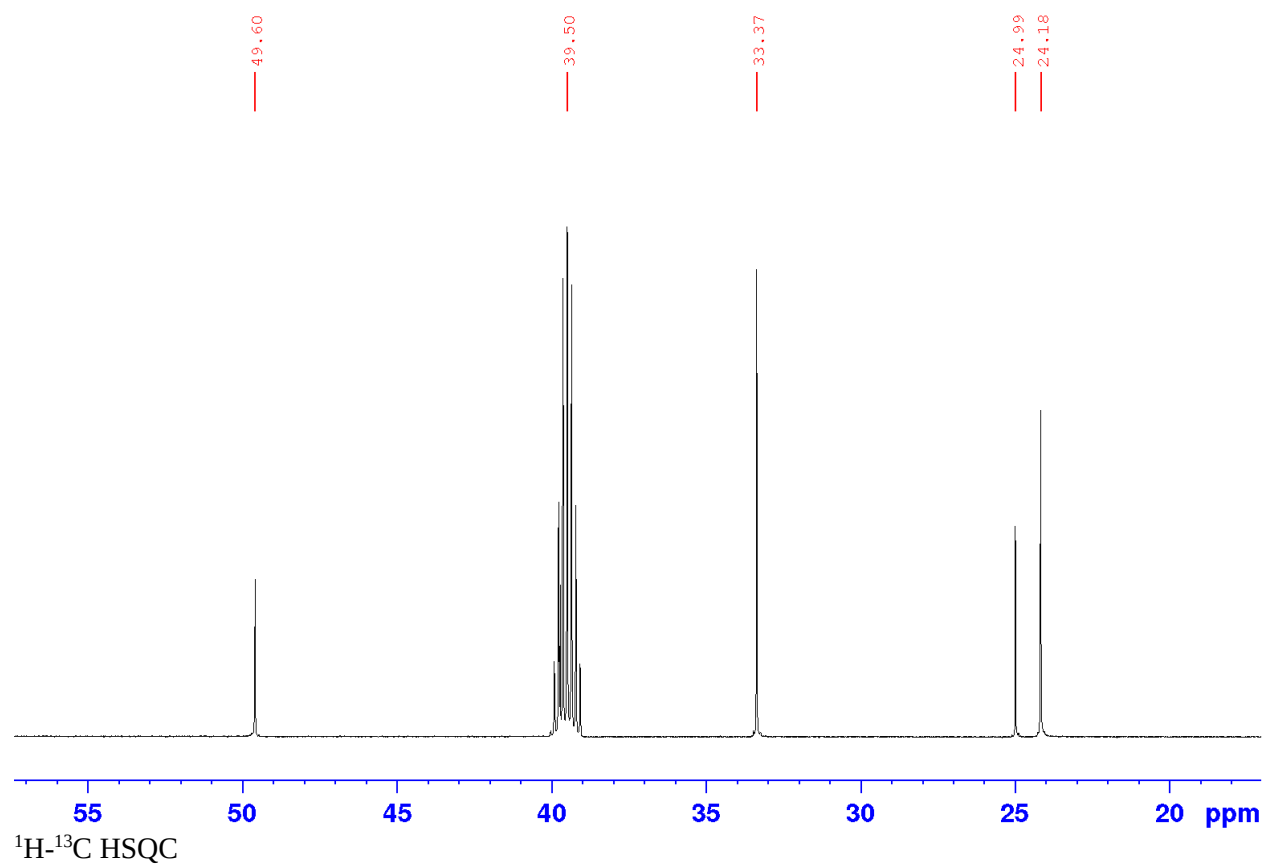


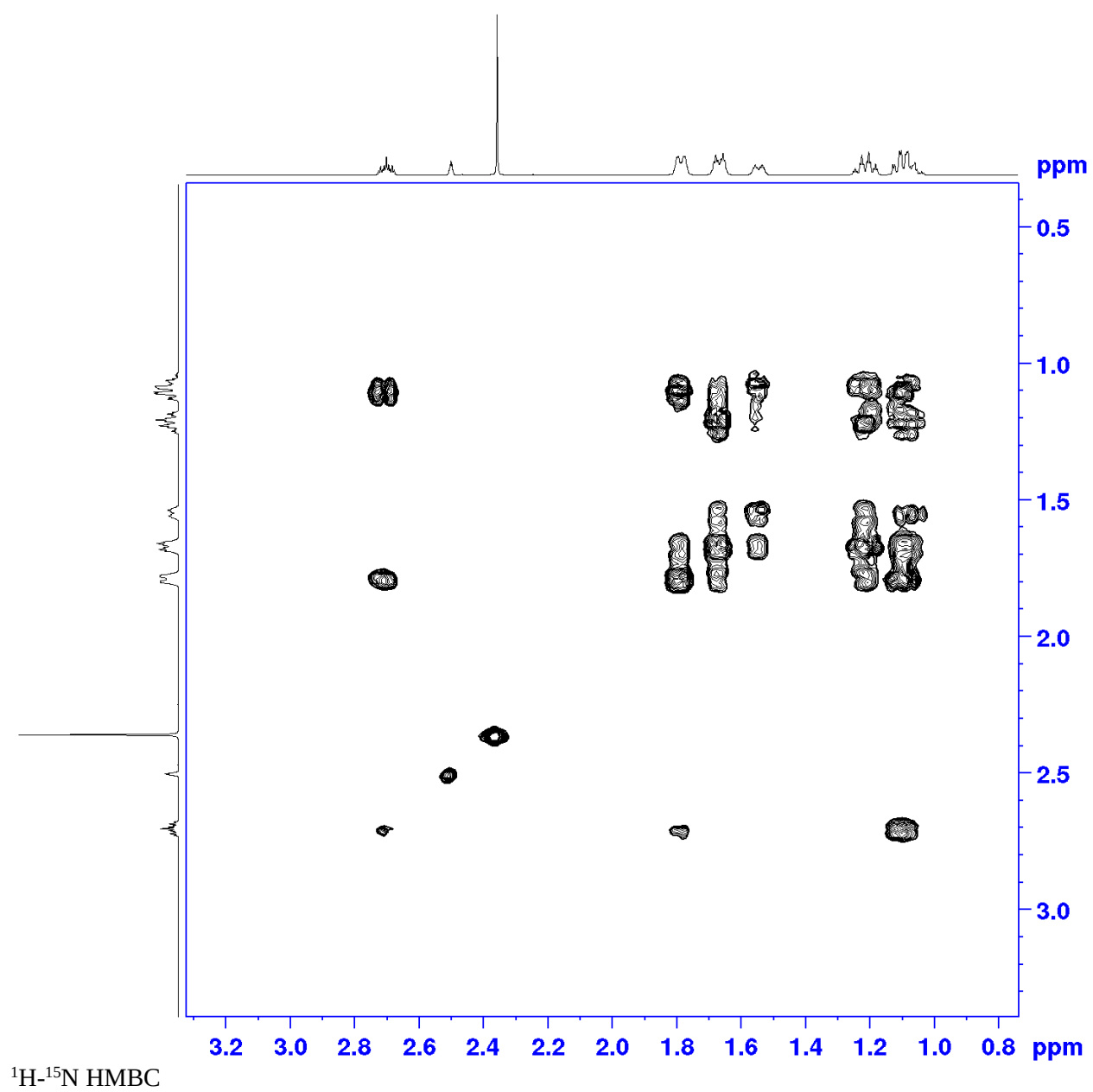


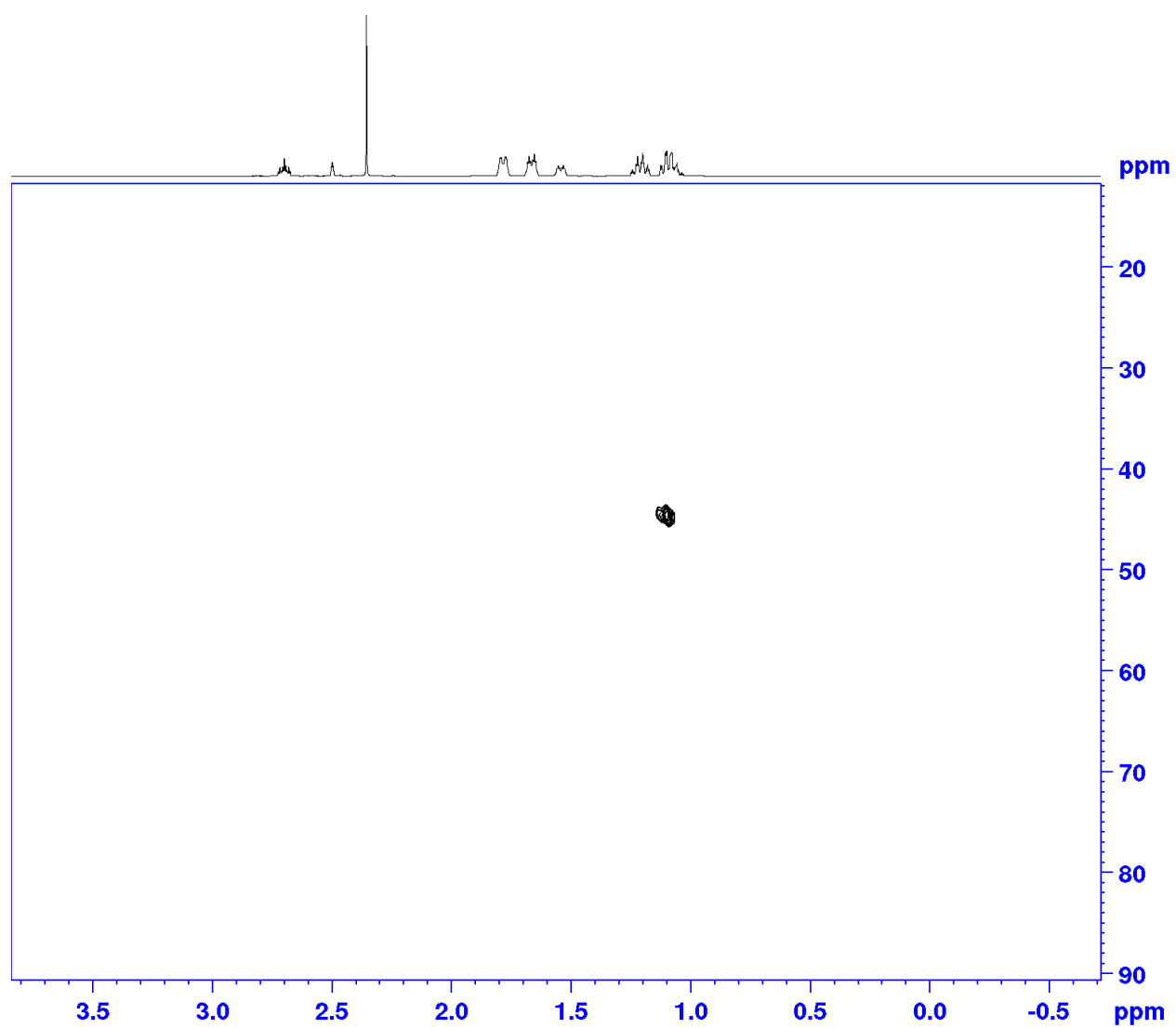
cyclohexanamine (**12**)

^1H



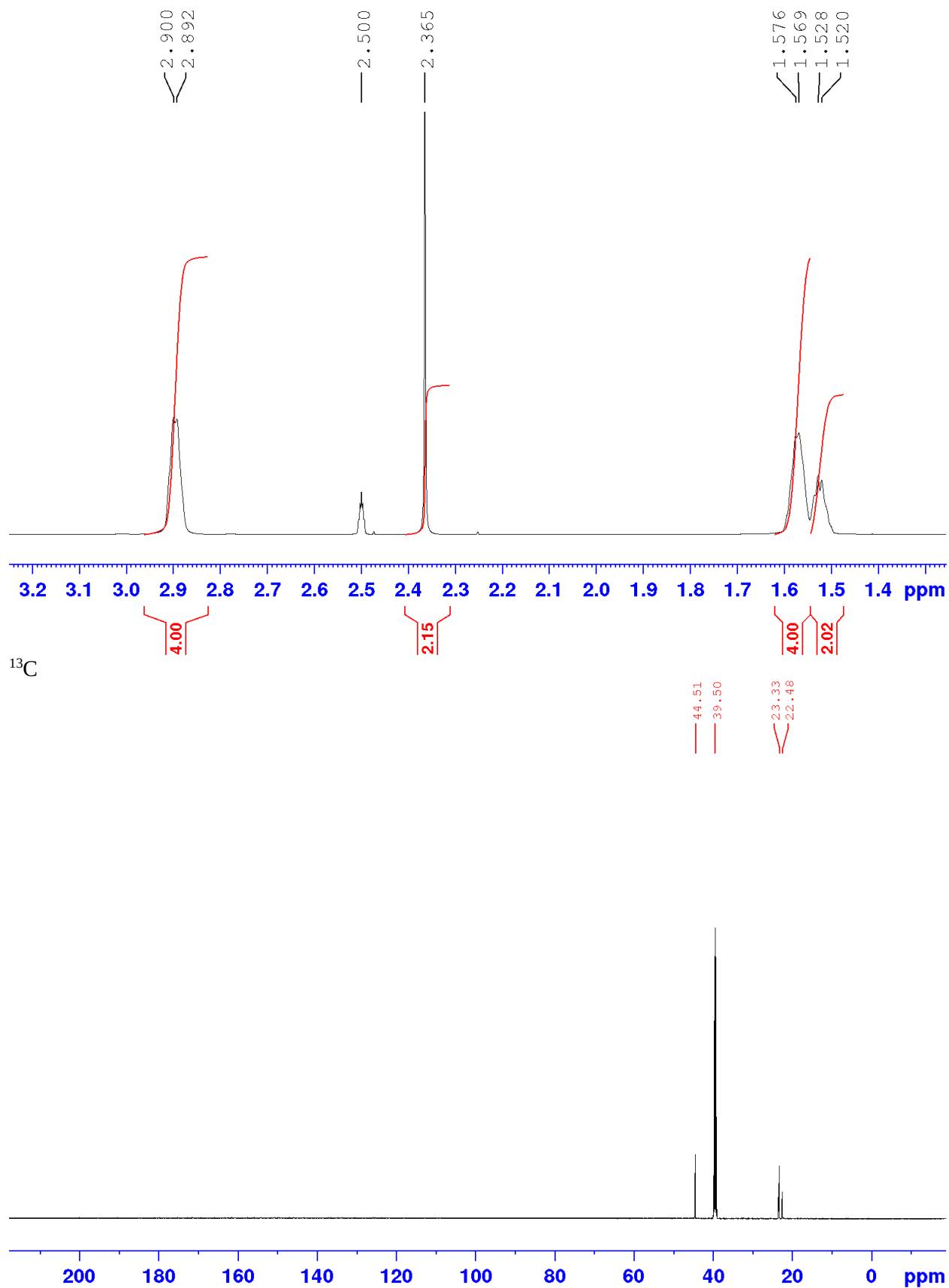




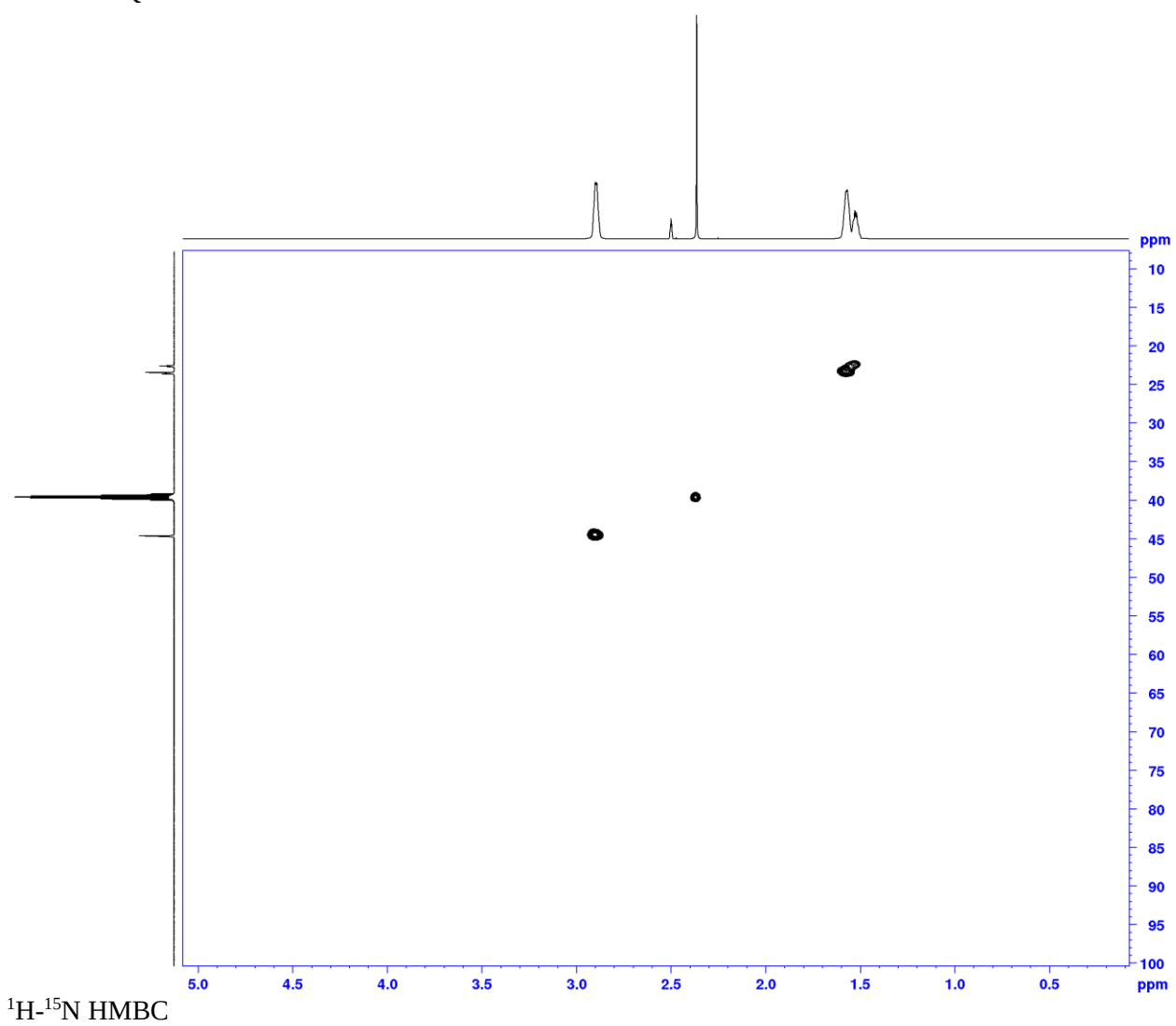


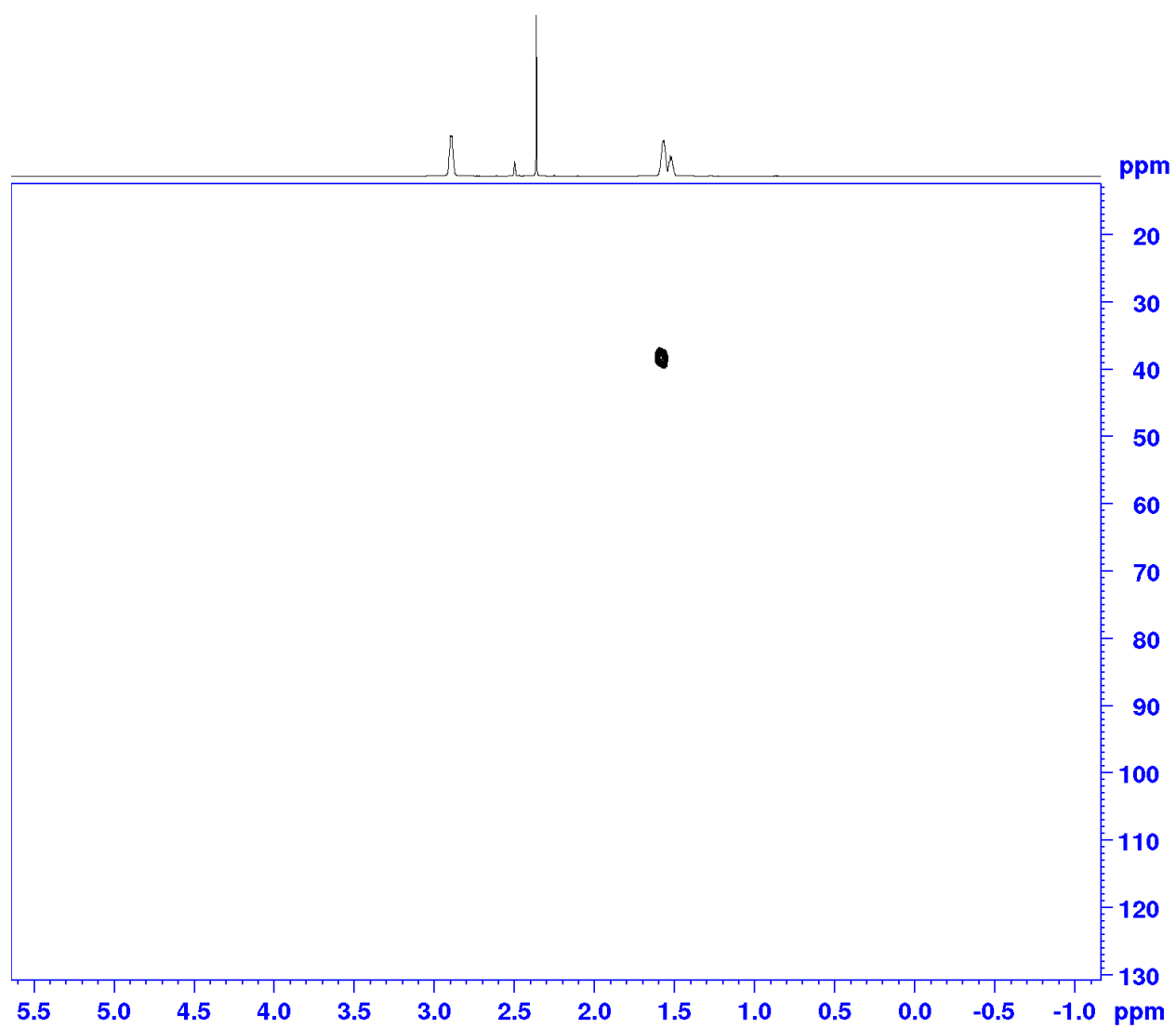
piperidine (13)

^1H



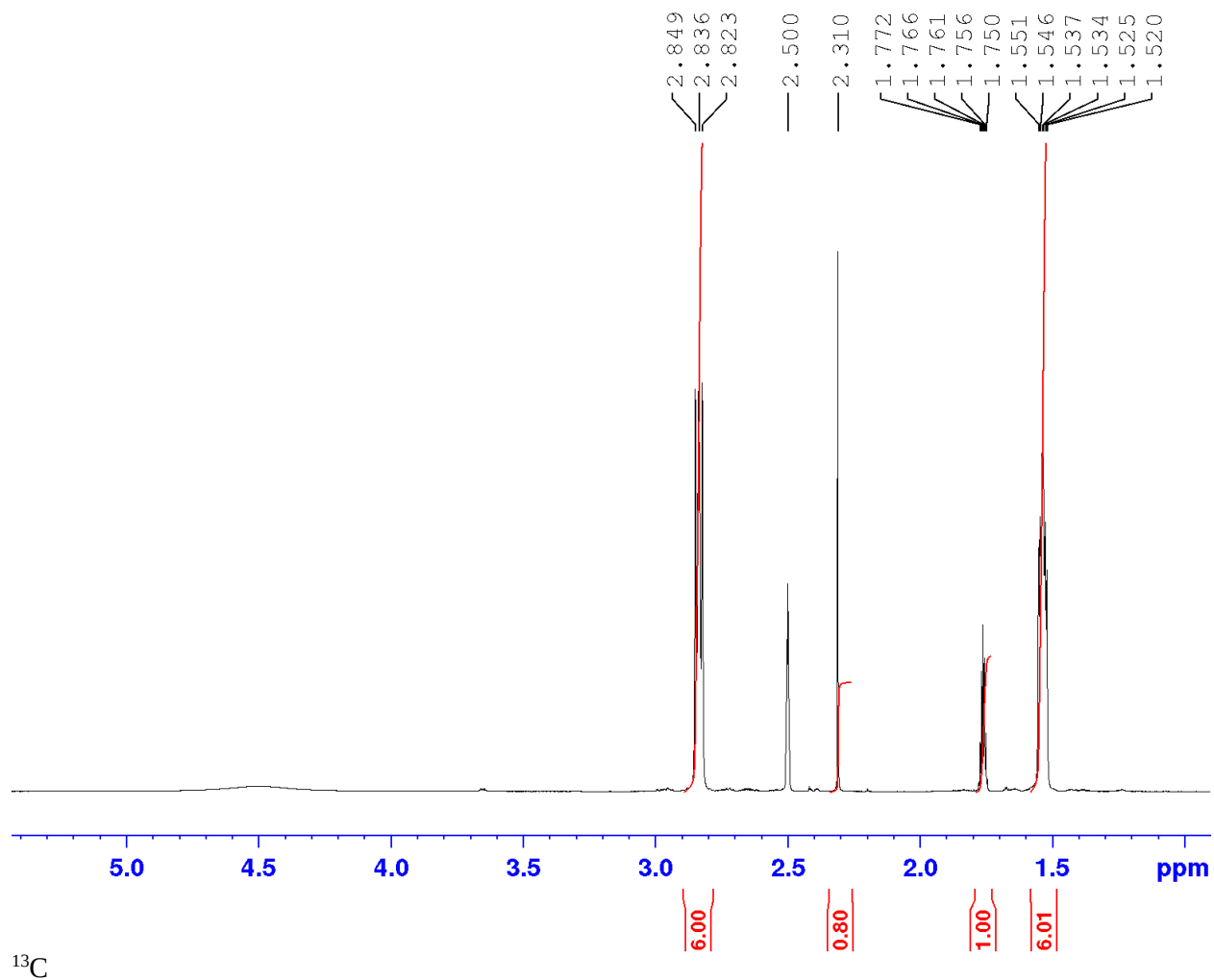
^1H - ^{13}C HSQC

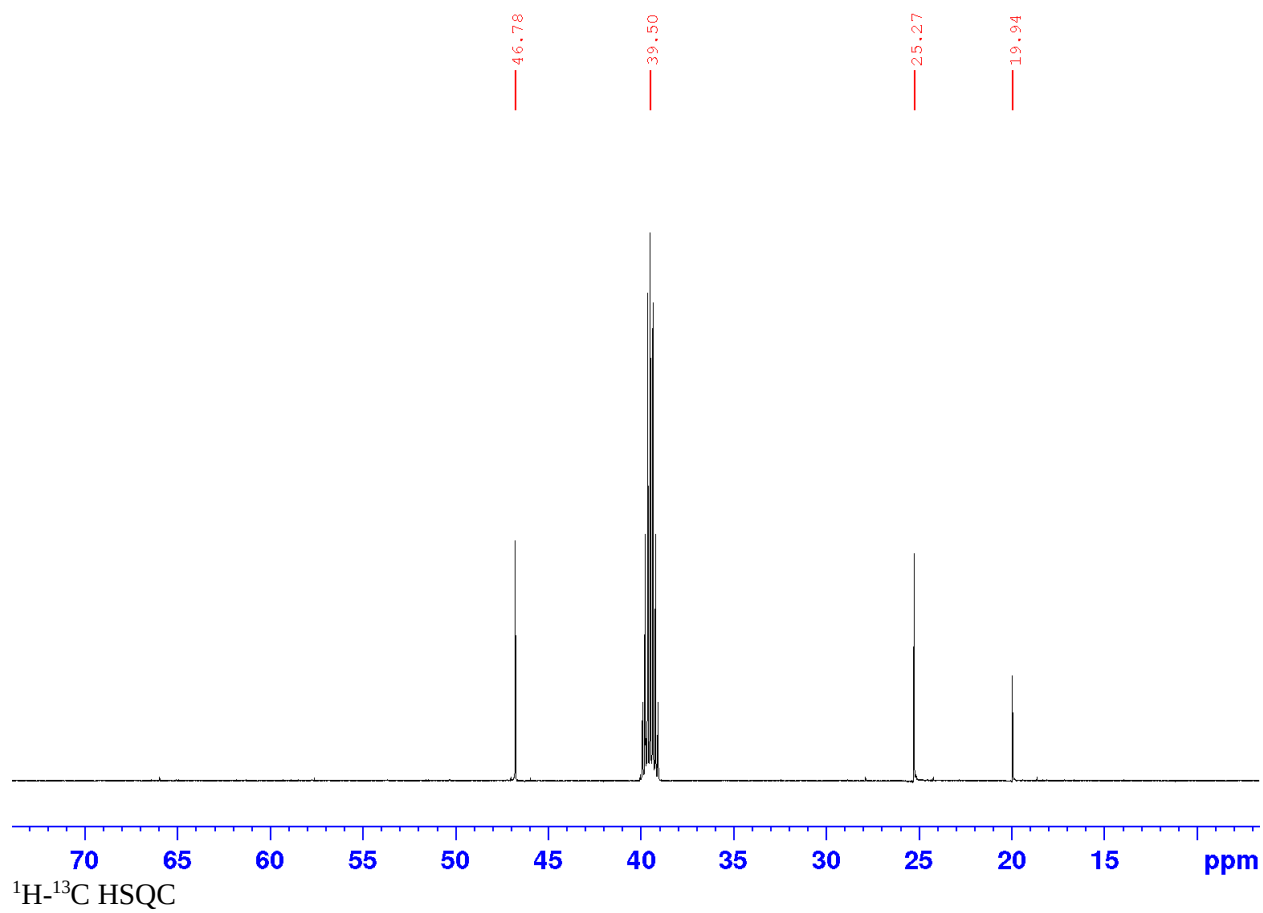


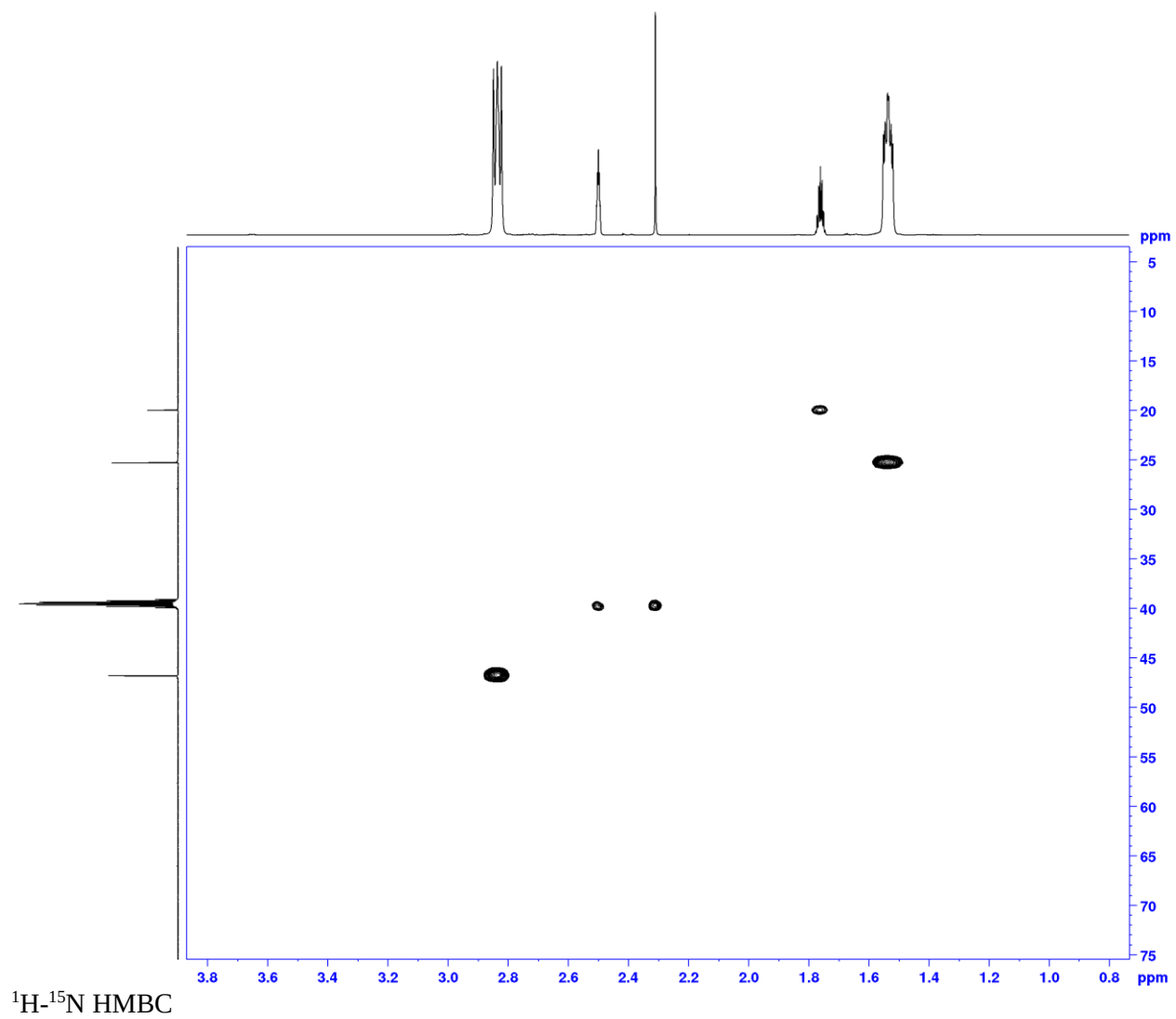


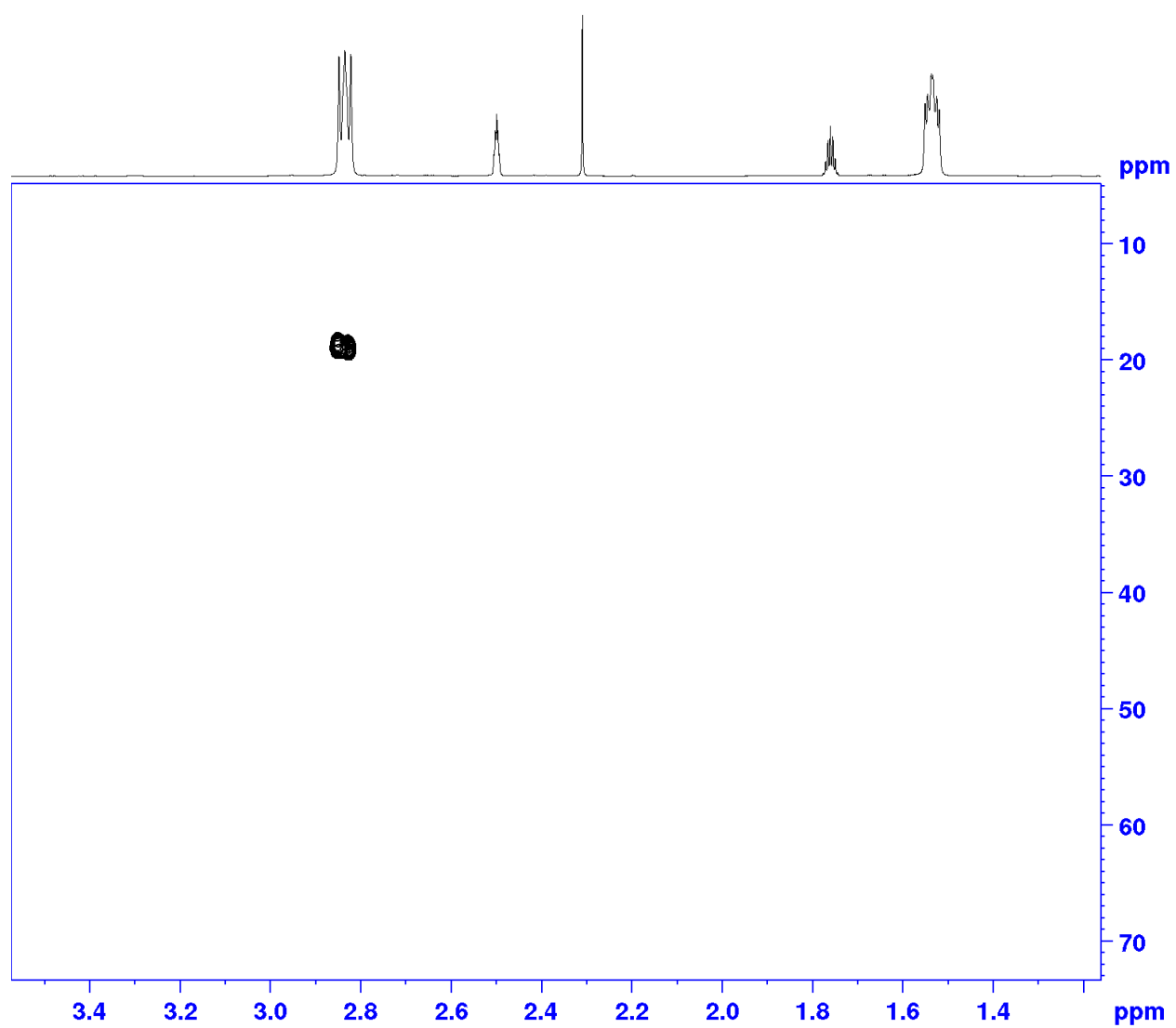
quinuclidine (**14**)

^1H



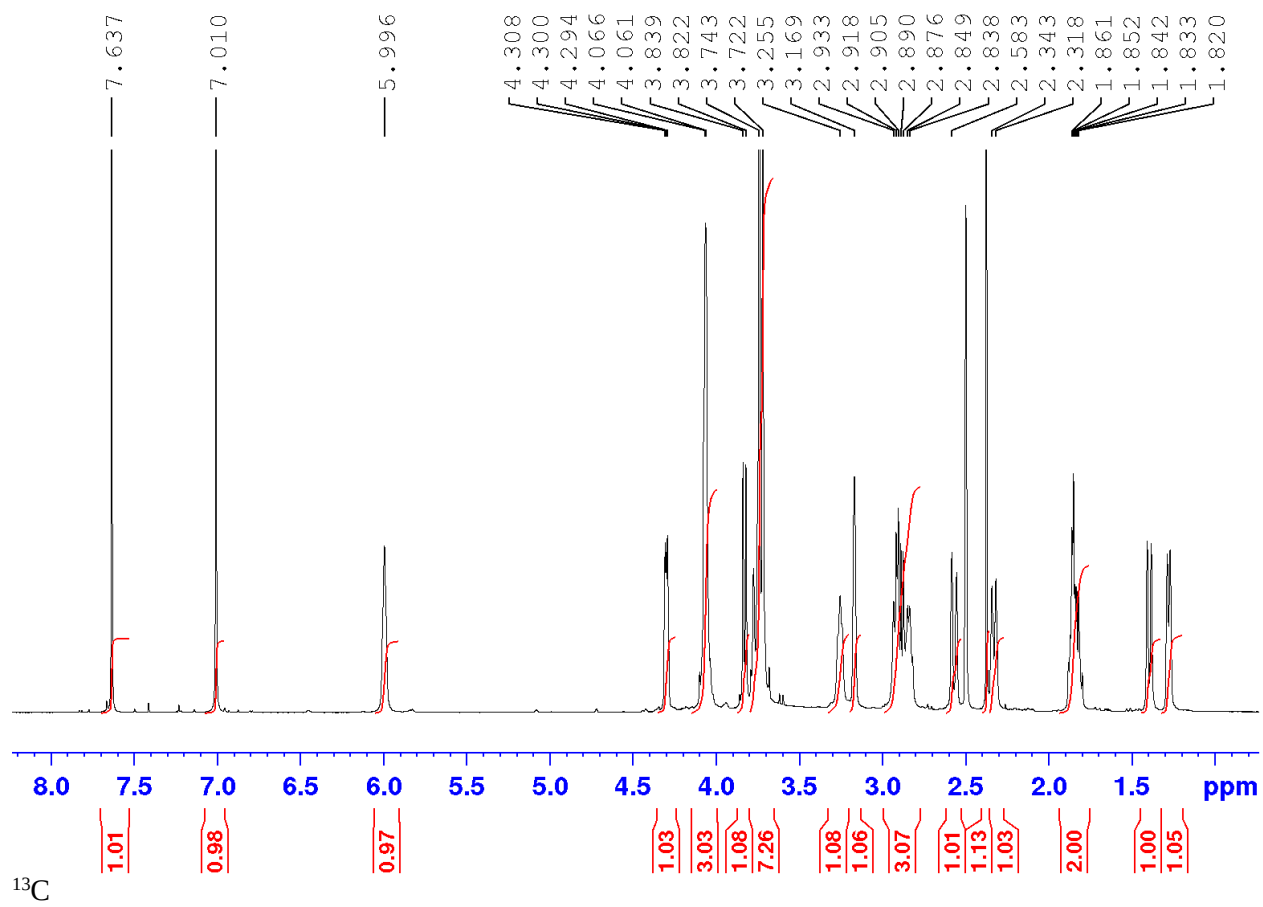


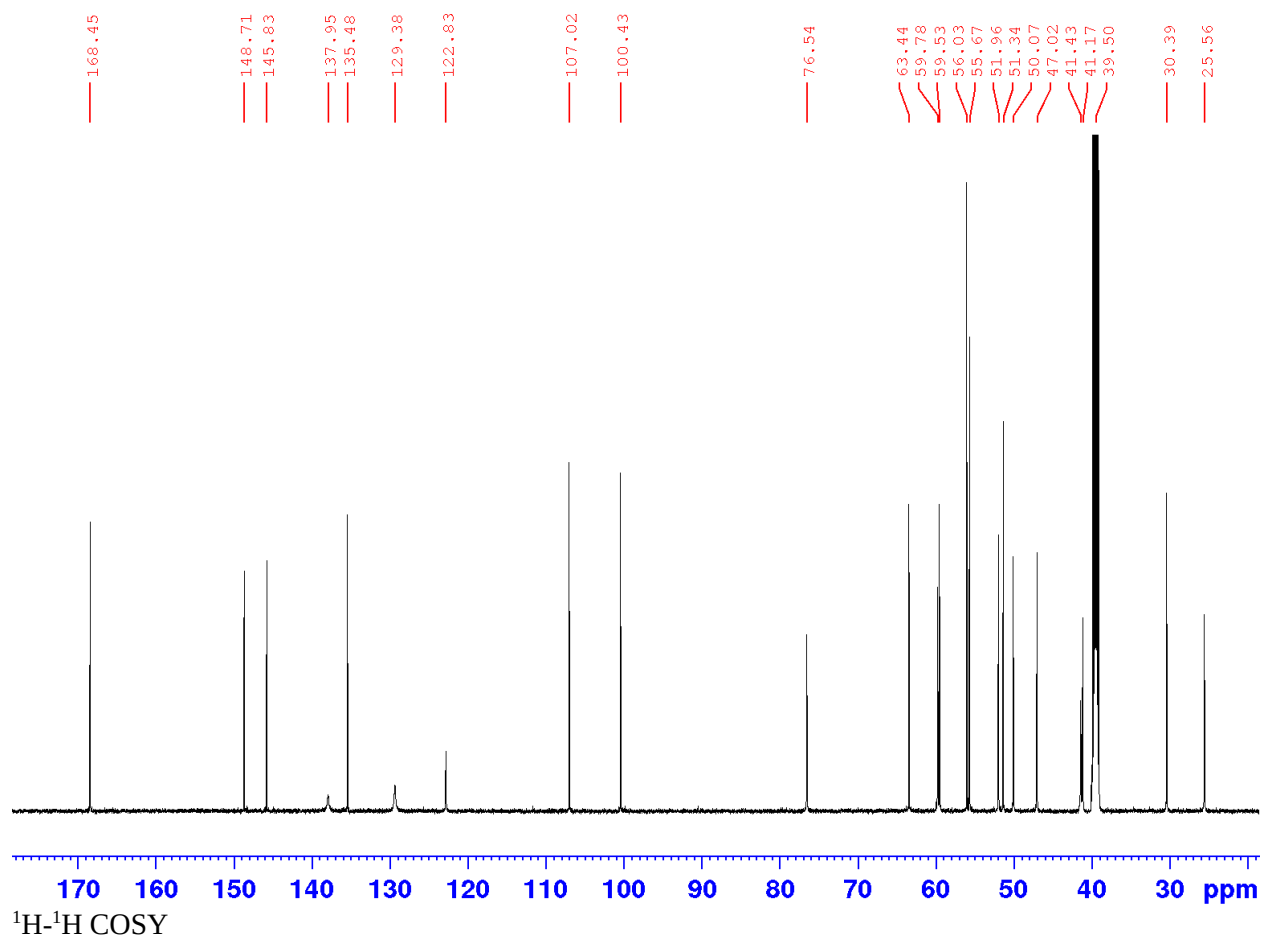


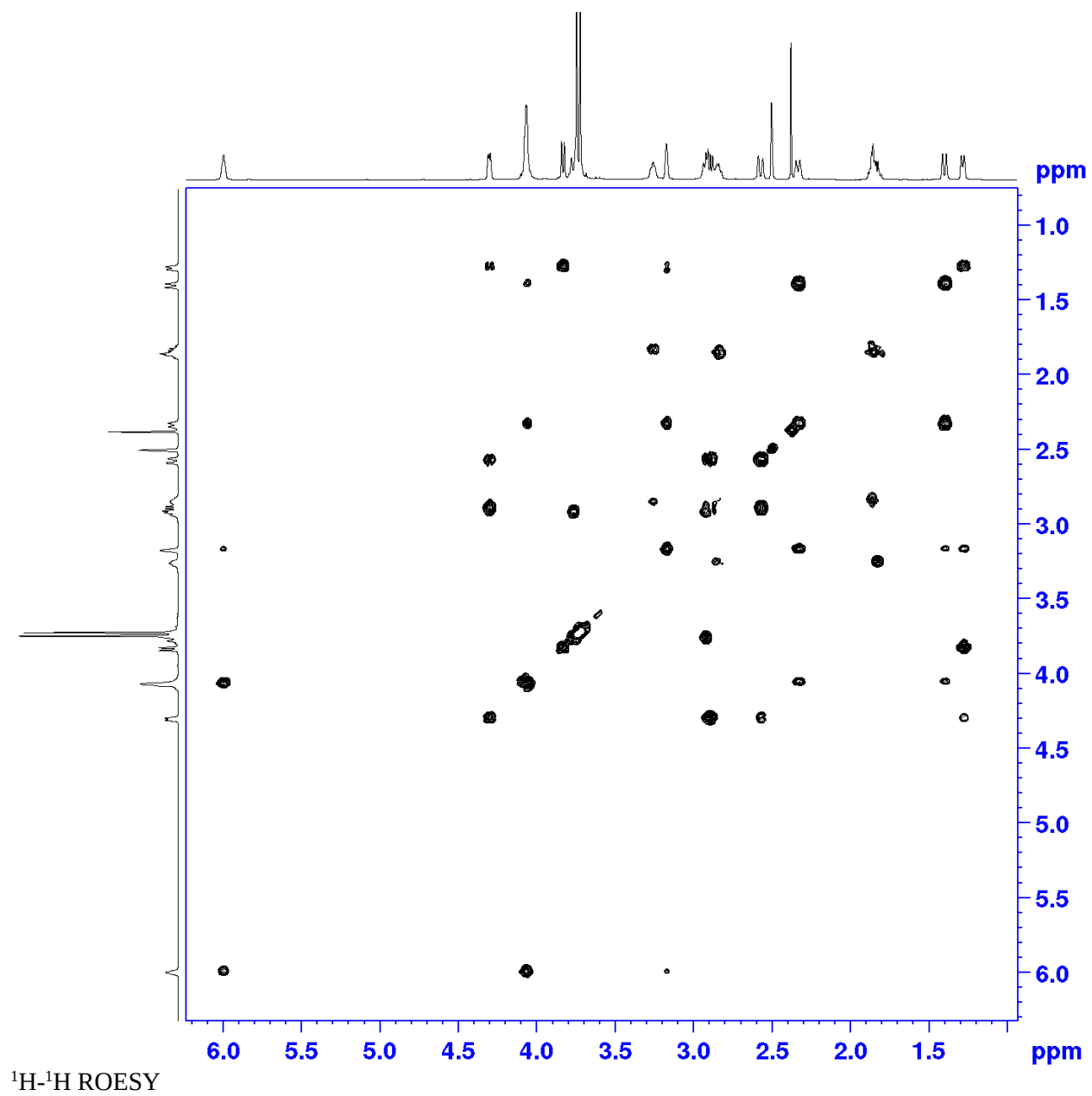


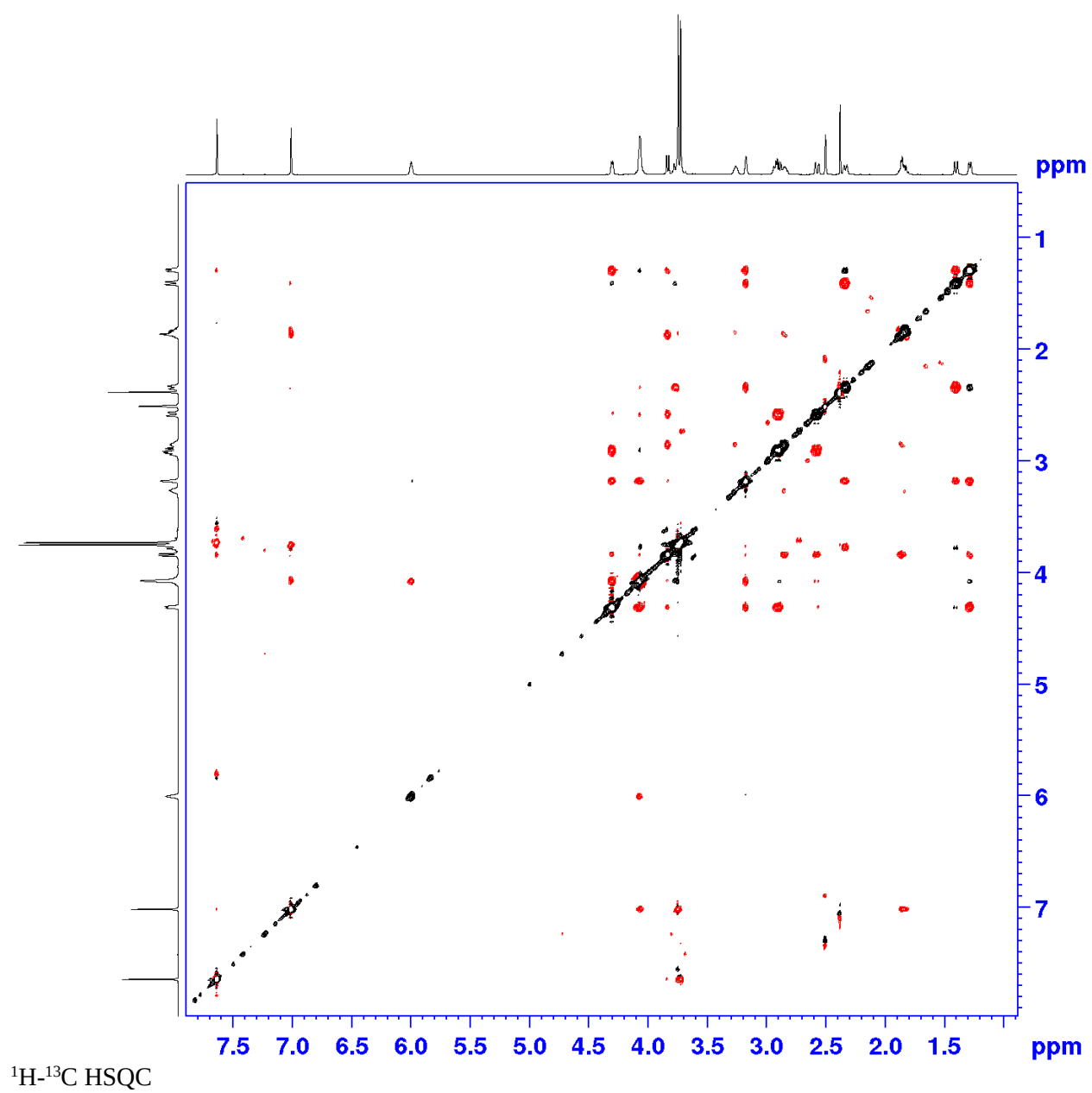
brucine (15) sample 1

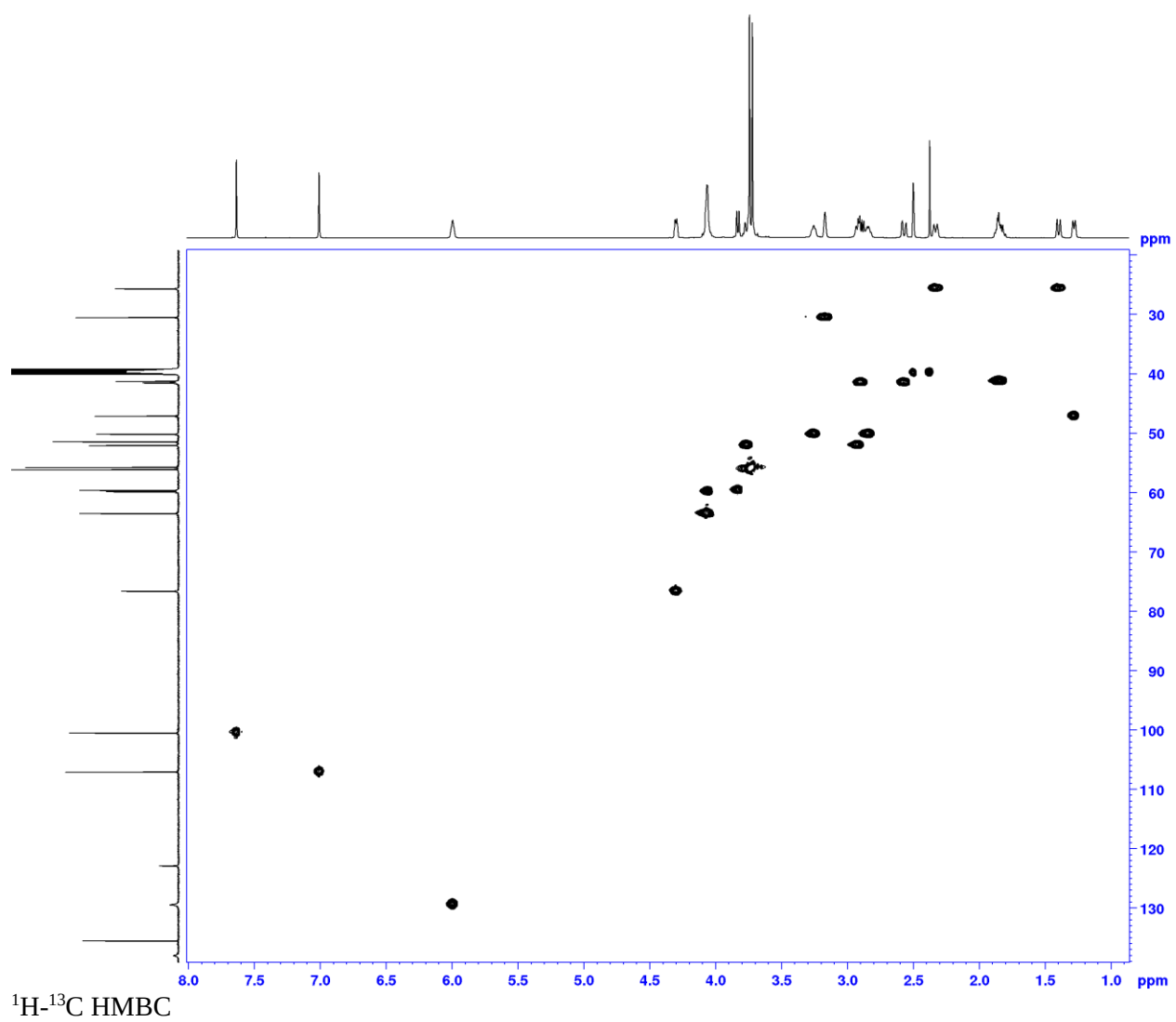
^1H

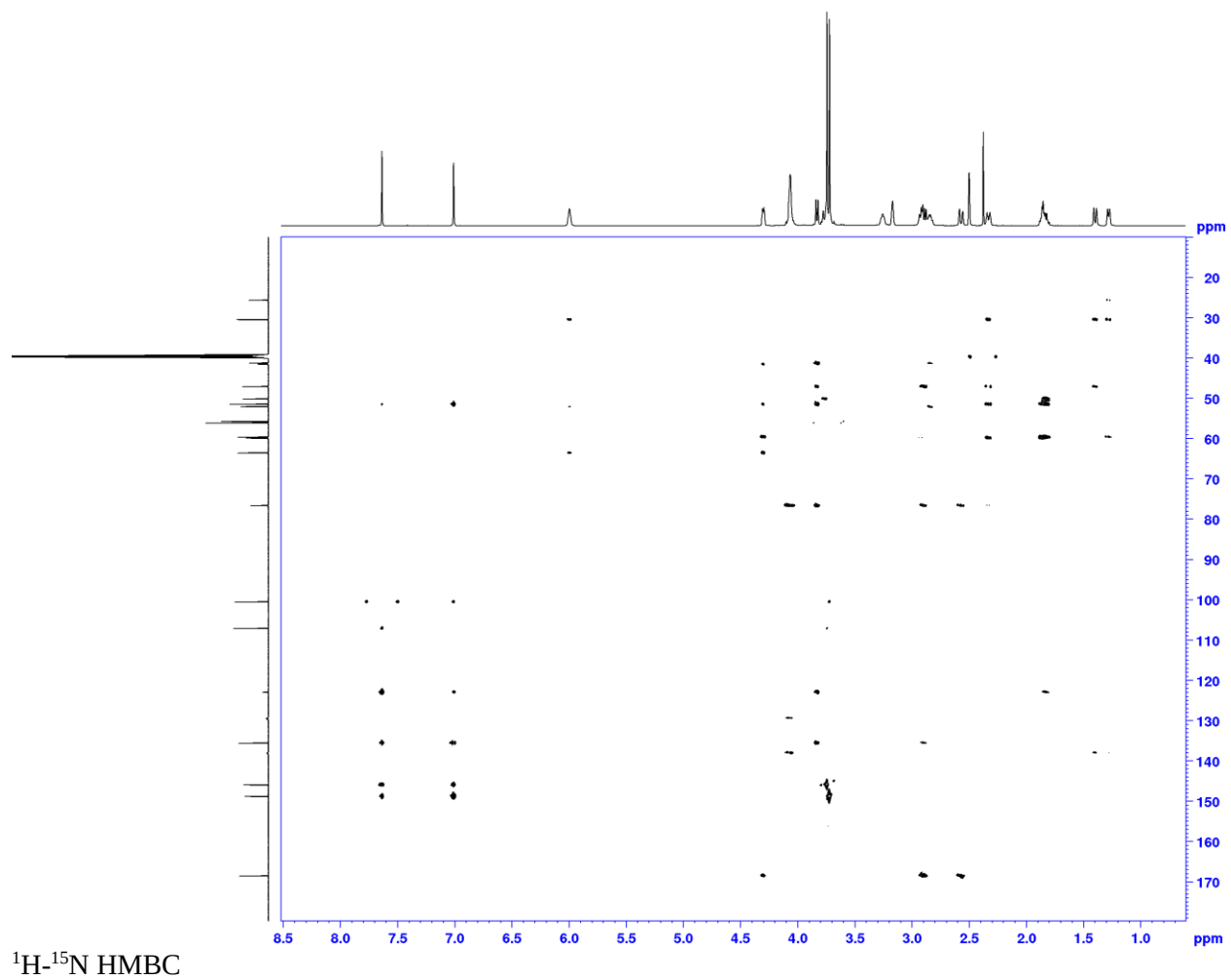


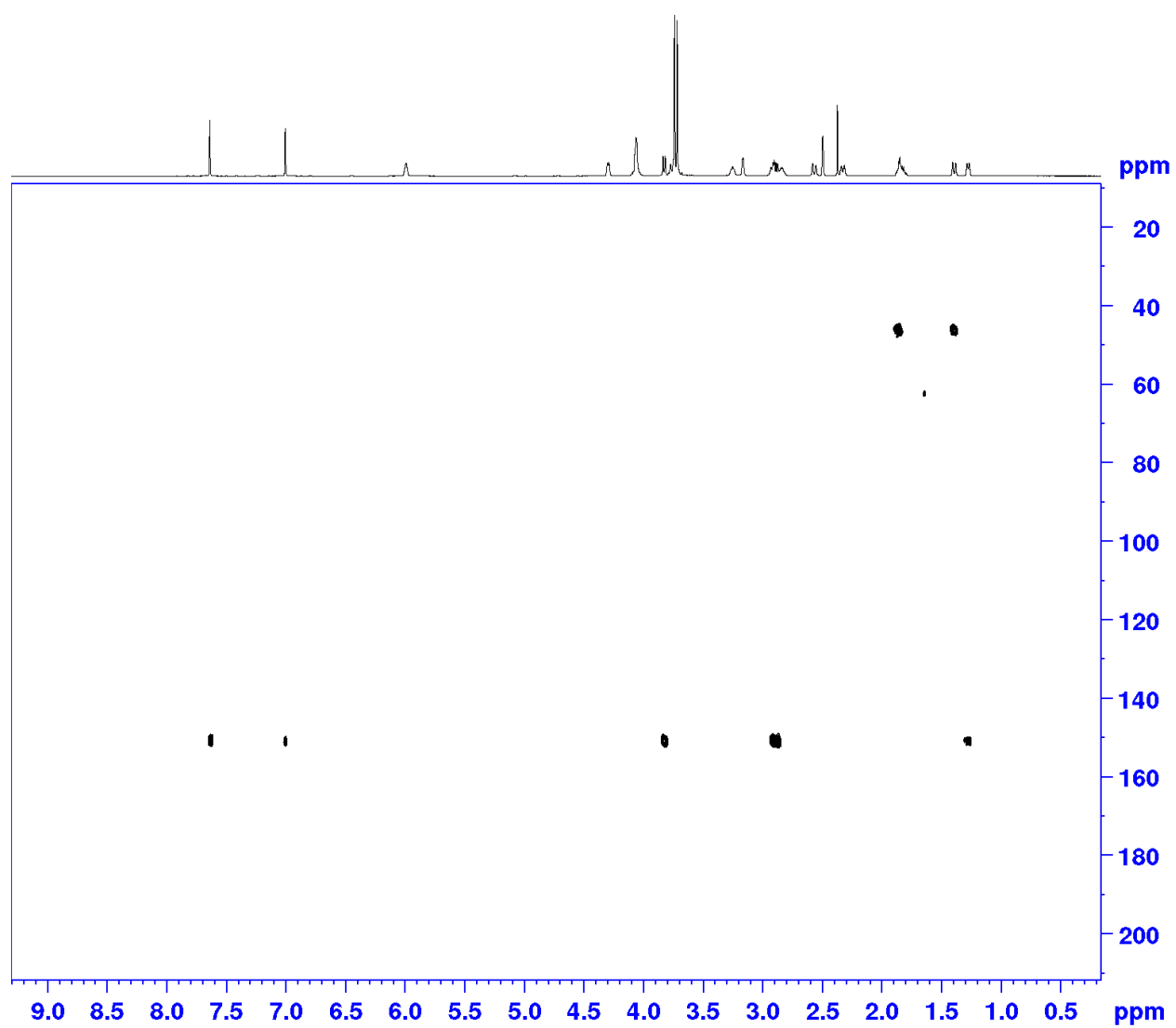






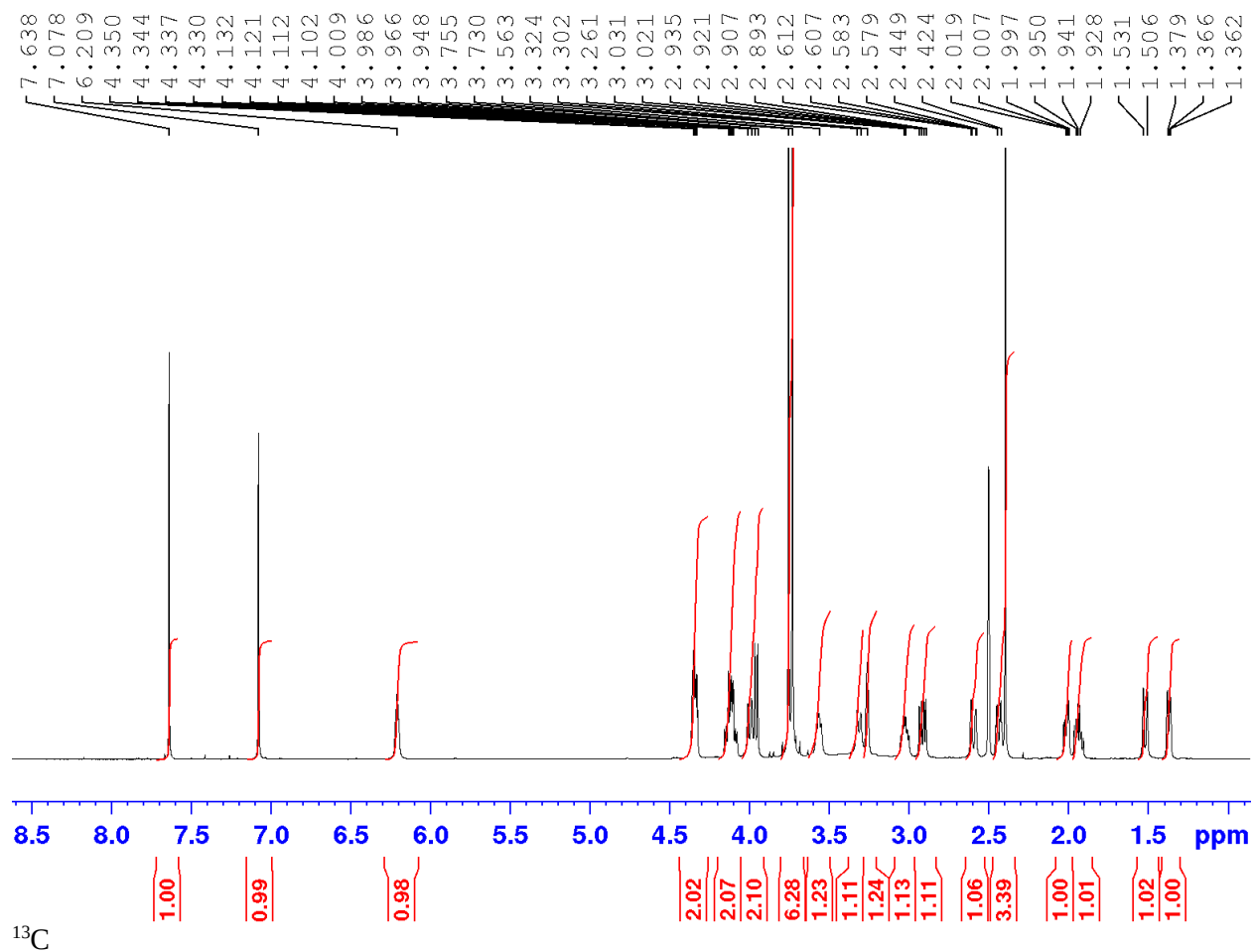


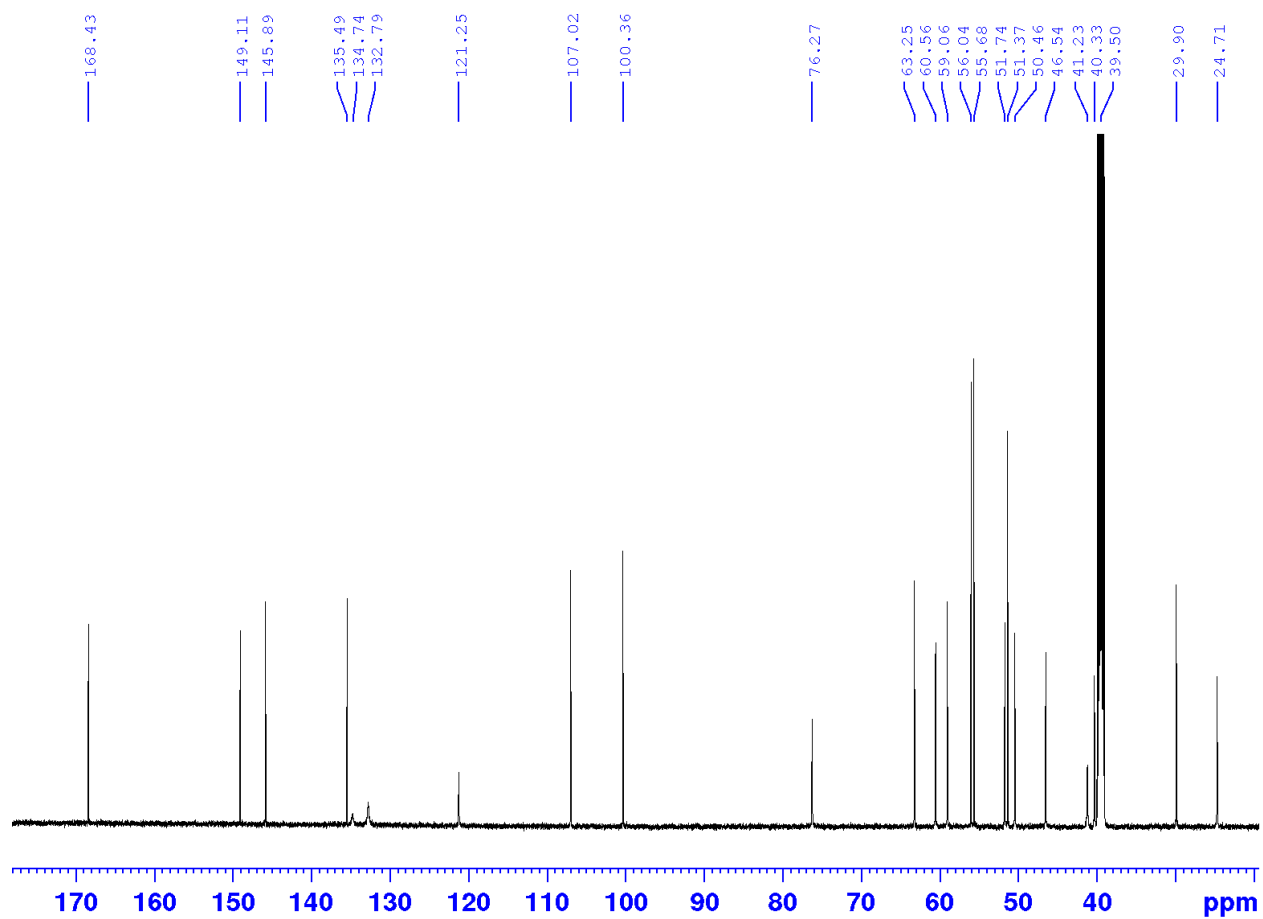




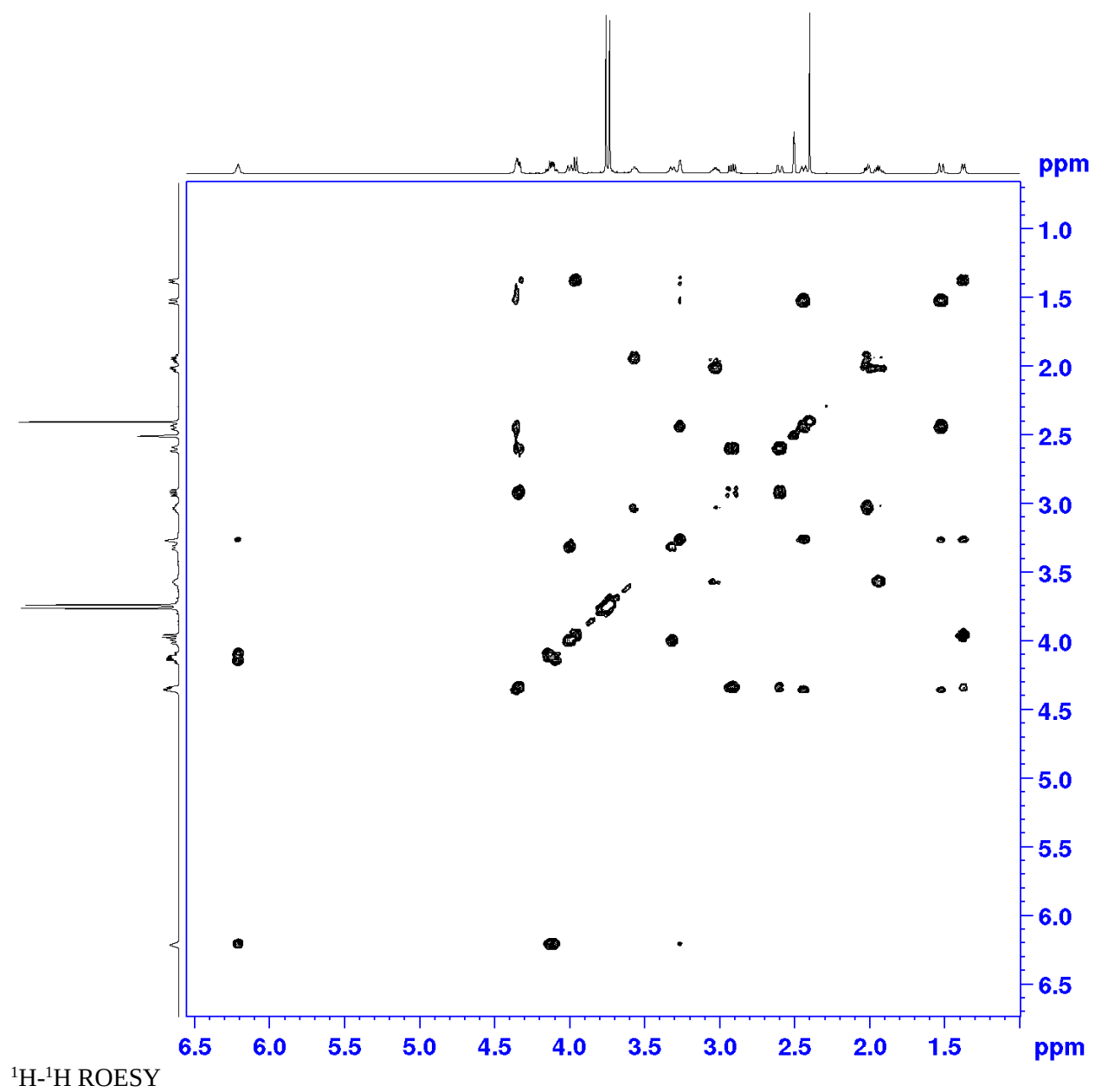
brucine (15) sample 2

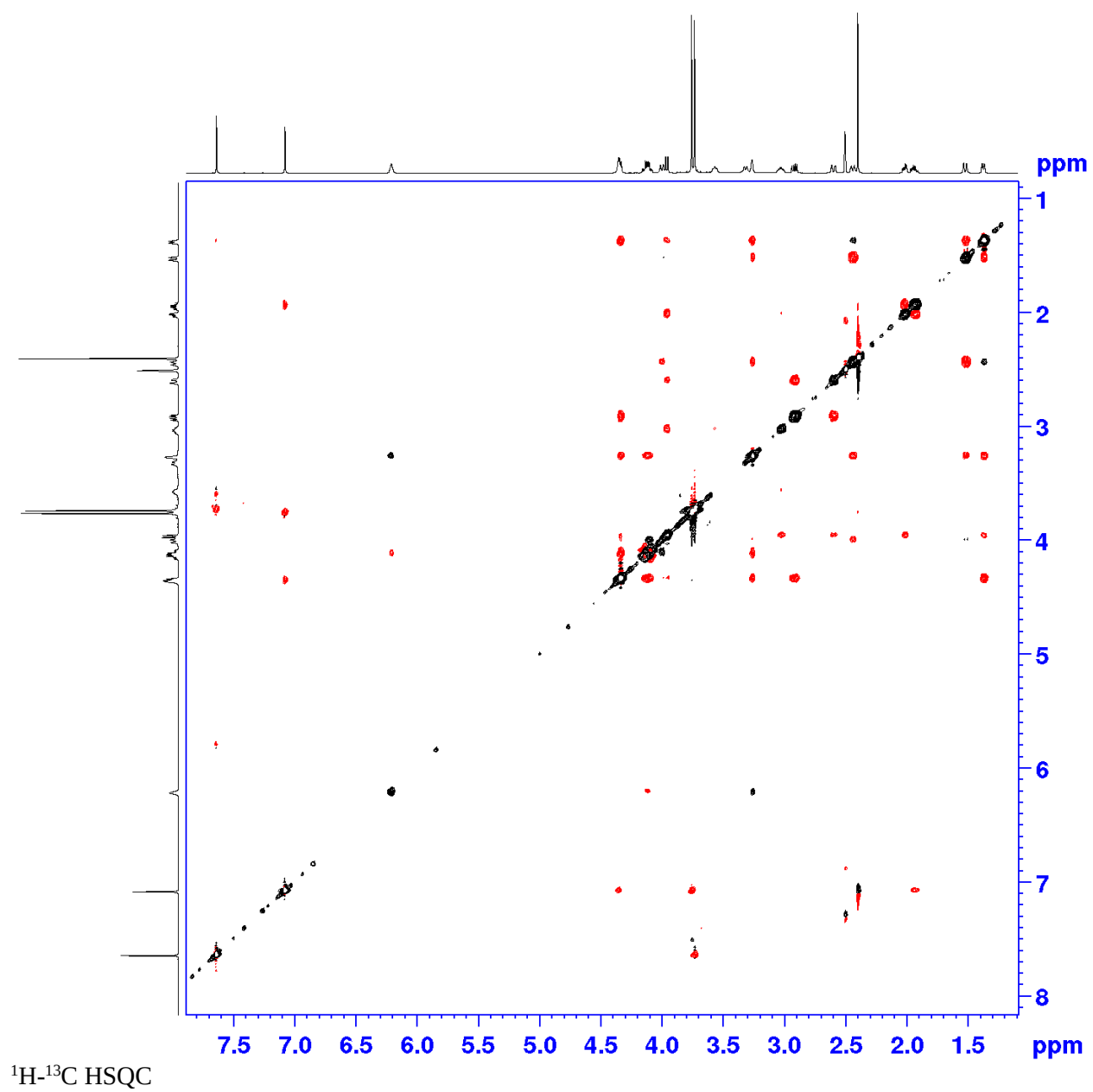
^1H

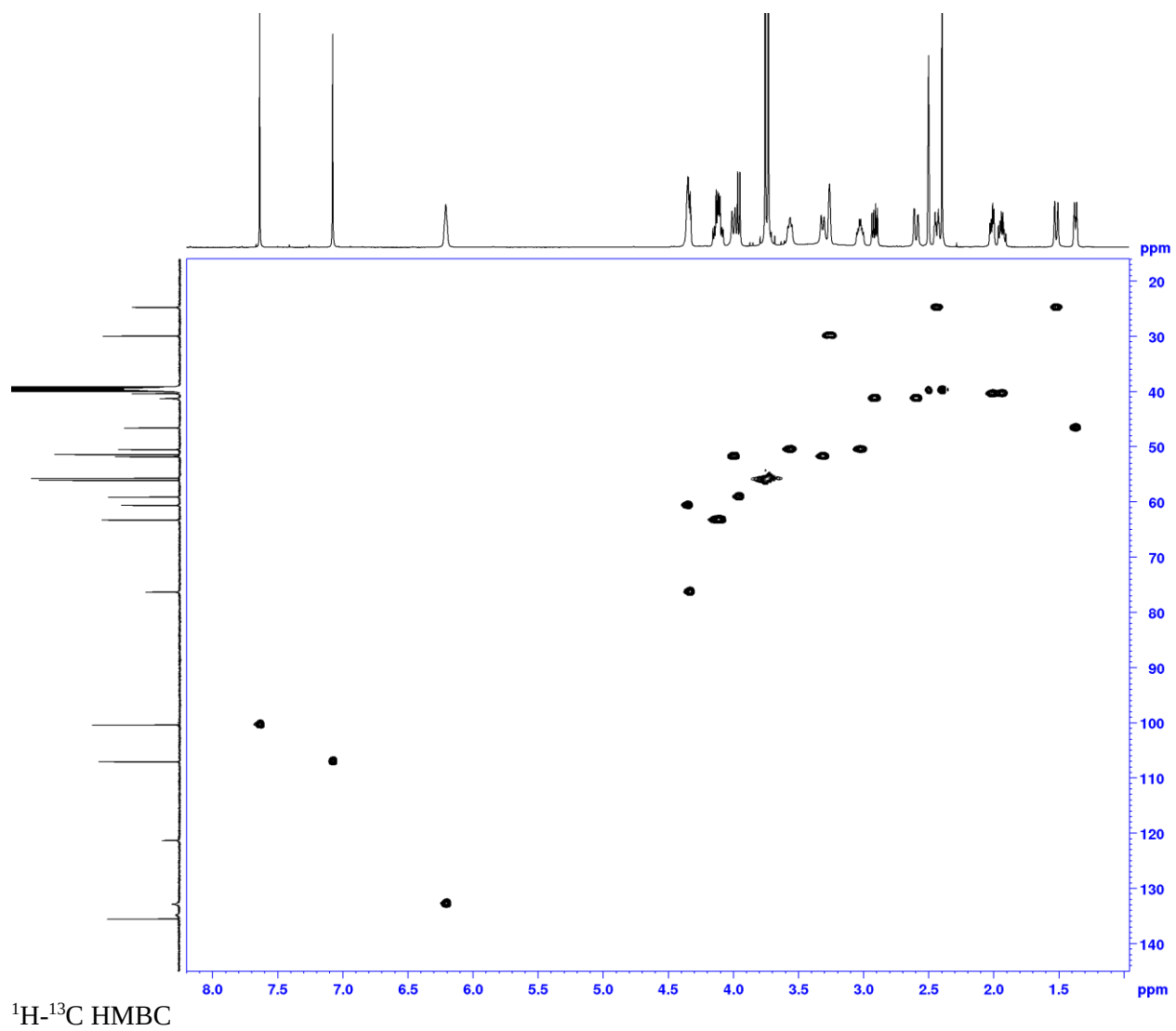


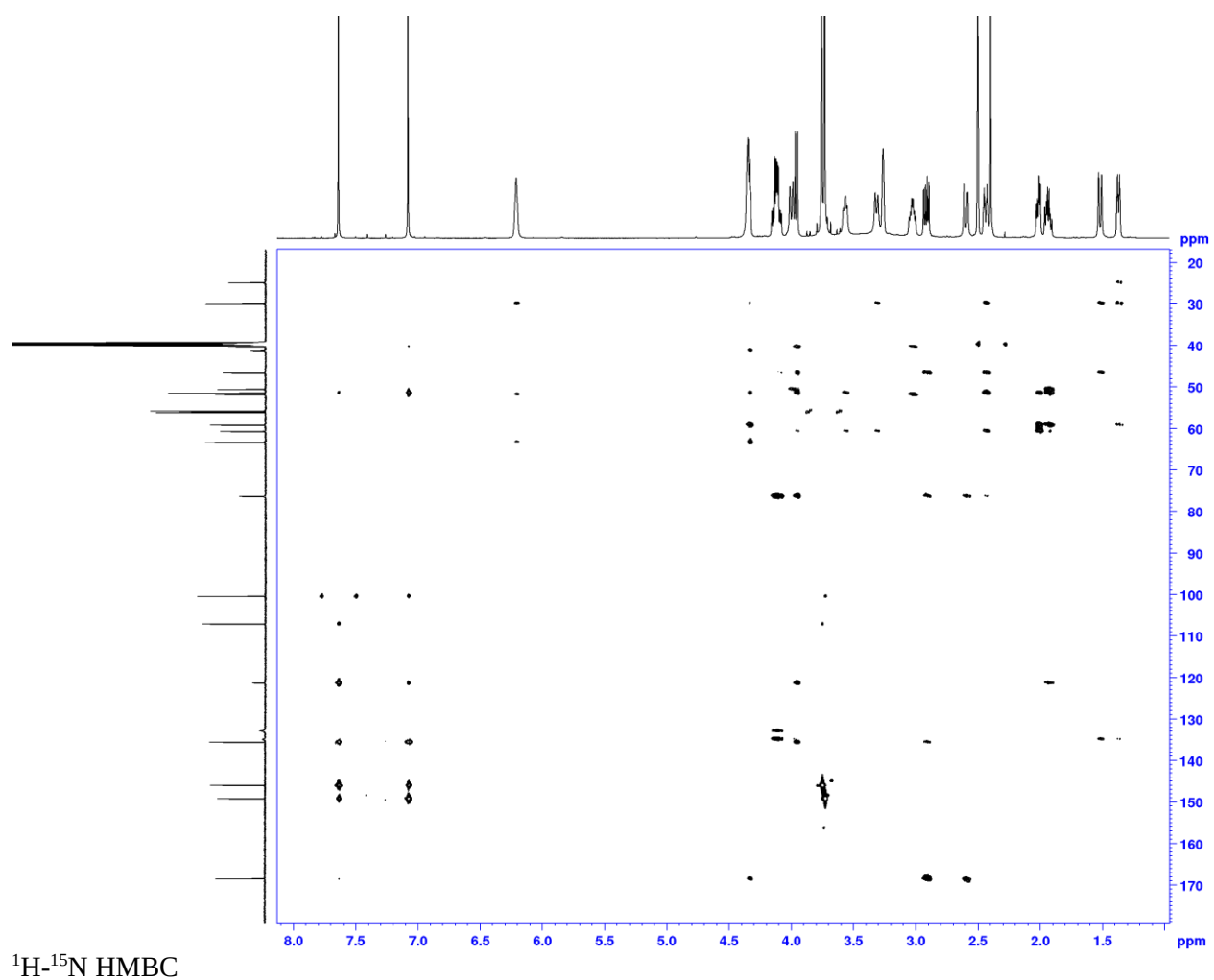


^1H - ^1H COSY

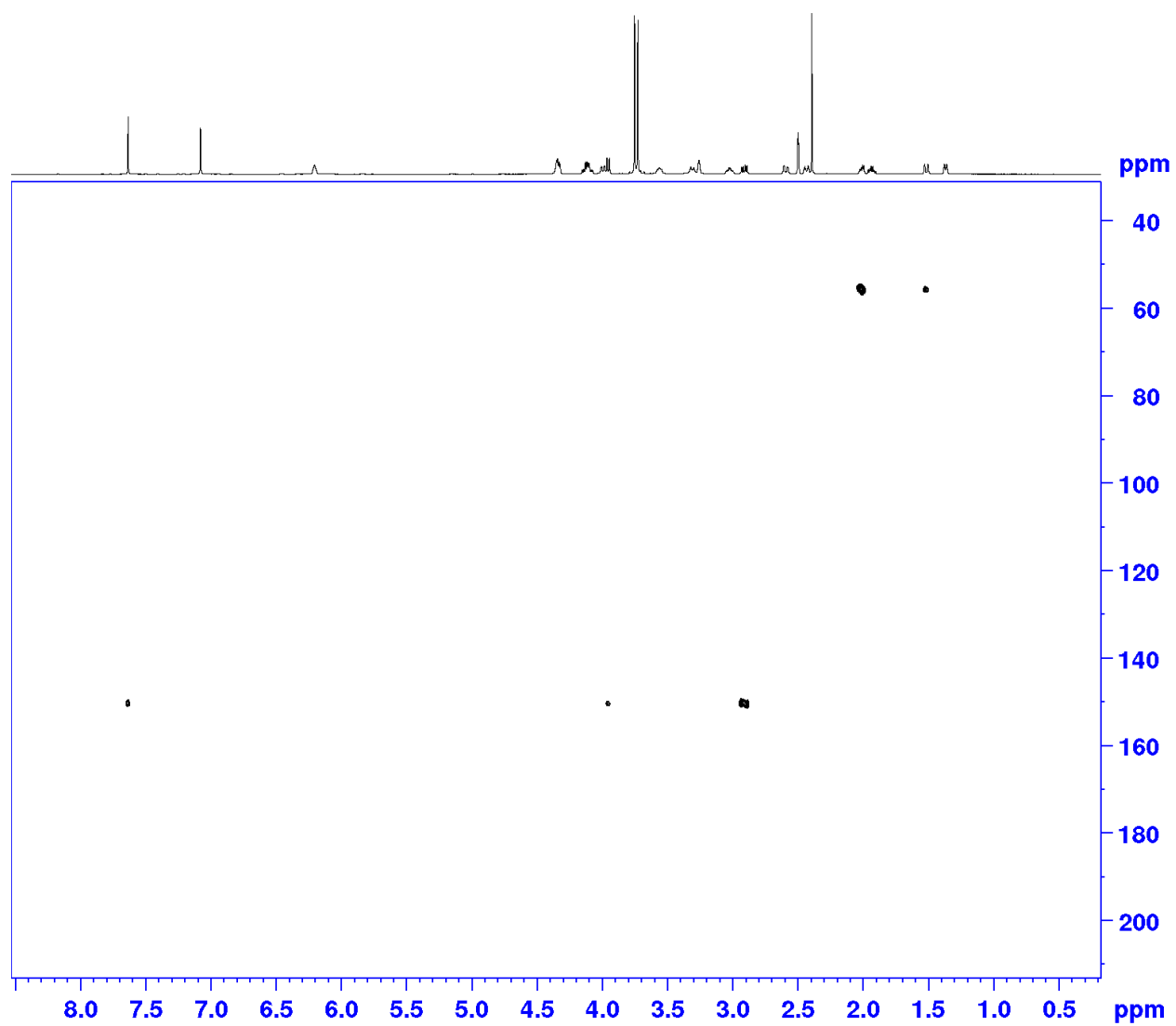






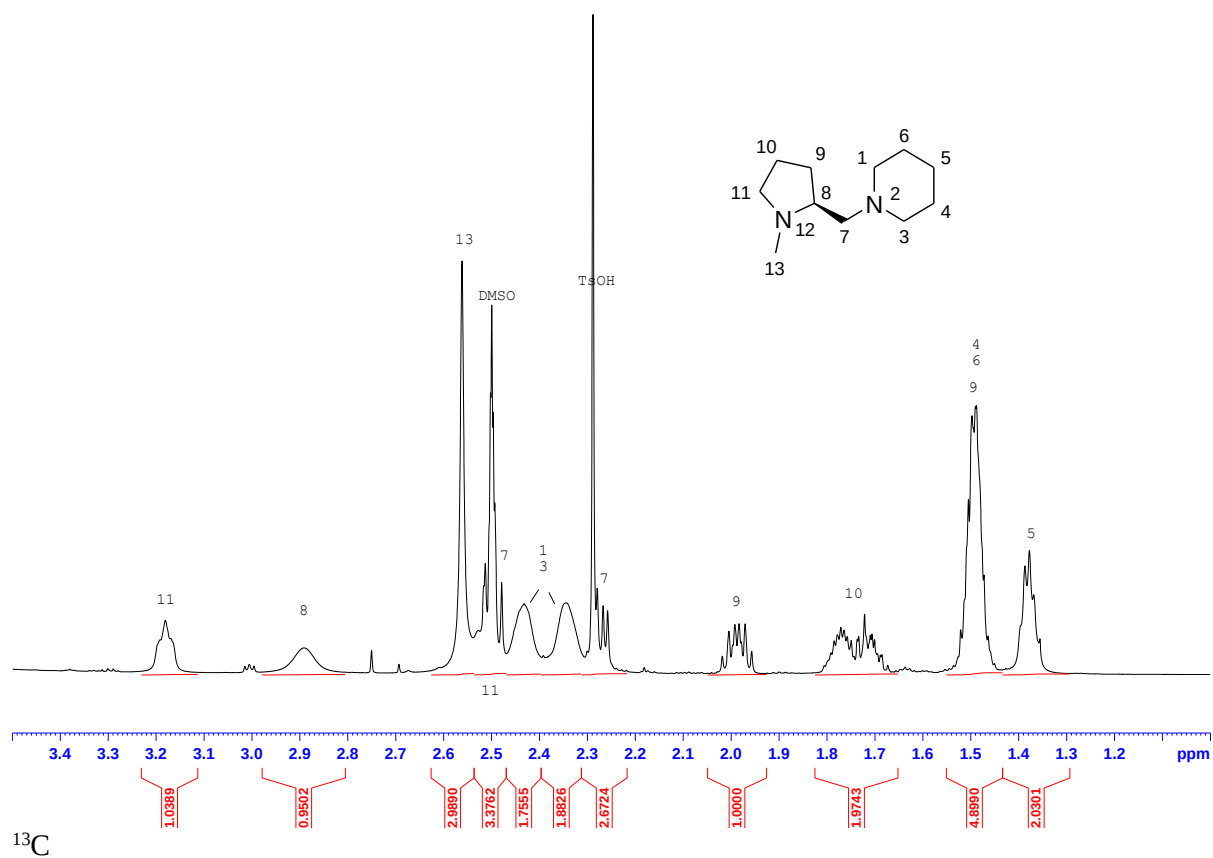


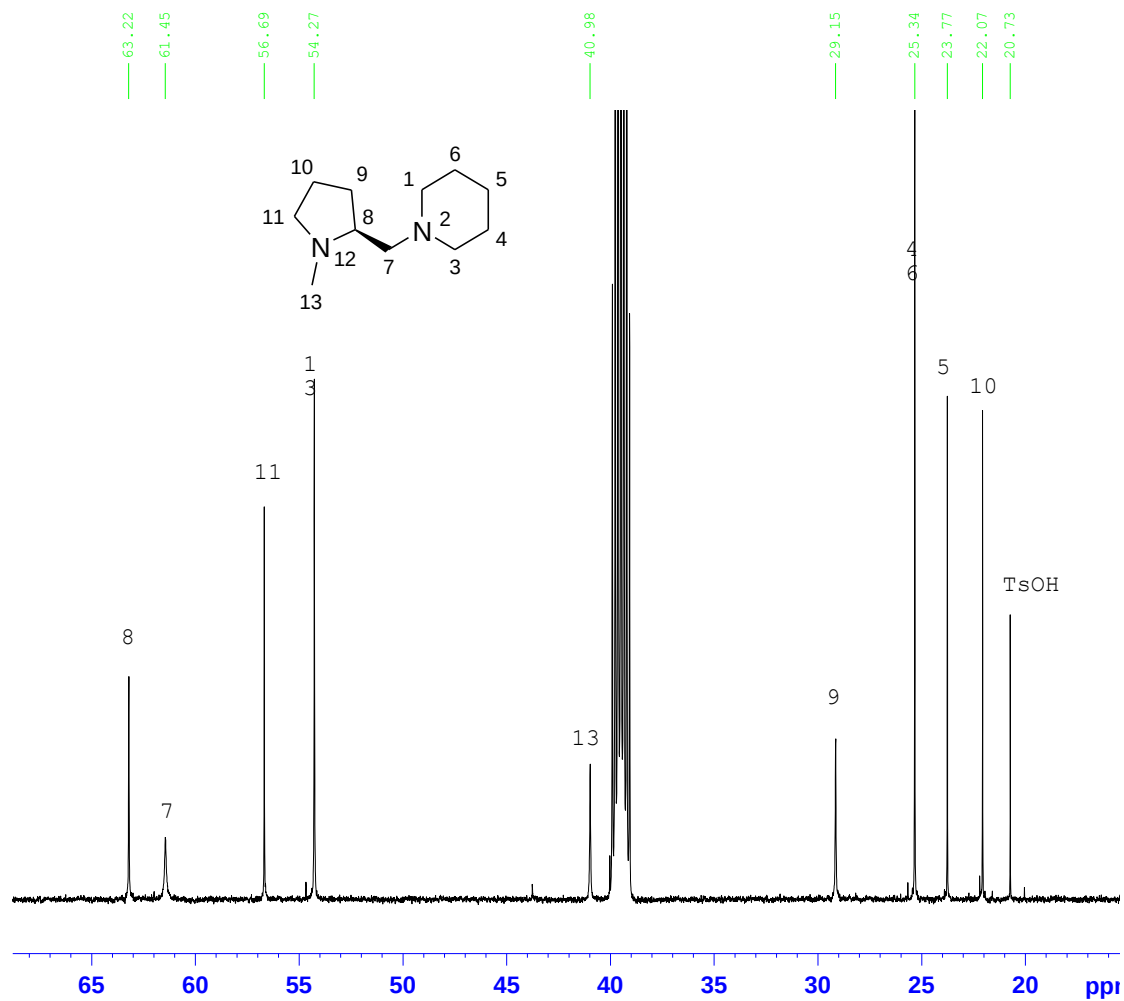
^1H - ^{15}N HMBC

1-(((S)-1-methylpyrrolidin-2-yl)methyl)piperidine (**16a**)

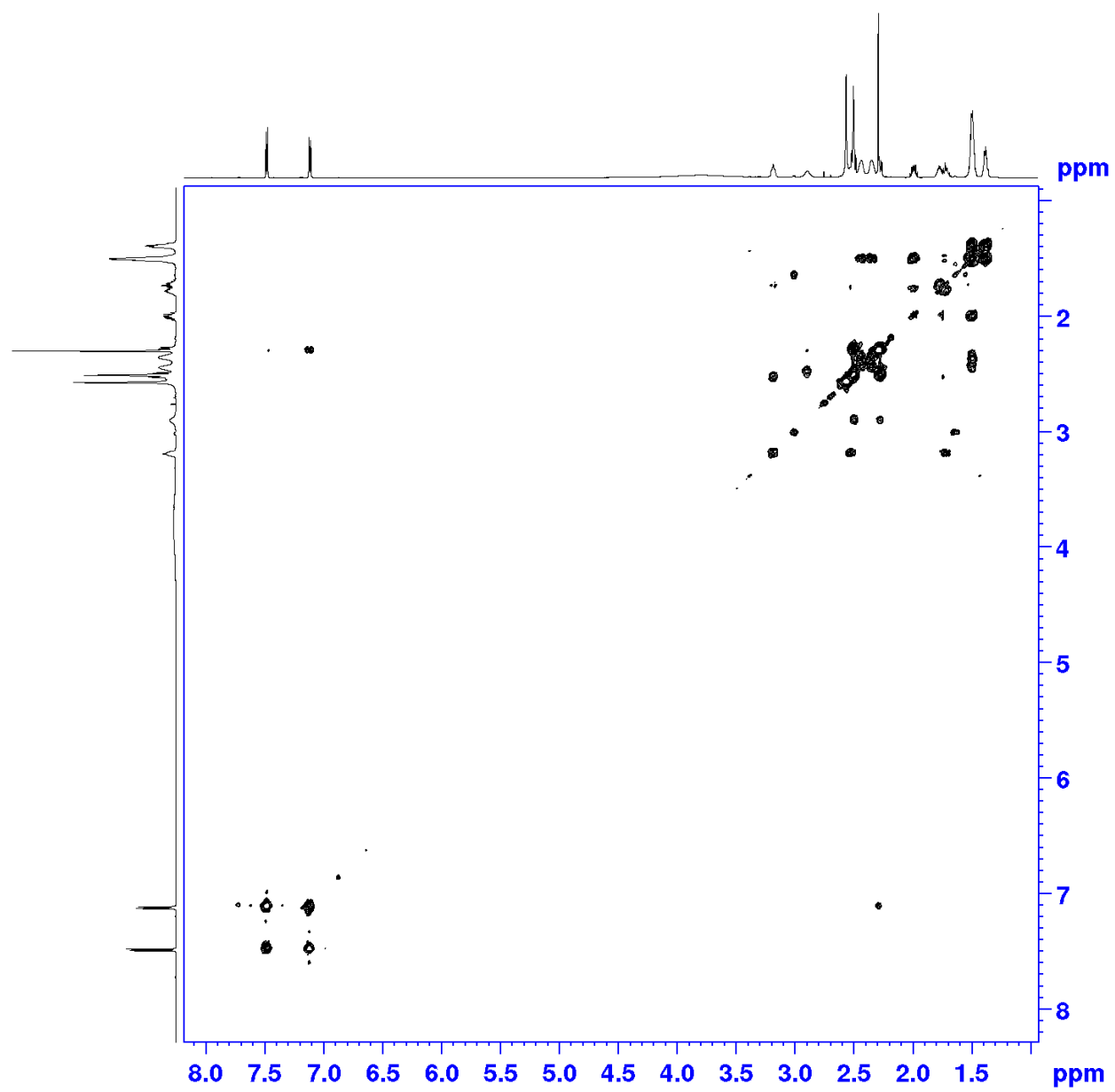
TsOH was used instead of MsOH in this sample

 ${}^1\text{H}$

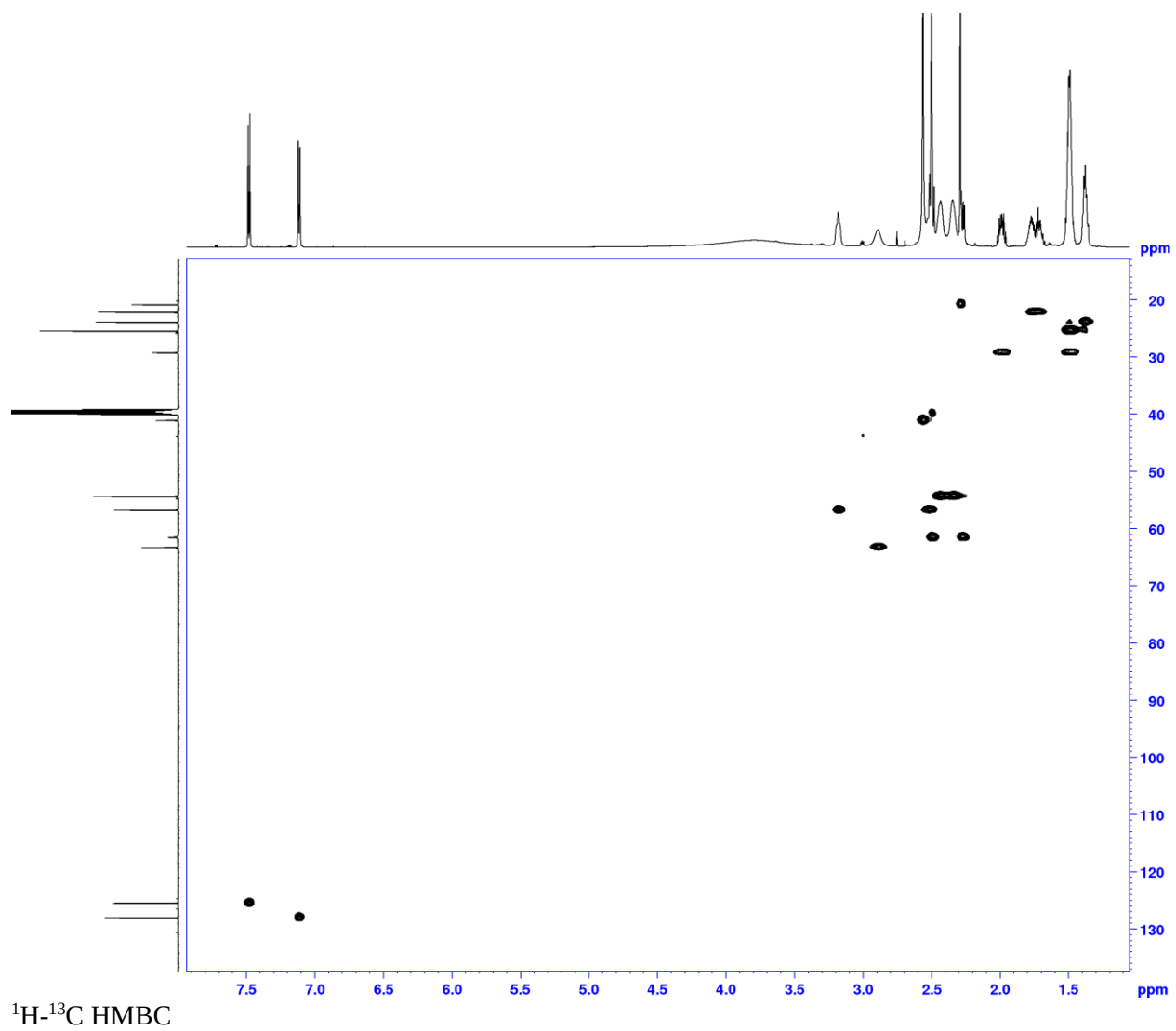


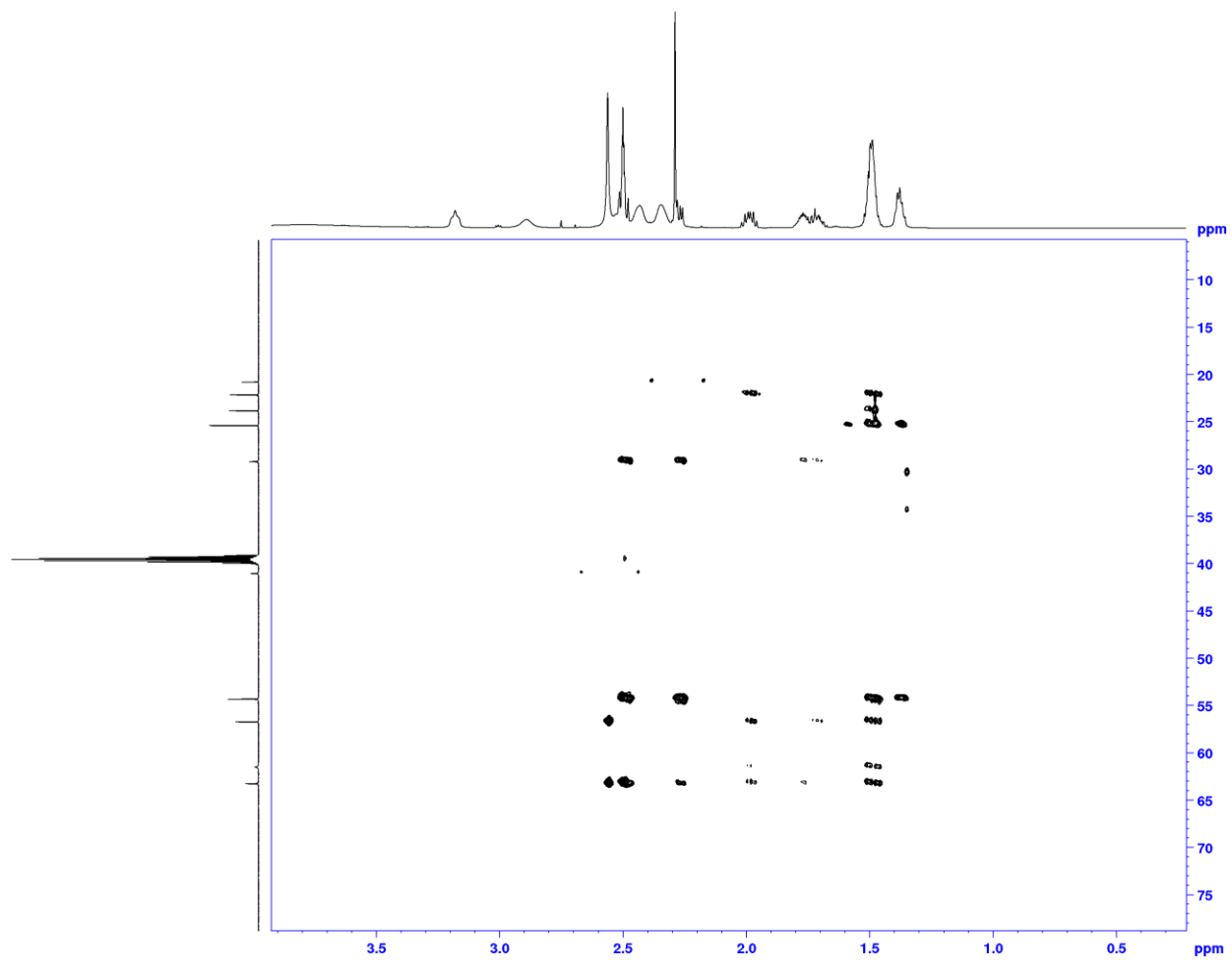


^1H - ^1H COSY



^1H - ^{13}C HSQC





^1H - ^{15}N HMBC

