Electronic Supplementary Material (ESI) for Polymer Chemistry.
This journal is © The Royal Society of Chemistry 2017

Supplementary Information

Effect of Trehalose Polymer Regioisomers on Protein Stabilization

Marco S. Messina,[a,b,‡] Jeong Hoon Ko,[a,b,‡], Zhongyue Yang,[a] M. Jane Strouse,[a] K. N. Houk,[a] and Heather D. Maynard[*,a,b]

[a]Department of Chemistry and Biochemistry, University of California, Los Angeles, 607 Charles E. Young Drive East, Los Angeles, California 90095-1569, United States.

[b]California NanoSystems Institute, University of California, Los Angeles, 570 Westwood Plaza, Los Angeles, California 90095-1569, United States.

*Correspondence to: maynard@chem.ucla.edu

Table of Contents

I. Synthesis

Synthesis of O2, O3, O4, and O6 using different bases – representative example

The reaction was conducted as in the experimental section of the manuscript, with different molar equivalents of base (entry 1 corresponds to the original condition). A representative reaction condition (entry 2) is detailed as follows: Potassium hydroxide (573 mg, 1.02×10^{-2} mol) was suspended in dry dimethyl sulfoxide (9.5 mL) and stirred at room temperature. Trehalose (437 mg, 1.28×10^{-3} mol) was then added and stirred until it dissolved. 4-Vinylbenzyl chloride (40 μL, 2.55×10^{-4} mol) was added dropwise. The reaction was stirred for 12 hours at 25 ˚C and was then precipitated into a mixture of cold hexanes (160 mL) and dichloromethane (40 mL). The precipitate was collected via filtration and dried under reduced pressure, and the resulting solid was analyzed by HPLC (40% MeOH in H_2O).

Table S1. Modulation of regioselectivity in monomer synthesis using different hydroxyl bases

Entry	Base		Regioisomer ratio O2 : O3 : O4 : O6[a]
	Base used	Mol. eq. relative to trehalose	
1	NaOH	8	1 : 0.21 : 3.38 : 1.42
2	KOH	8	1 : 0.24 : 1.49 : 1.44
3	NaOH	1	1 : 0.36 : 1.45 : 1.34
4	KOH	1	1 : 0.35 : 1.02 : 1.36

[a] Ratio calculated from HPLC chromatogram AUC.

Synthesis of O2, O3, O4, and O6 in water or at a higher temperature

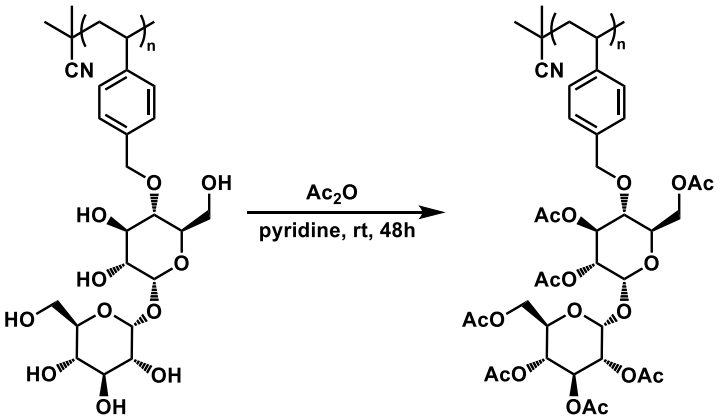
The reaction was conducted as in the experimental section of the manuscript, except at a different temperature (50 °C) or in water. Briefly, 8 equivalents of NaOH and 1 equivalent of trehalose were dissolved in DMSO (to make 0.15 M trehalose), and 0.2 equivalent of 4-vinylbenzyl chloride was added dropwise and the reaction was allowed to stir for 15 to 21 hours at respective temperature. The reaction was neutralized with dilute hydrochloric acid, and analyzed by LC-MS. The reactions in water was conducted both with (entry 3) and without (entry 2) the phase transfer catalyst (tetrabutylammonium hydrogensulfate) at 0.2 molar equivalents with respect to the added trehalose.

Table S2. The effect of solvent and temperature on regioselectivity

Entry	Solvent	Temperature	Additive	Regioisomer ratio O2 + O3[a] : O4 : O6[b]
1	DMSO	50 °C	None	1 : 2.27 : 2.12
2	Water	23 °C	None	1 : 3.78 : 4.61
3	Water	23 °C	Tetrabutylammonium hydrogensulfate	1 : 2.01 : 3.34

[a] Due to the low overall yield and weak signal, O2 and O3 peaks were overlapping.
[b] Ratio calculated from UPLC-MS chromatogram.

Representative Polymer Acetylation: Acetylation of P4

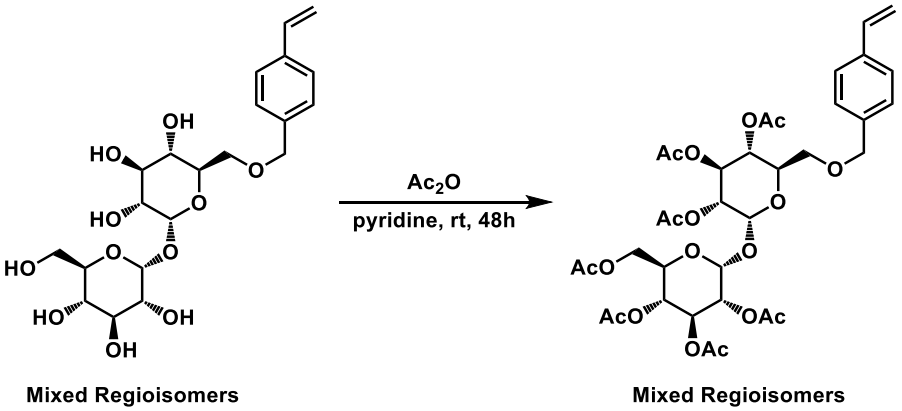


P4 (11.5 mg, 25.1 μmol, 1 eq.) was dissolved in dry pyridine (1.0 mL) and added to a dry and degassed round bottom flask. After five minutes of stirring, acetic anhydride (59.3 μL, 0.627 mmol, 25 eq.) was added dropwise. The solution stirred at room temperature for 48 hours. After 48 hours, the polymer was precipitated twice from cold diethyl ether. The precipitate was then collected and freeze-dried from benzene to afford product as a white powder. The polymer was characterized by DMF GPC.

Deacetylated polymer molecular weight was calculated using the following equation:

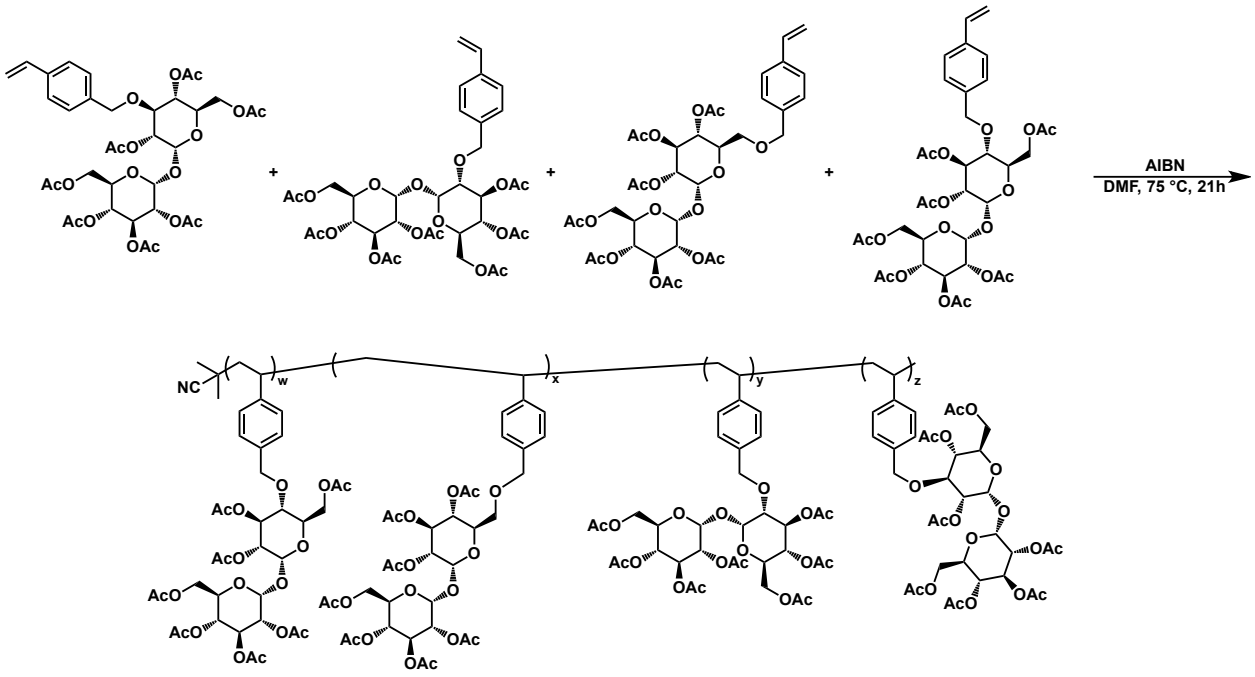
$[M_n \text{ P-OH}] = [M_n \text{ P-OAc}]*((\text{MW O}_{\text{monomer}})/(\text{MW OAc}_{\text{monomer}}))$.

Representative Monomer Acetylation: Acetylation of OA (OA-OAc)



OA (199.6 mg, 0.435 mmol, 1 eq.) was dissolved in dry pyridine (1.4 mL) and added to a dry and degassed round bottom flask. After five minutes of stirring, acetic anhydride (823 μL, 8.70 mmol, 20 eq.) was added dropwise. The solution was stirred at room temperature for 48 hours. After 48 hours, solvent was removed under reduced pressure to yield a white solid. The solid was dissolved in dichloromethane (≈10 mL) and washed with H_2O (≈10 mL) once. Organic layer was collected and washed with brine (≈10 mL) once. The organic layer was collected, dried over $MgSO_4$, and filtered. Solvent was removed under reduced pressure and flash chromatography was performed (dichloromethane:ethyl acetate; 9:1) to afford product as a white solid. Yield= 72%.

Free Radical Polymerization of OA-OAc (PA-OAc)



OA (690.0 mg, 0.917 mmol, 43 eq.) and AIBN (3.5 mg, 21.0 μmol, 1eq.) were dissolved in DMF (3.06 mL). The mixture was added to a dry Schlenk tube and subjected to five freeze-pump-thaw cycles. Polymerization was started by immersing the Schlenk tube in a 75 °C oil bath. After 21 hours, the polymer was precipitated from cold diethyl ether. Crude solid was collected via filtration and rinsed with cold diethyl ether to afford the product as a white solid.

Representative Polymer Acetyl Deprotection: Deprotection of PA-OAc

PA-OAc (73.4 mg, 97.5 μmol, 1 eq.) was dissolved in $CHCl_3$ (2 mL) and MeOH (2mL). To this was added sodium methoxide (27 μL, 0.488 mmol, 5 eq.) dropwise. The solution was stirred at room temperature for 2 hours. After two hours, the precipitate was collected via centrifugation and dried. Resulting white solid was dissolved in water (~10 mL) and neutralized with 0.1 N HCl. Product was purified via dialysis (MWCO= 3,500 Da) for three days. Lyophilization afforded product as a fluffy white solid.

II. Characterization of Small Molecules

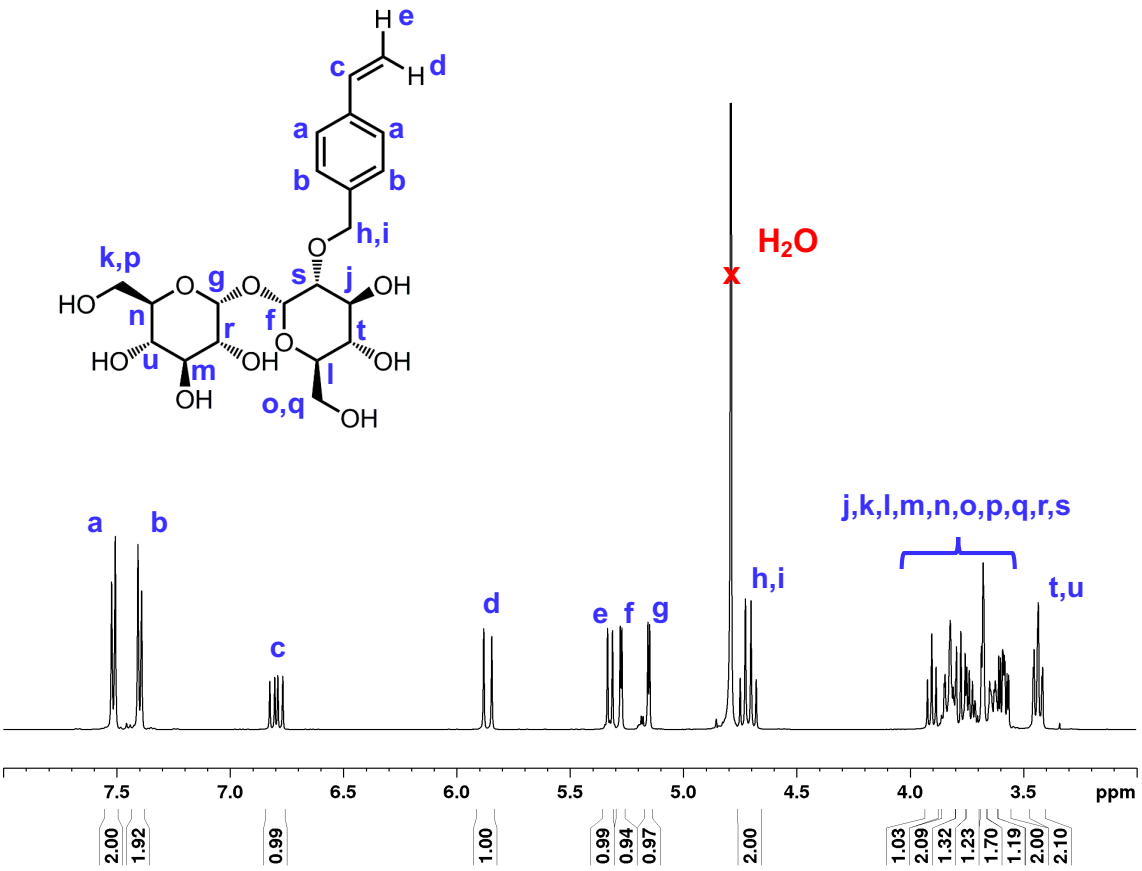


Figure S1. ^{1}H NMR spectrum of **O2** in D_2O at 298 K.

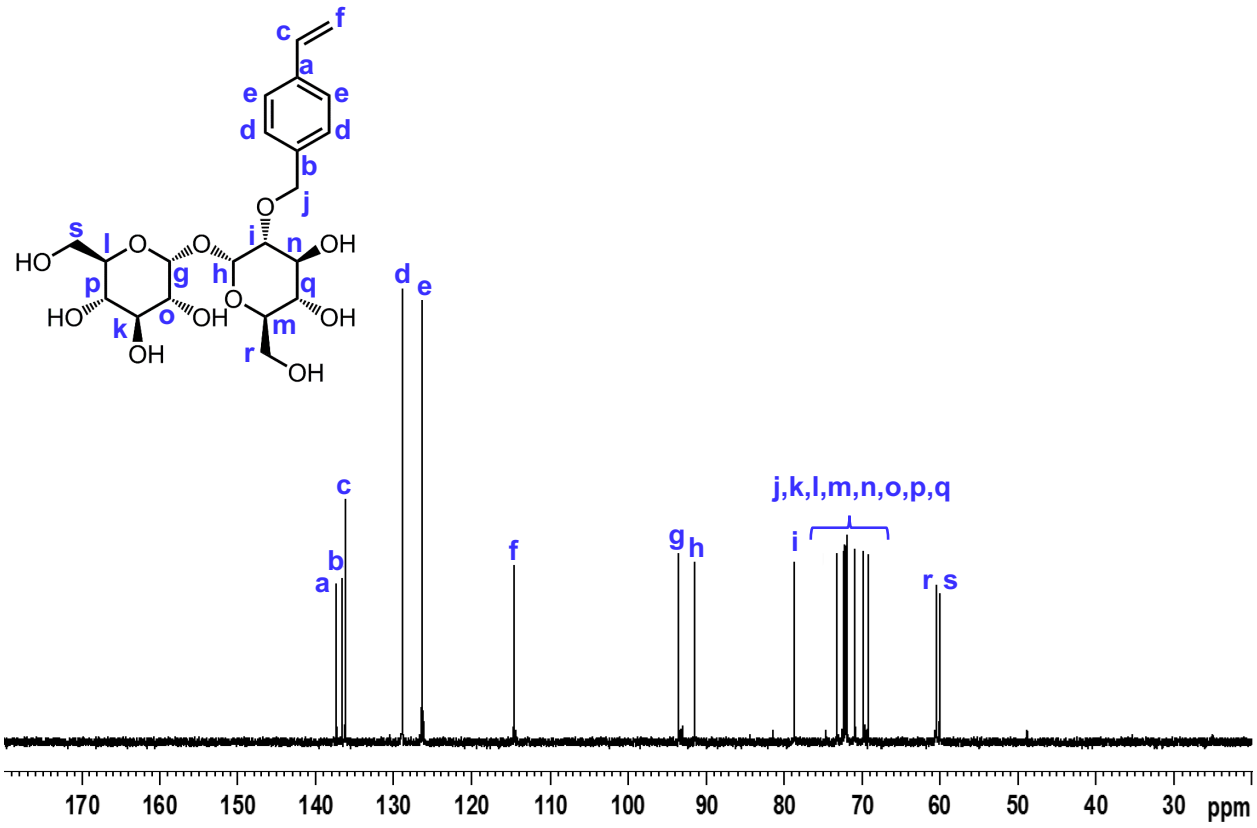


Figure S2. ^{13}C NMR spectrum of **O2** in D_2O at 298 K.

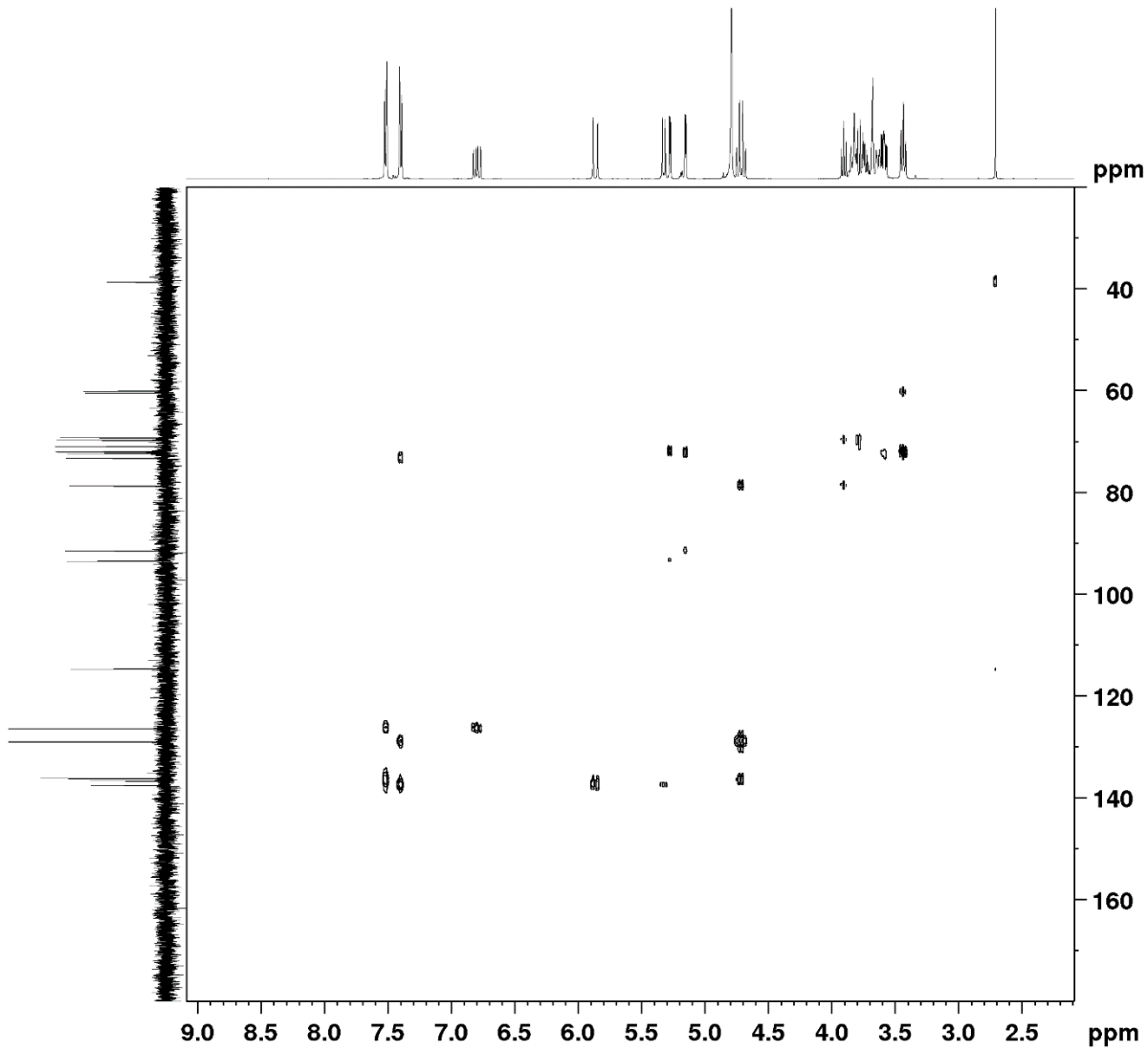


Figure S3. HMBC spectrum of **O2** in D2O at 298 K**.**

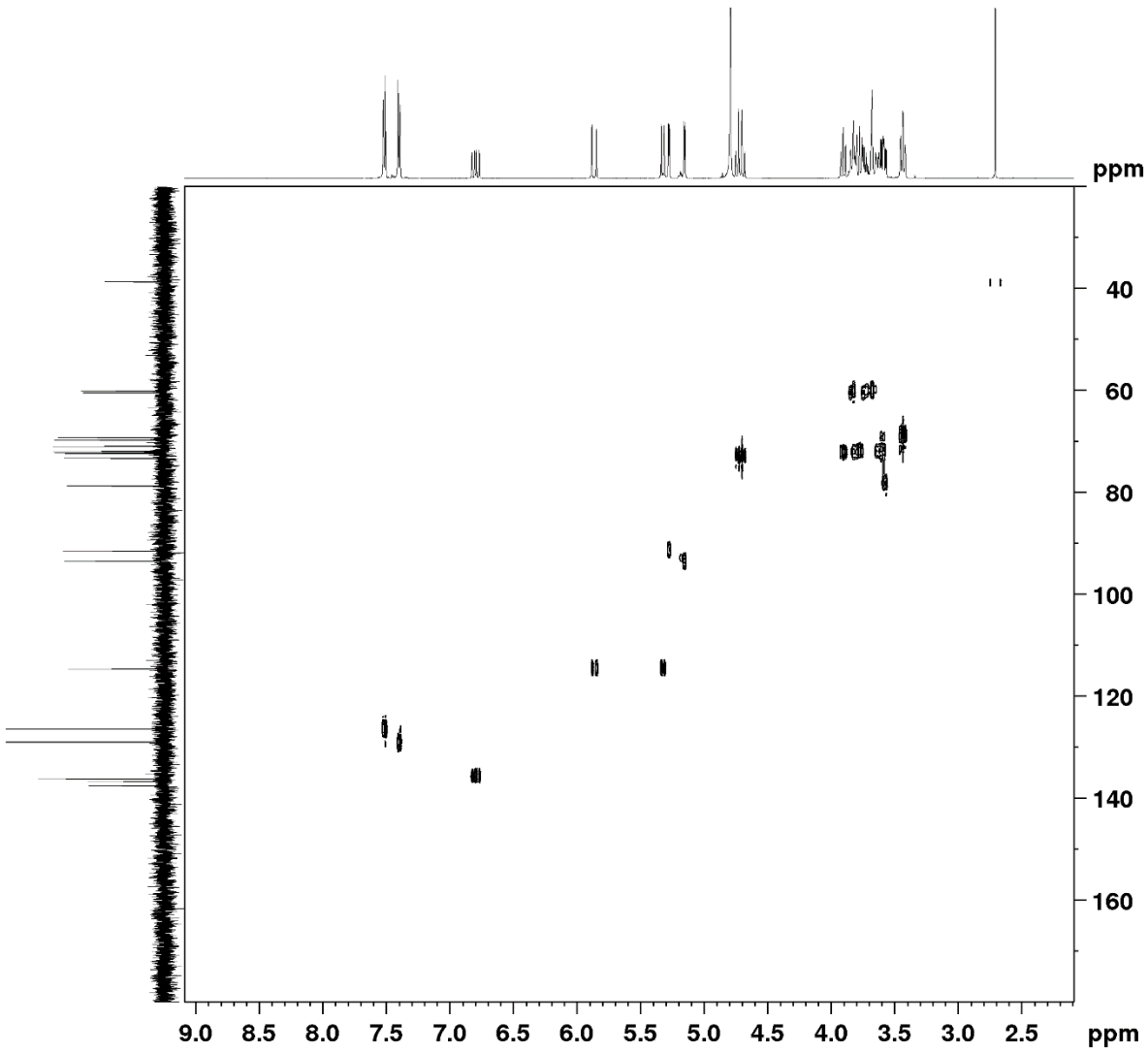


Figure S4. HSQC spectrum of **O2** in D_2O at 298 K.

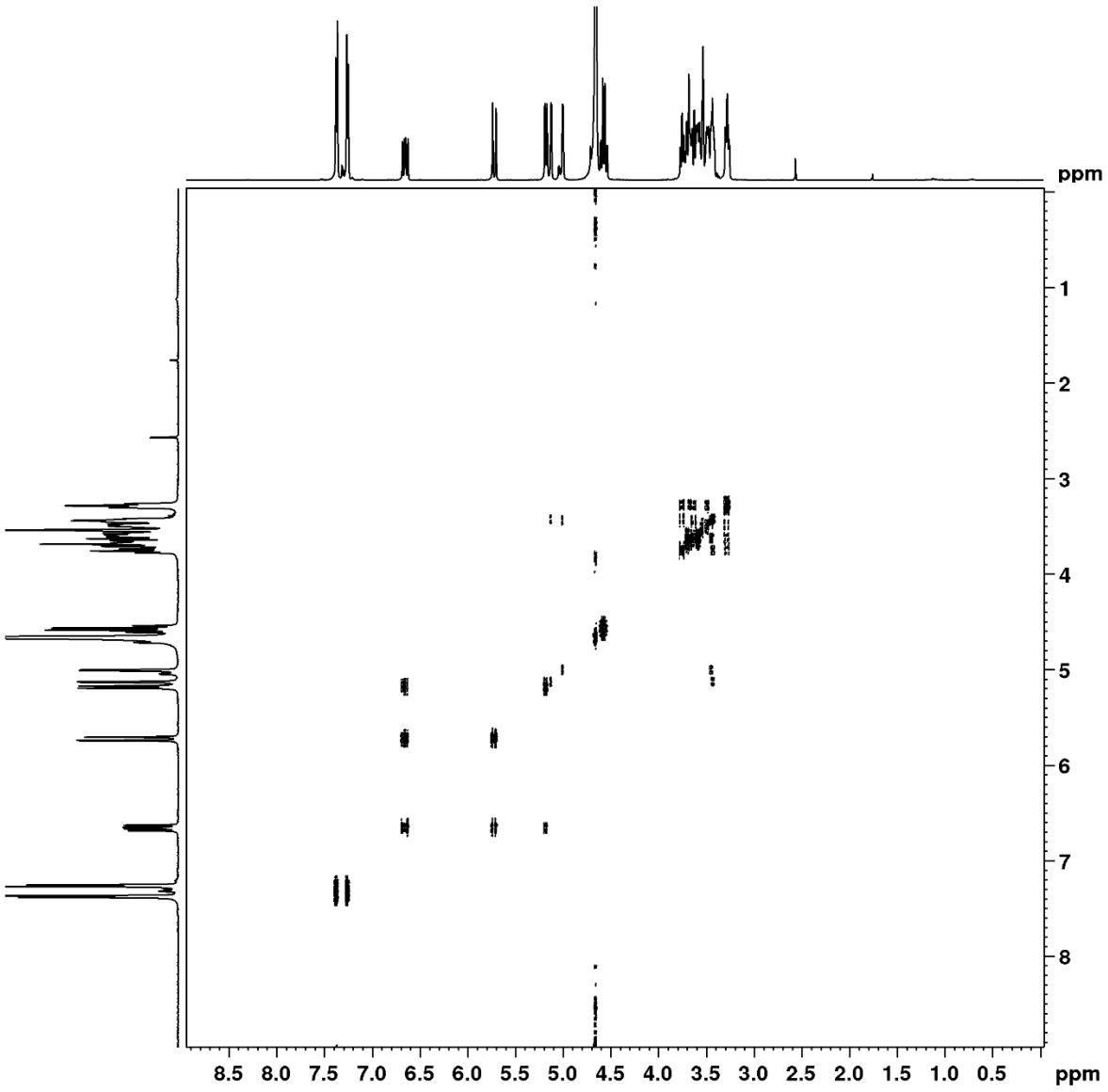


Figure S5. COSY spectrum of **O2** in D_2O at 298 K.

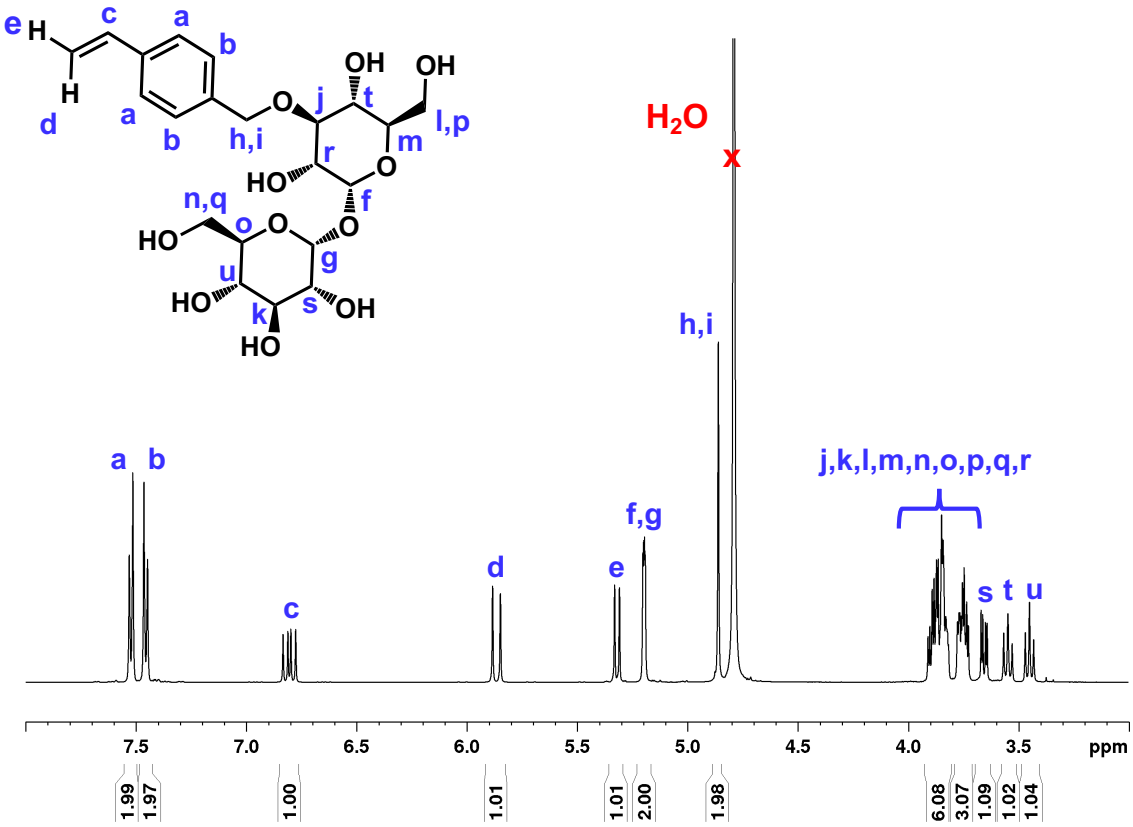


Figure S6. ^{1}H NMR spectrum of **O3** in D_2O at 298 K.

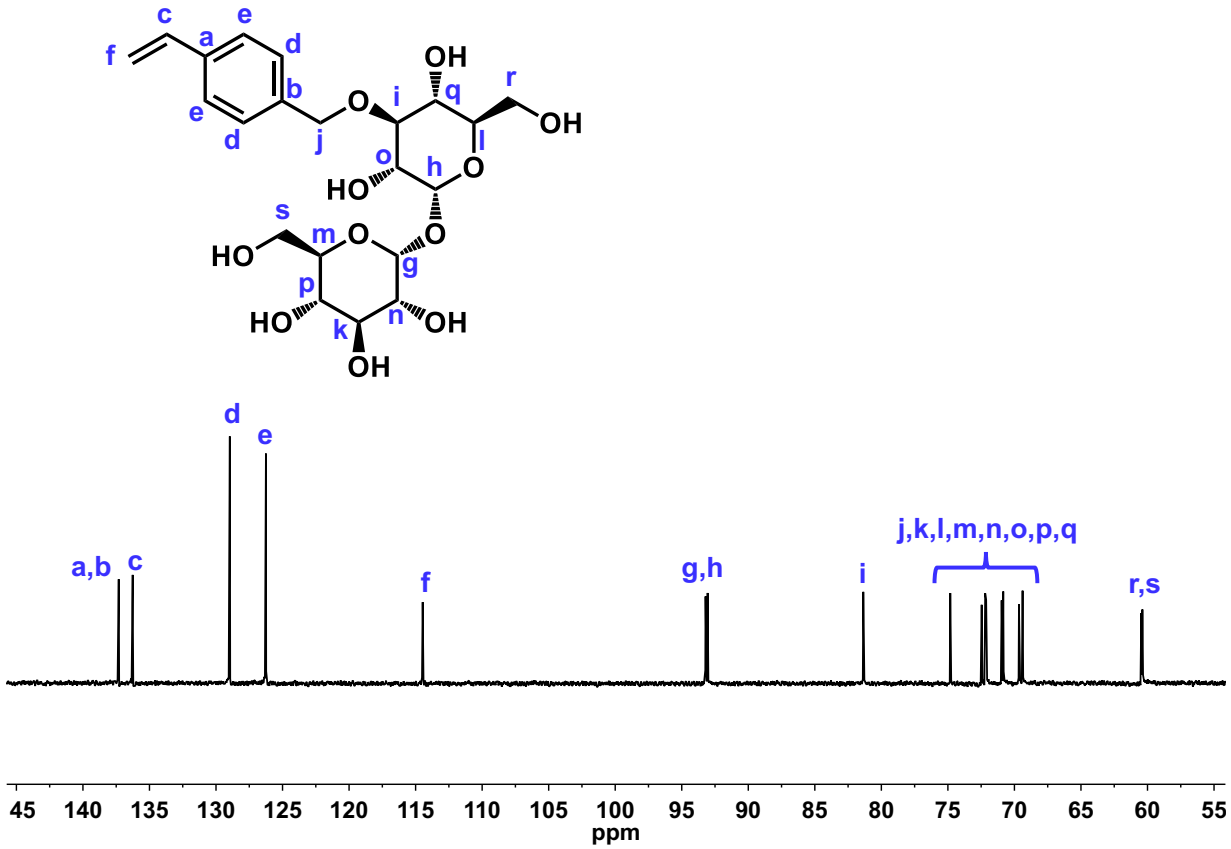


Figure S7. ^{13}C NMR spectrum of **O3** in D_2O at 298 K.

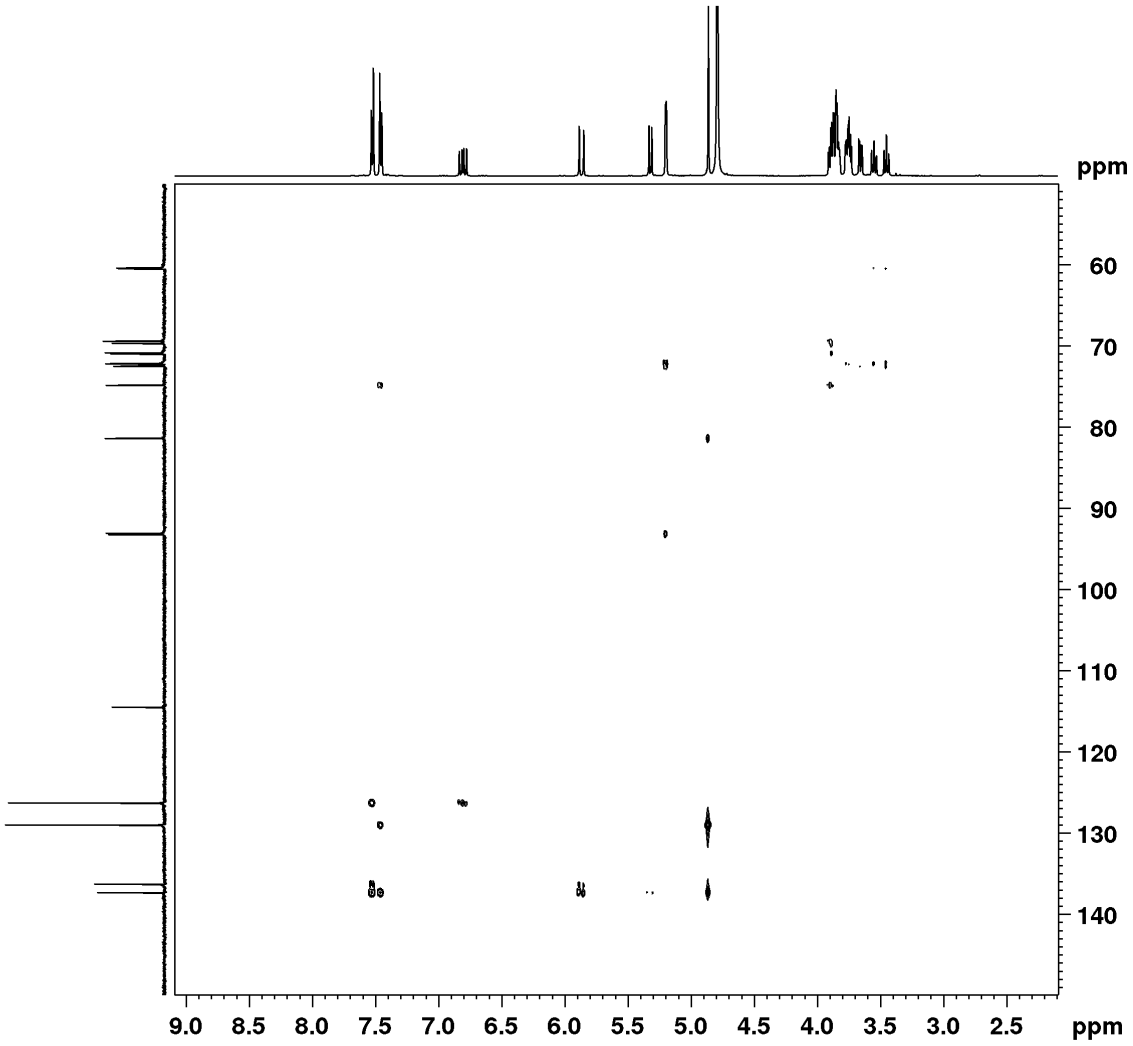


Figure S8. HMBC spectrum of **O3** in D_2O at 298 K.

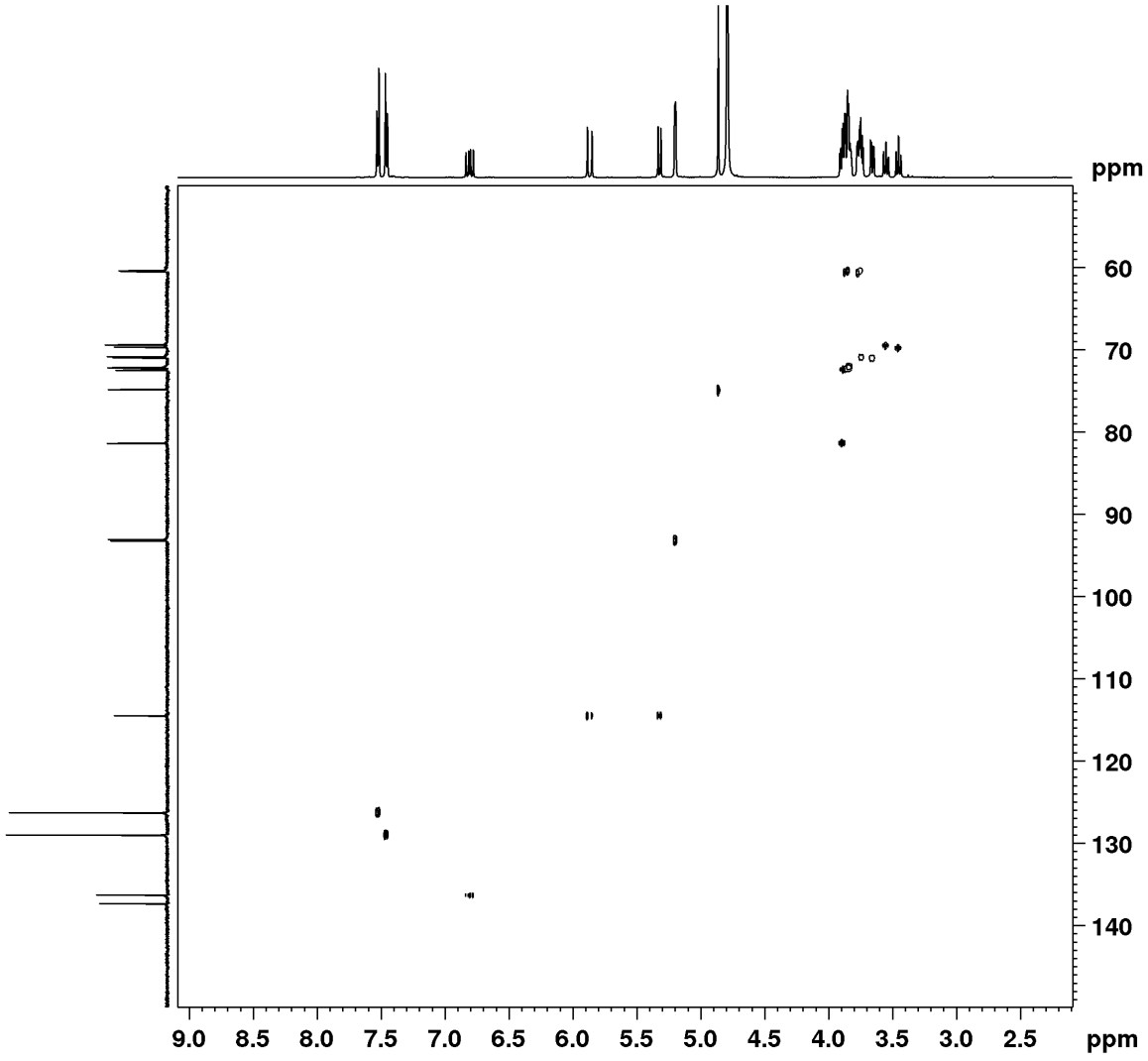


Figure S9. HSQC spectrum of **O3** in D_2O at 298 K.

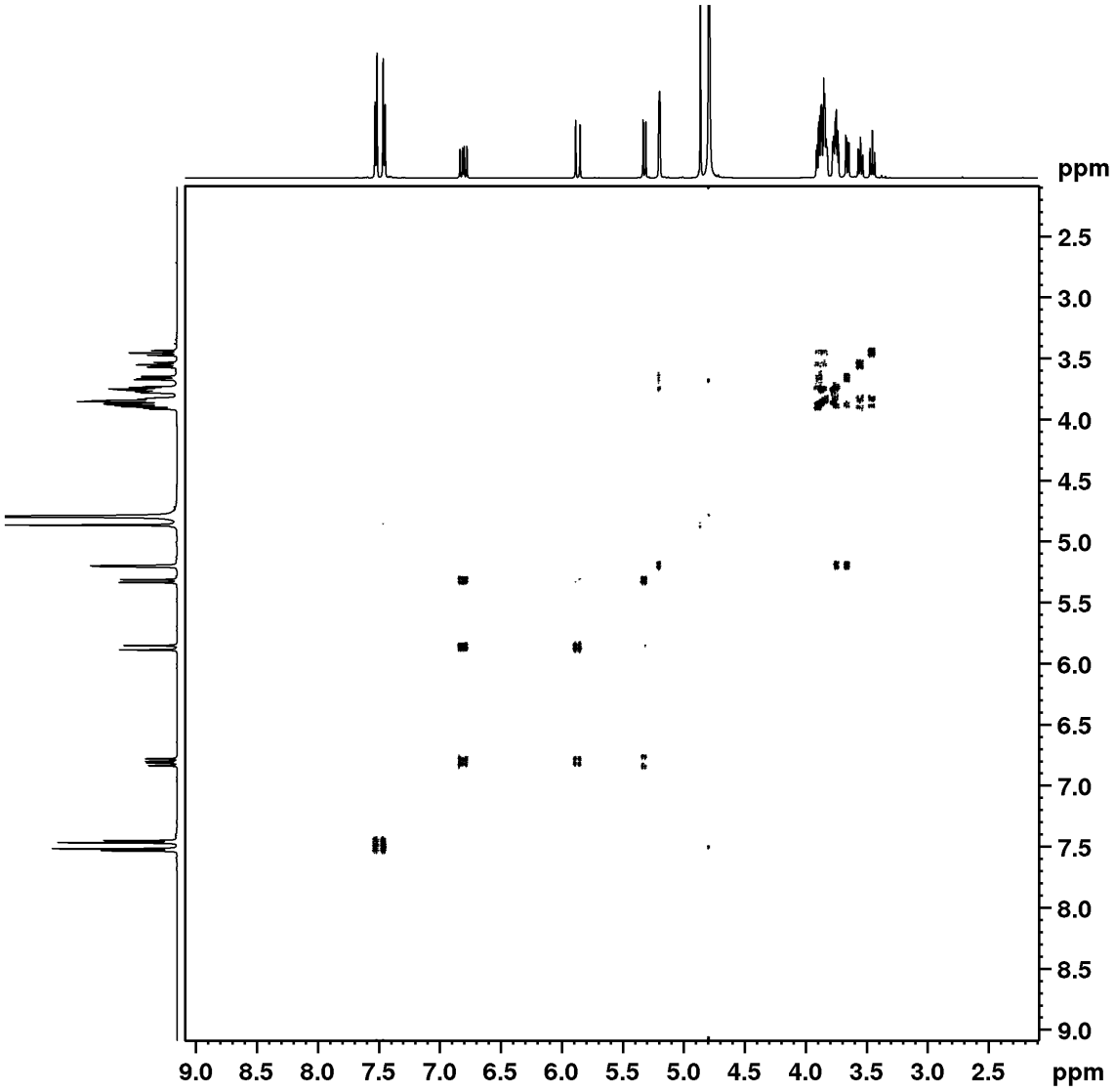


Figure S10. COSY spectrum of **O3** in D_2O at 298 K.

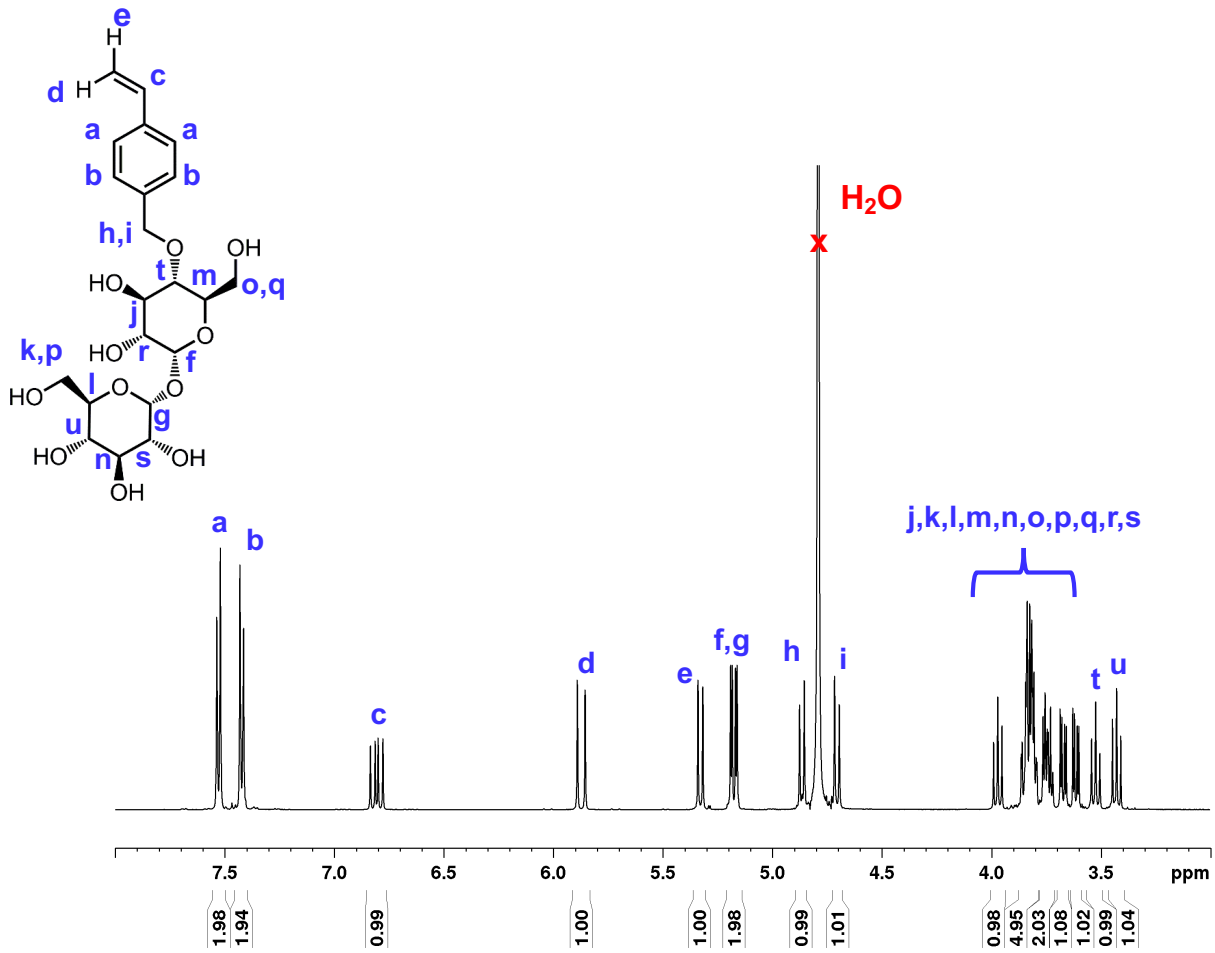


Figure S11. ^{1}H NMR spectrum of **O4** in D_2O at 298 K.

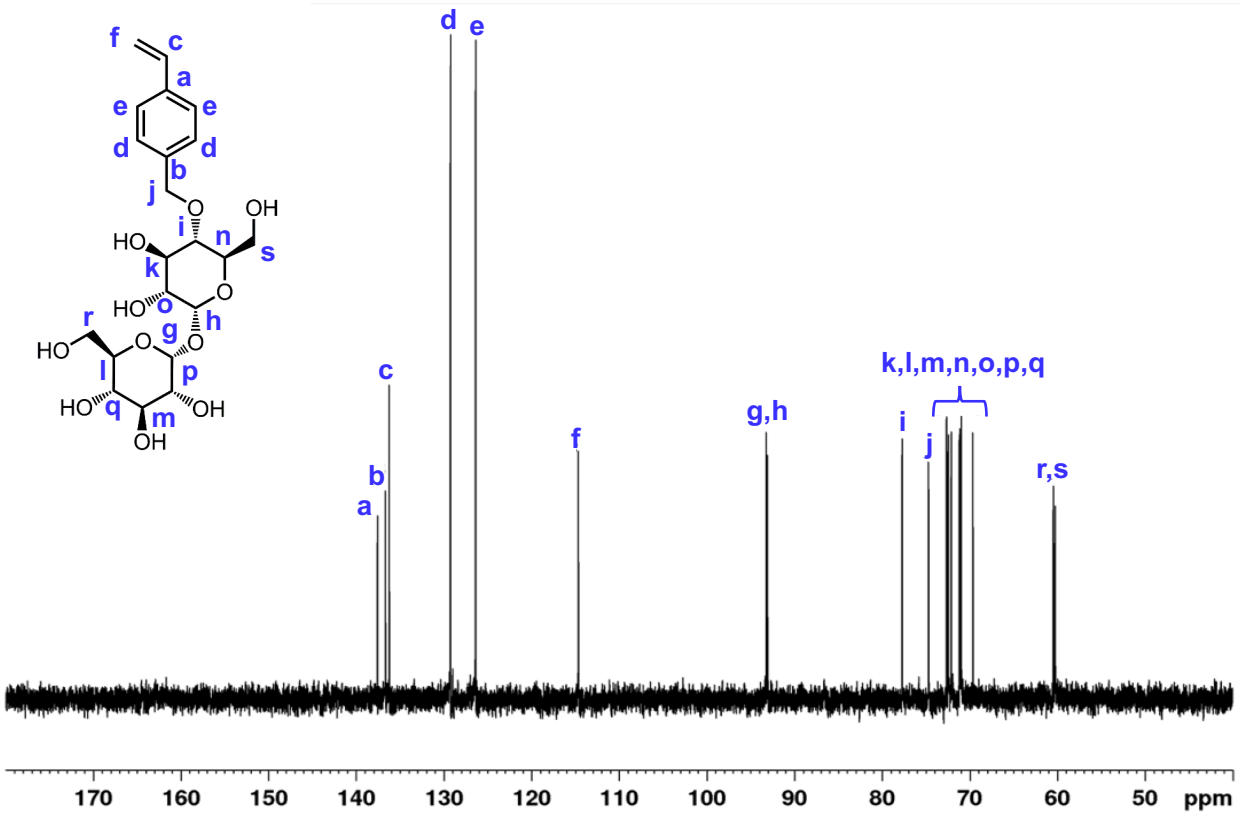


Figure S12. ^{13}C NMR spectrum of **O4** in D_2O at 298 K.

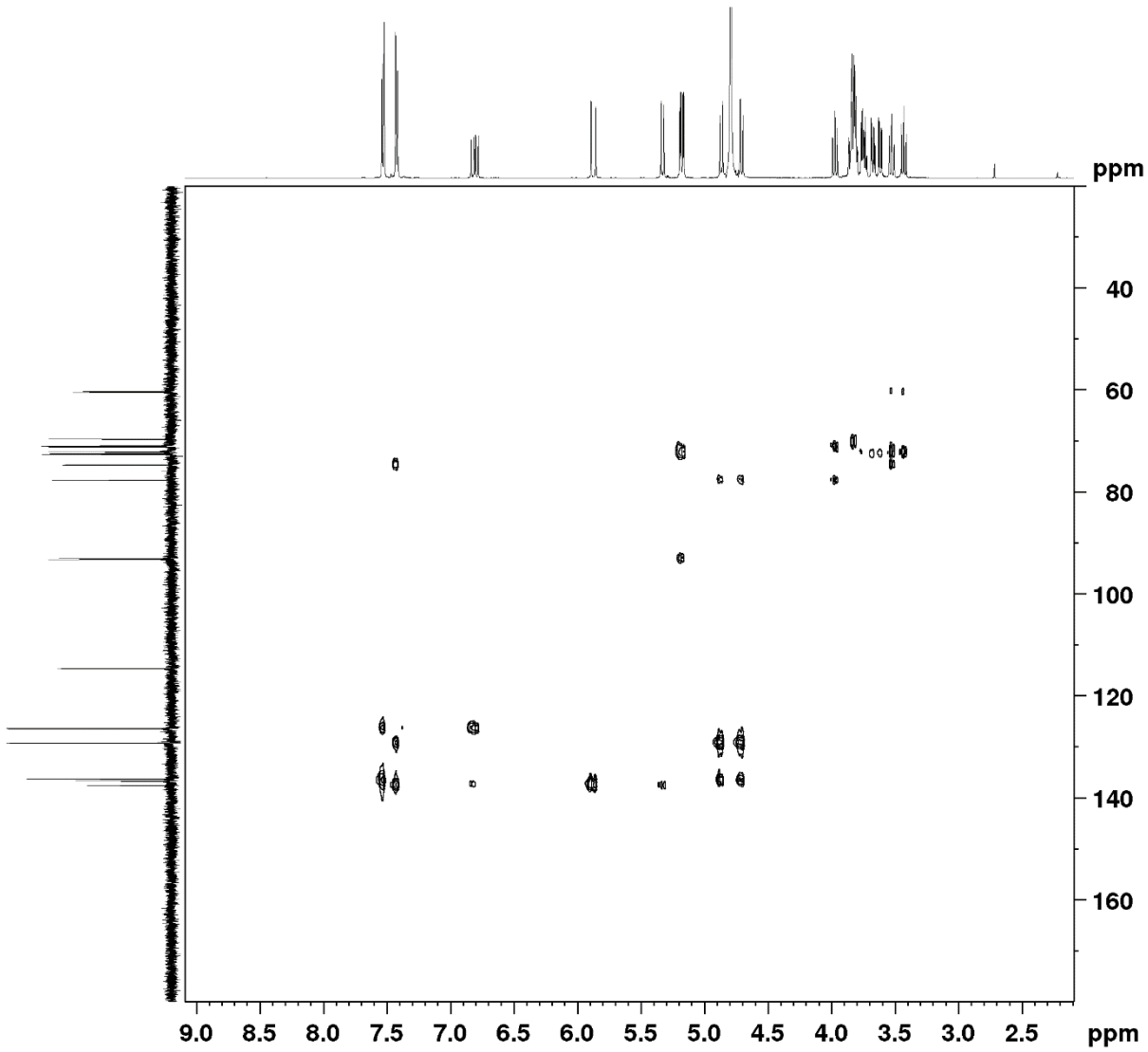


Figure S13. HMBC spectrum of **O4** in D_2O at 298 K.

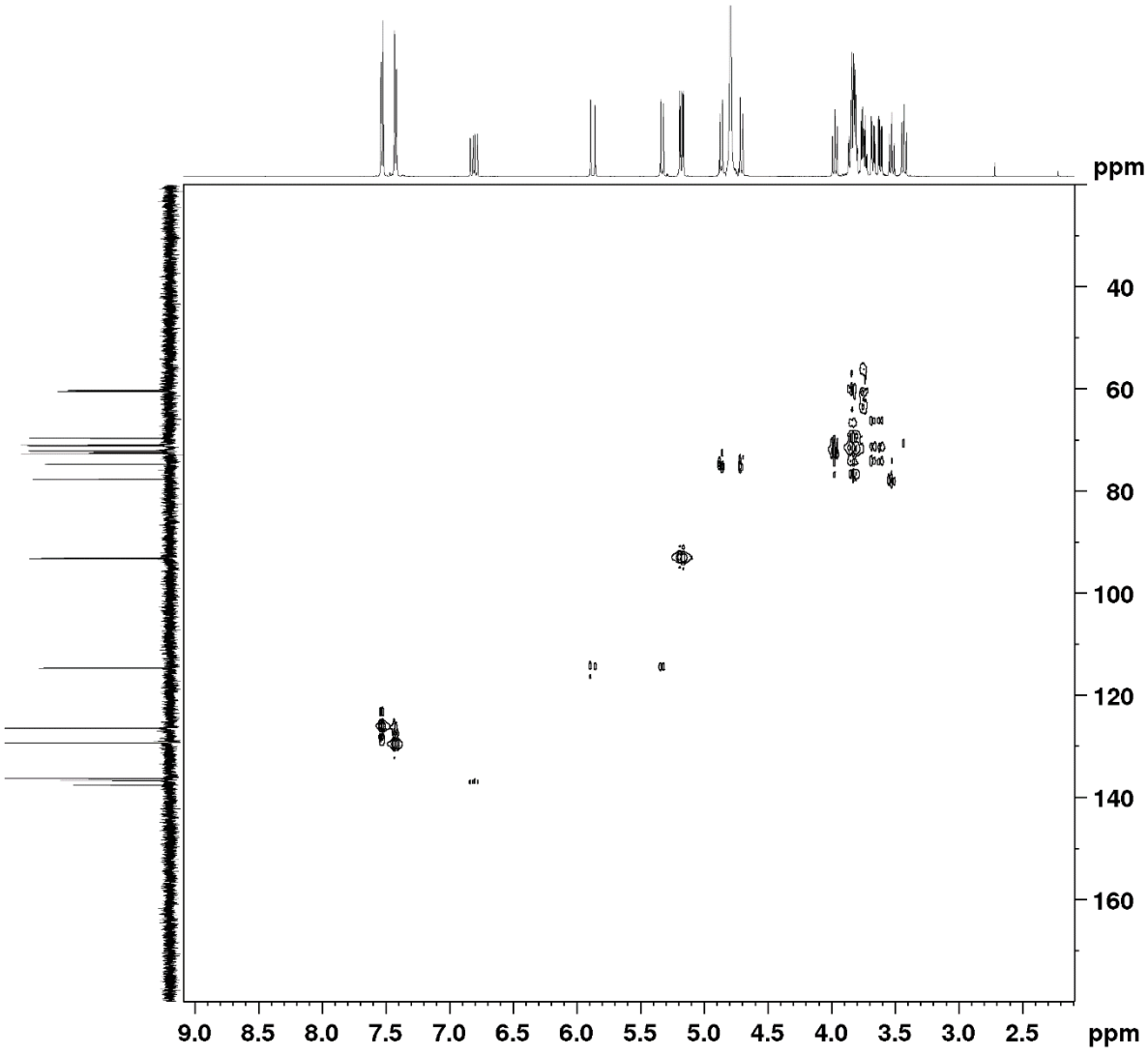


Figure S14. HSQC spectrum of **O4** in D_2O at 298 K.

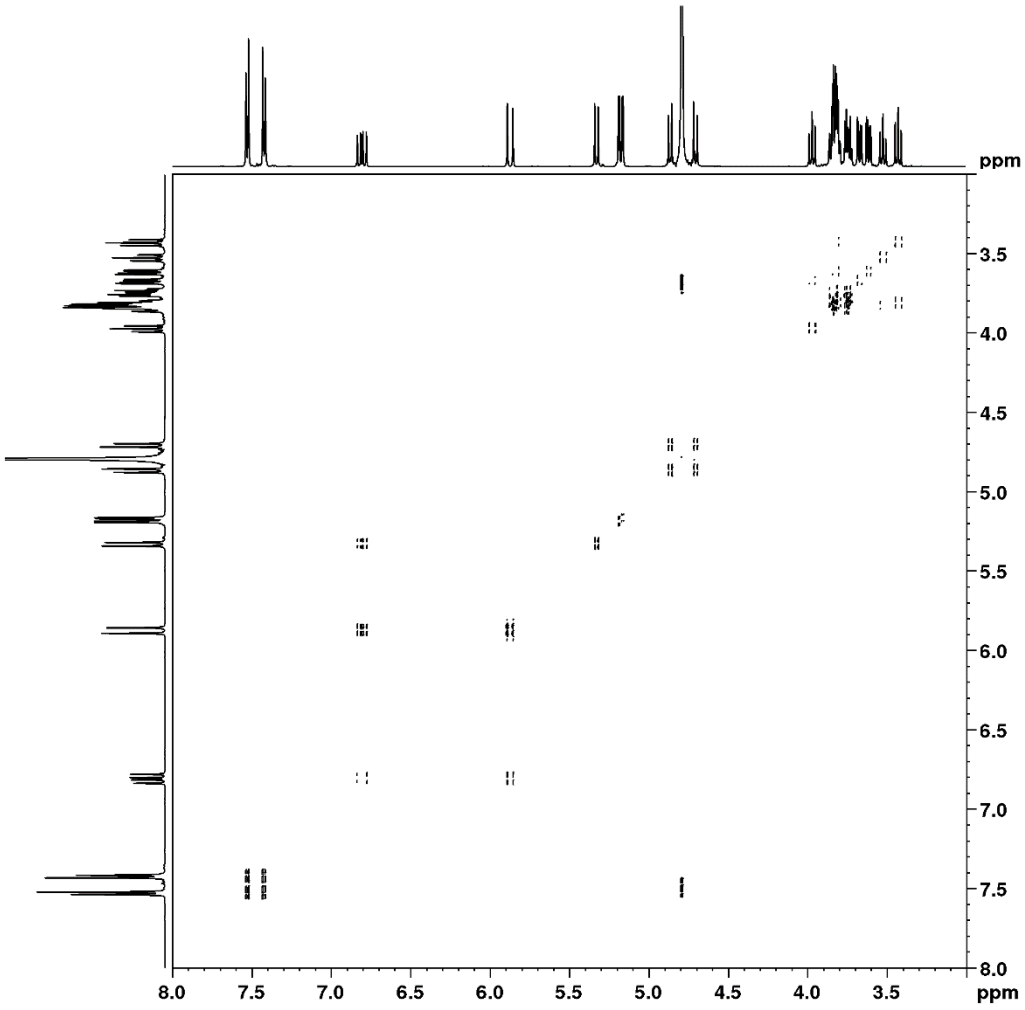


Figure S15. COSY spectrum of **O4** in D_2O at 298 K.

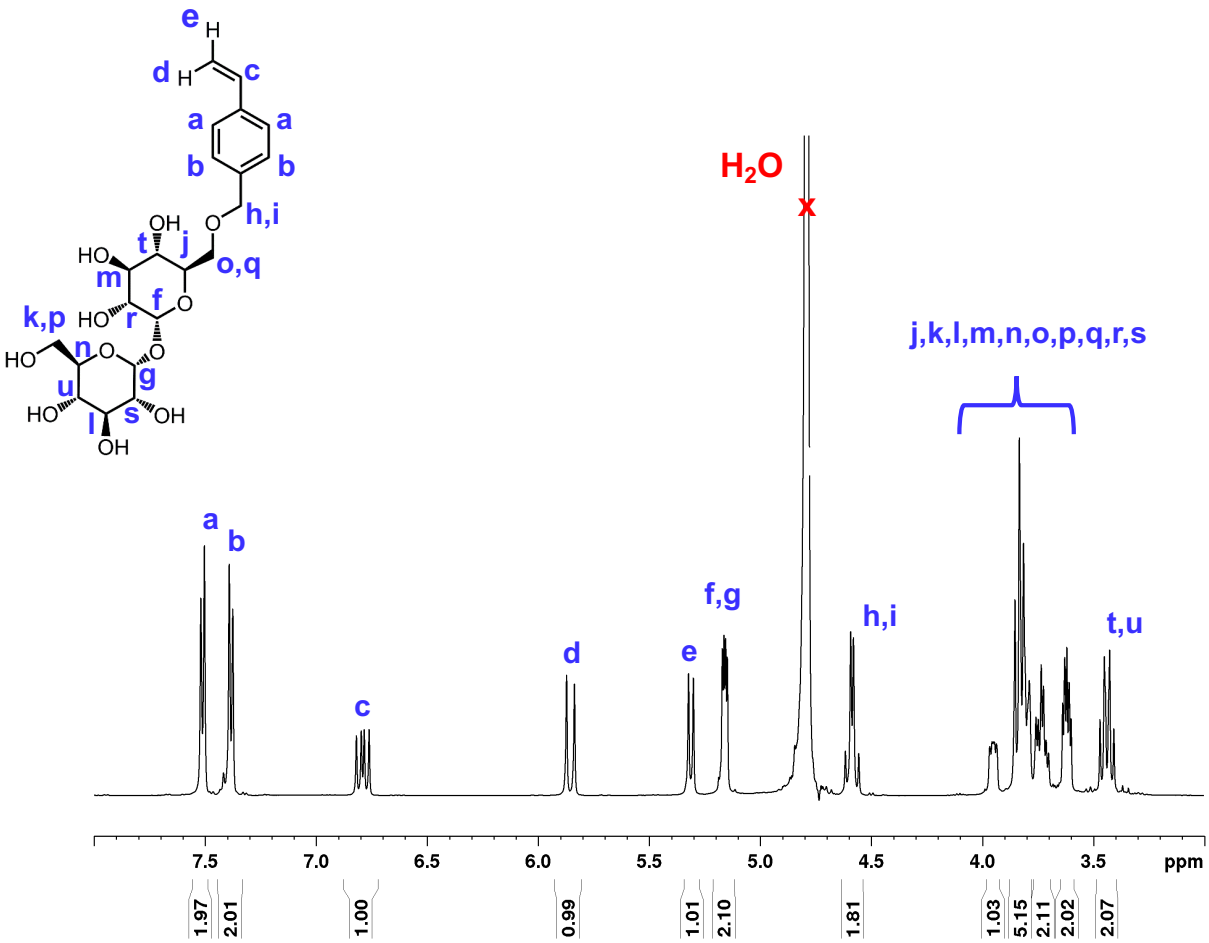


Figure S16. ^{1}H NMR spectrum of **O6** in D_2O at 298 K.

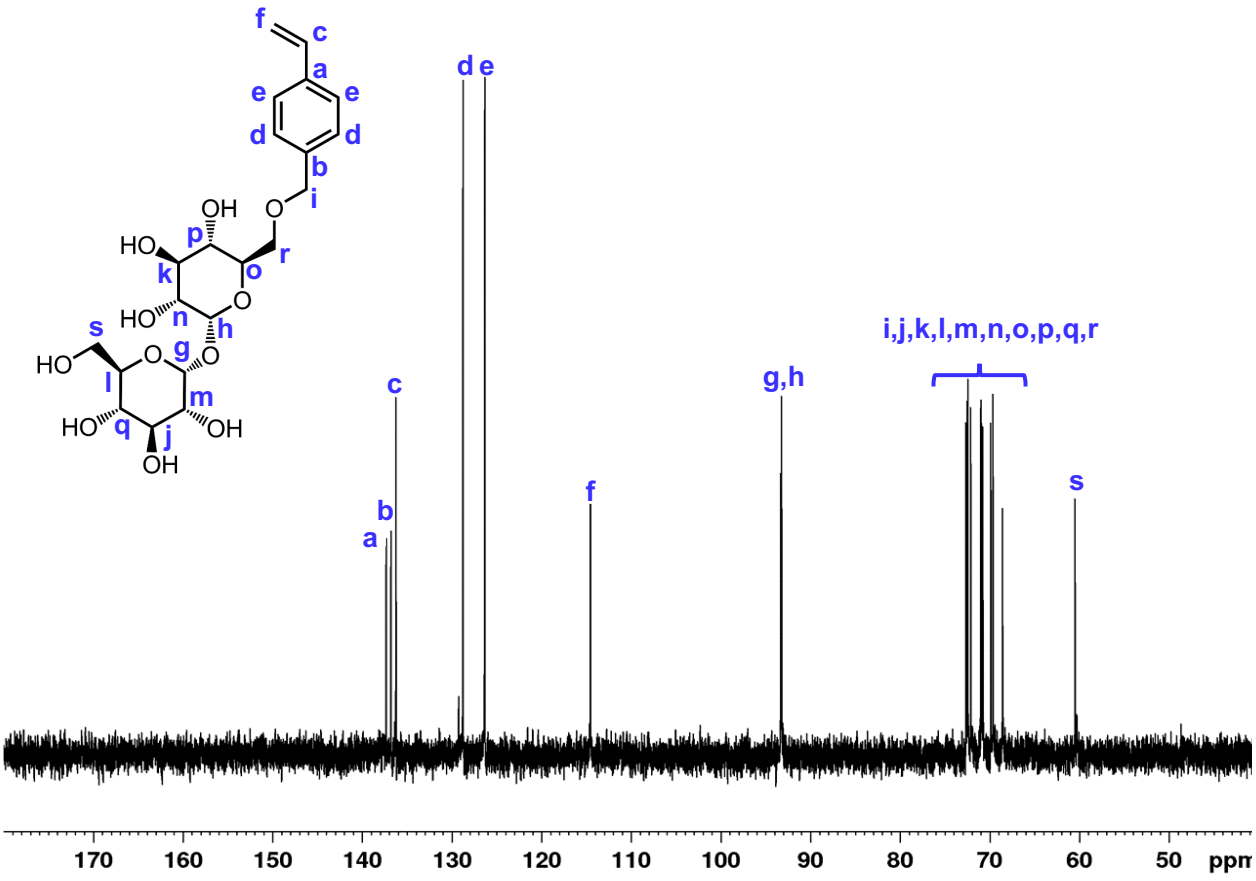


Figure S17. ^{13}C NMR spectrum of **O6** in D_2O at 298 K.

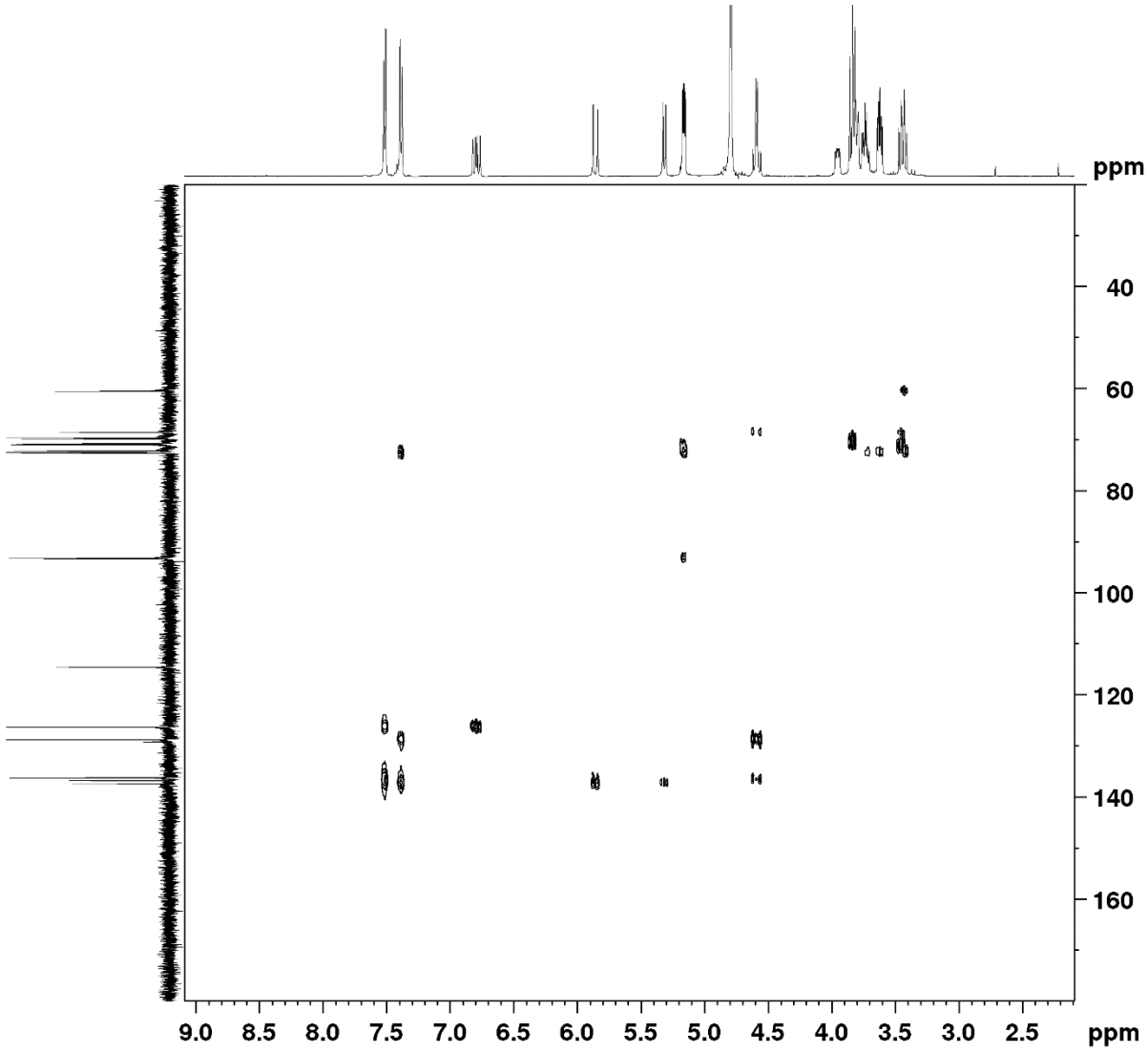


Figure S18. HMBC spectrum of **O6** in D_2O at 298 K.

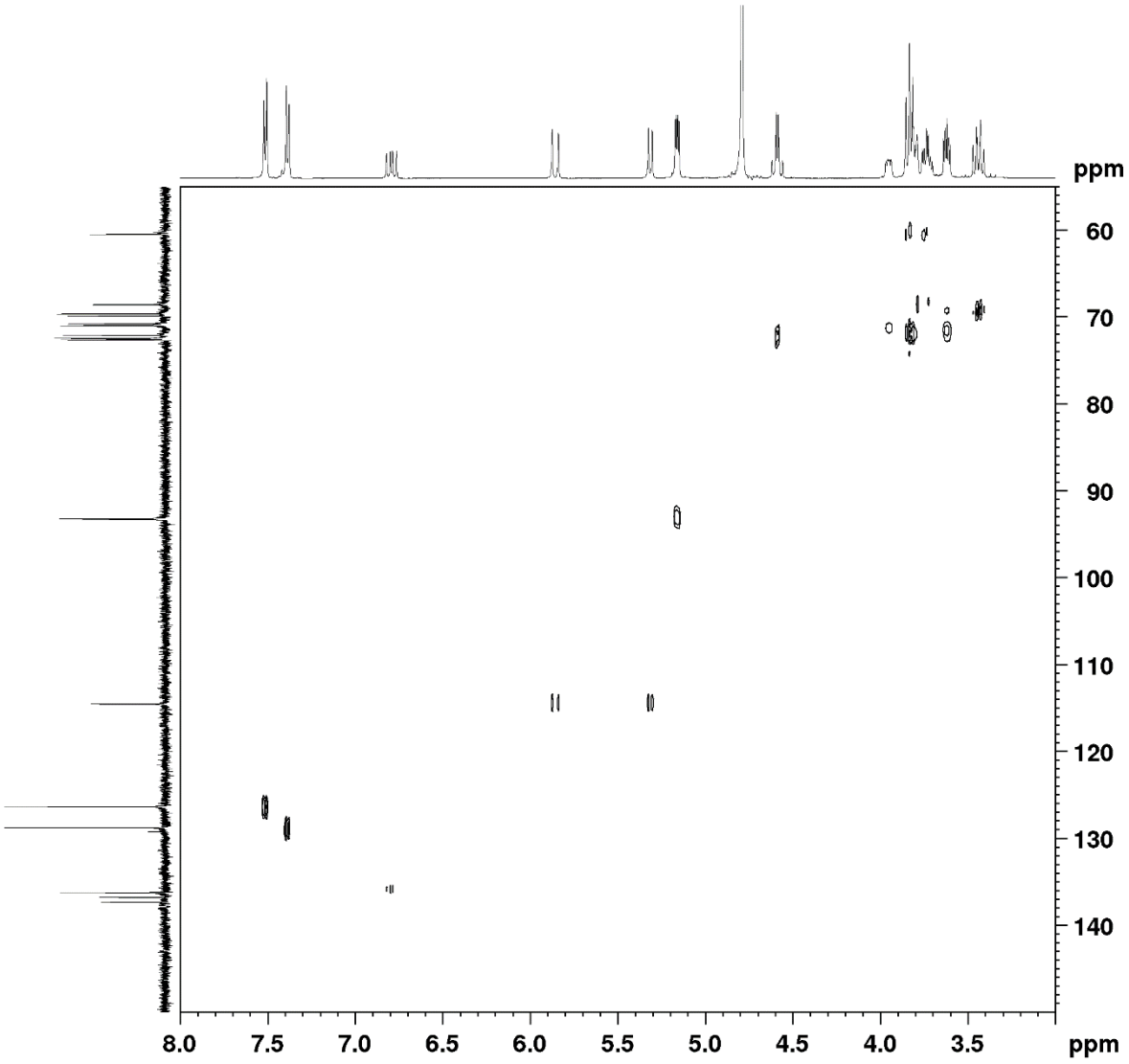


Figure S19. HSQC spectrum of **O6** in D_2O at 298 K.

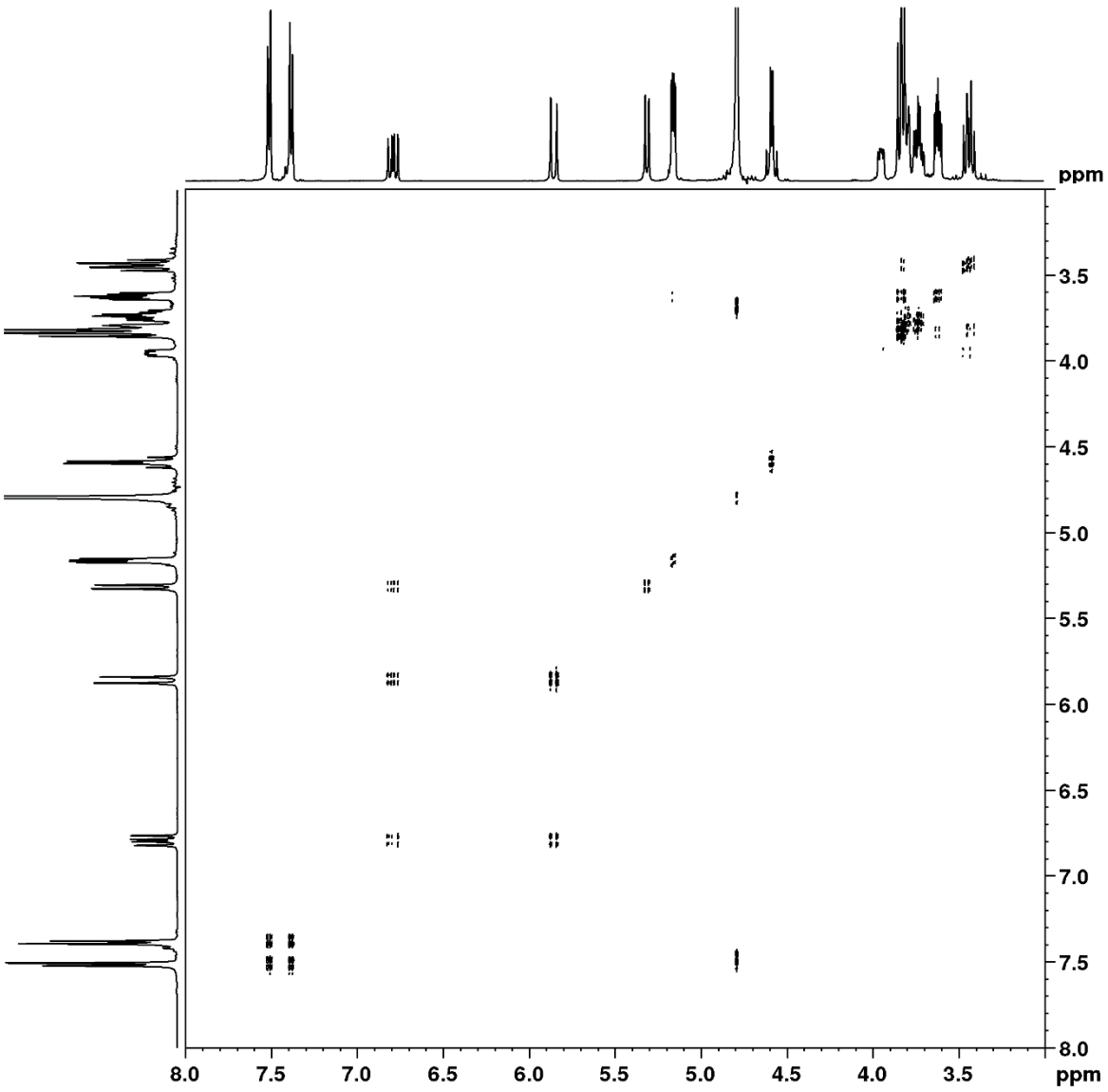


Figure S20. COSY spectrum of **O6** in D_2O at 298 K.

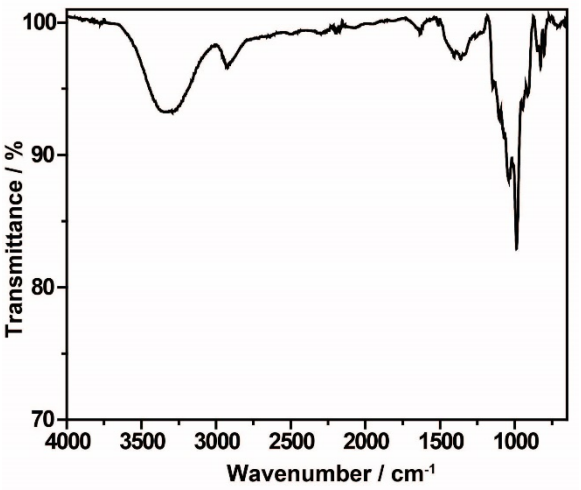


Figure S21. IR spectrum of **O2**.

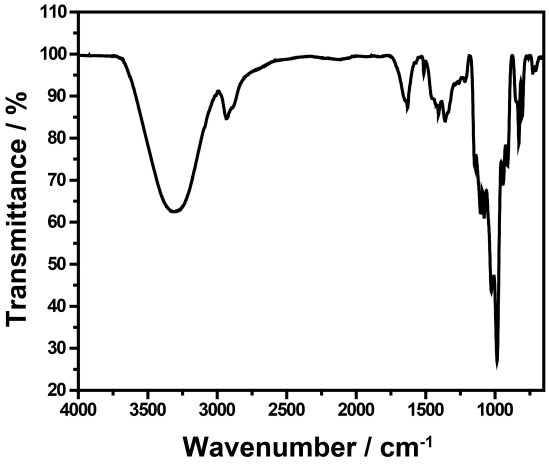


Figure S22. IR spectrum of **O3**.

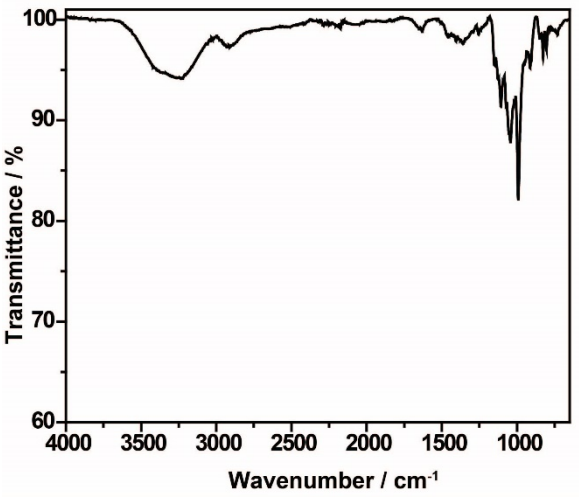


Figure S23. IR spectrum of **O4**.

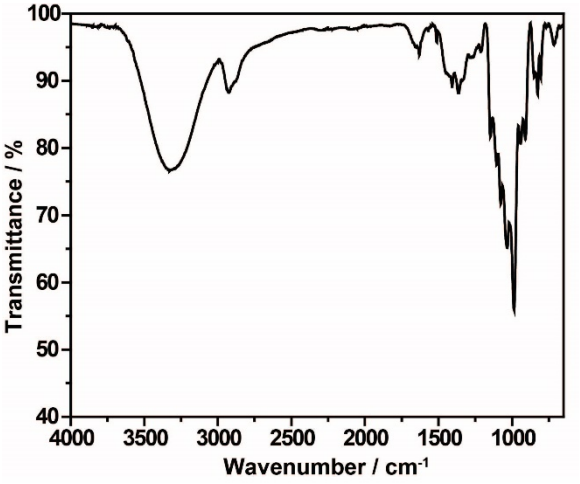


Figure S24. IR spectrum of **O6**.

III. Polymer Characterization

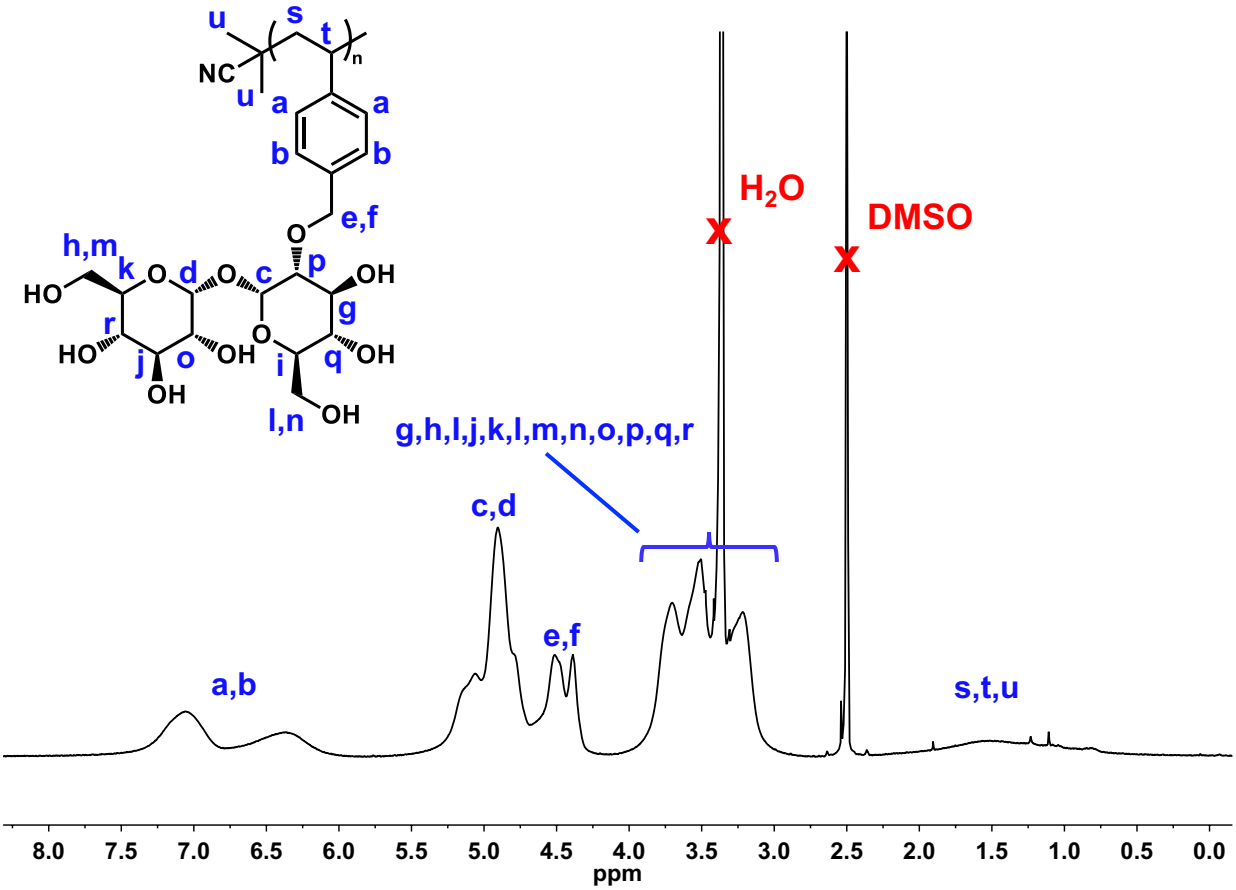


Figure S25. ^{1}H NMR spectrum of **P2** in DMSO-d_6 at 298K.

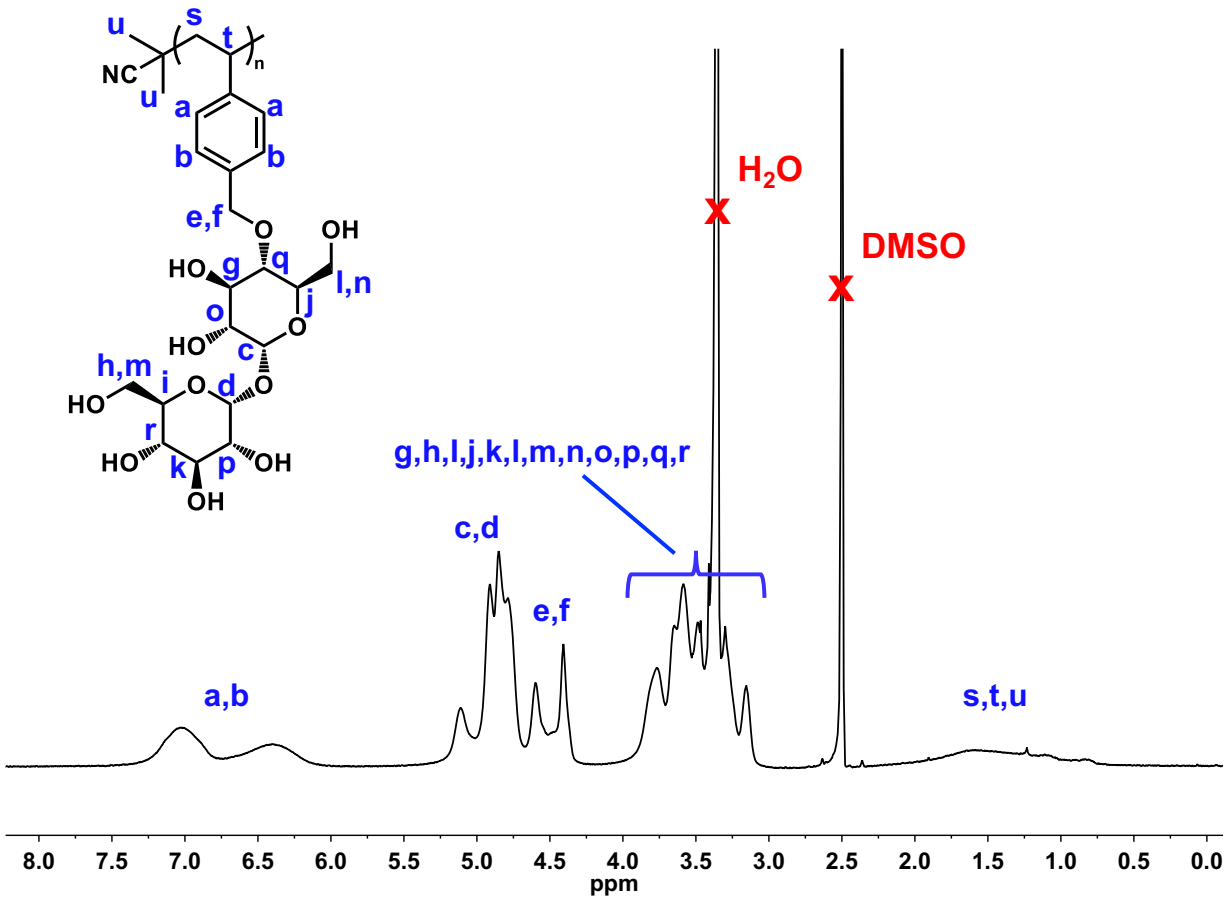


Figure S26. ^{1}H NMR spectrum of **P4** in DMSO-d_6 at 298K.

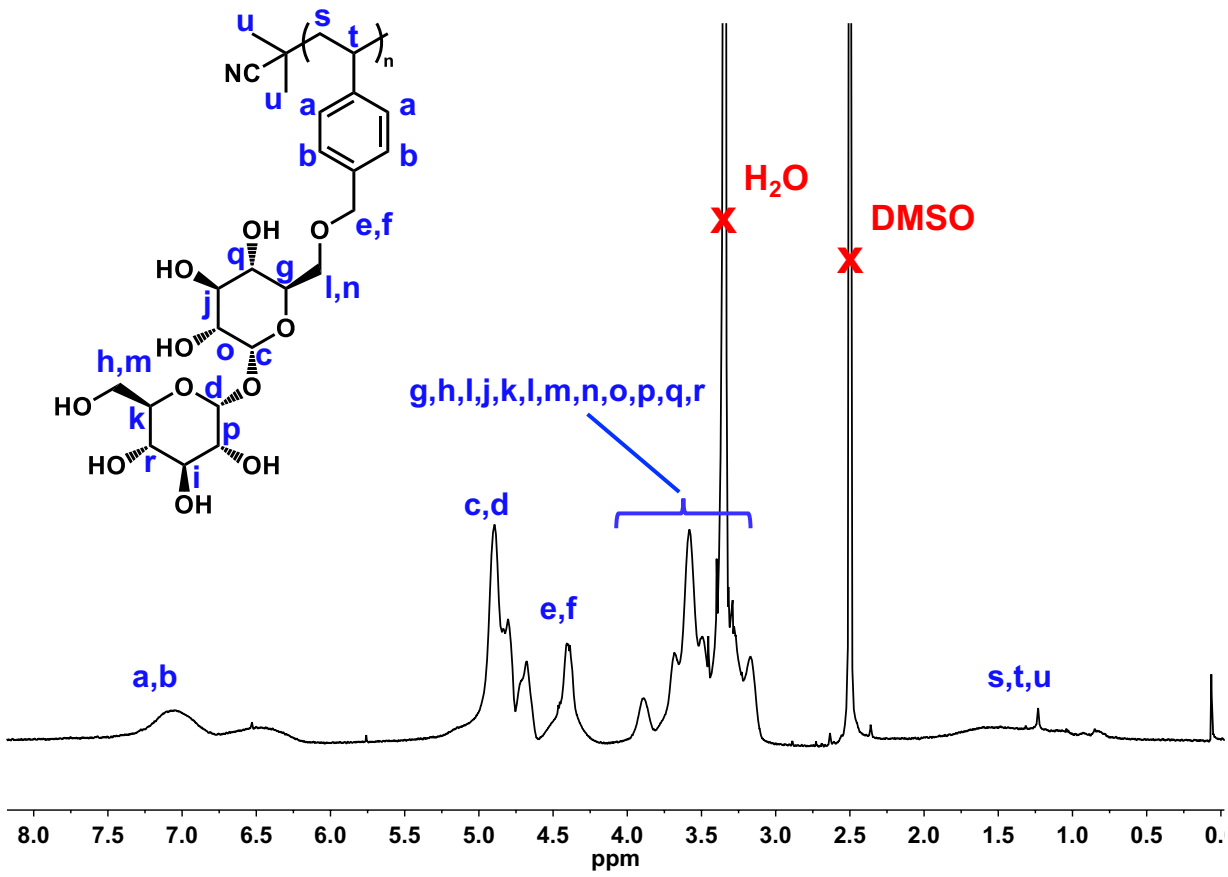


Figure S27. ^{1}H NMR spectrum of **P6** in DMSO-d_6 at 298K.

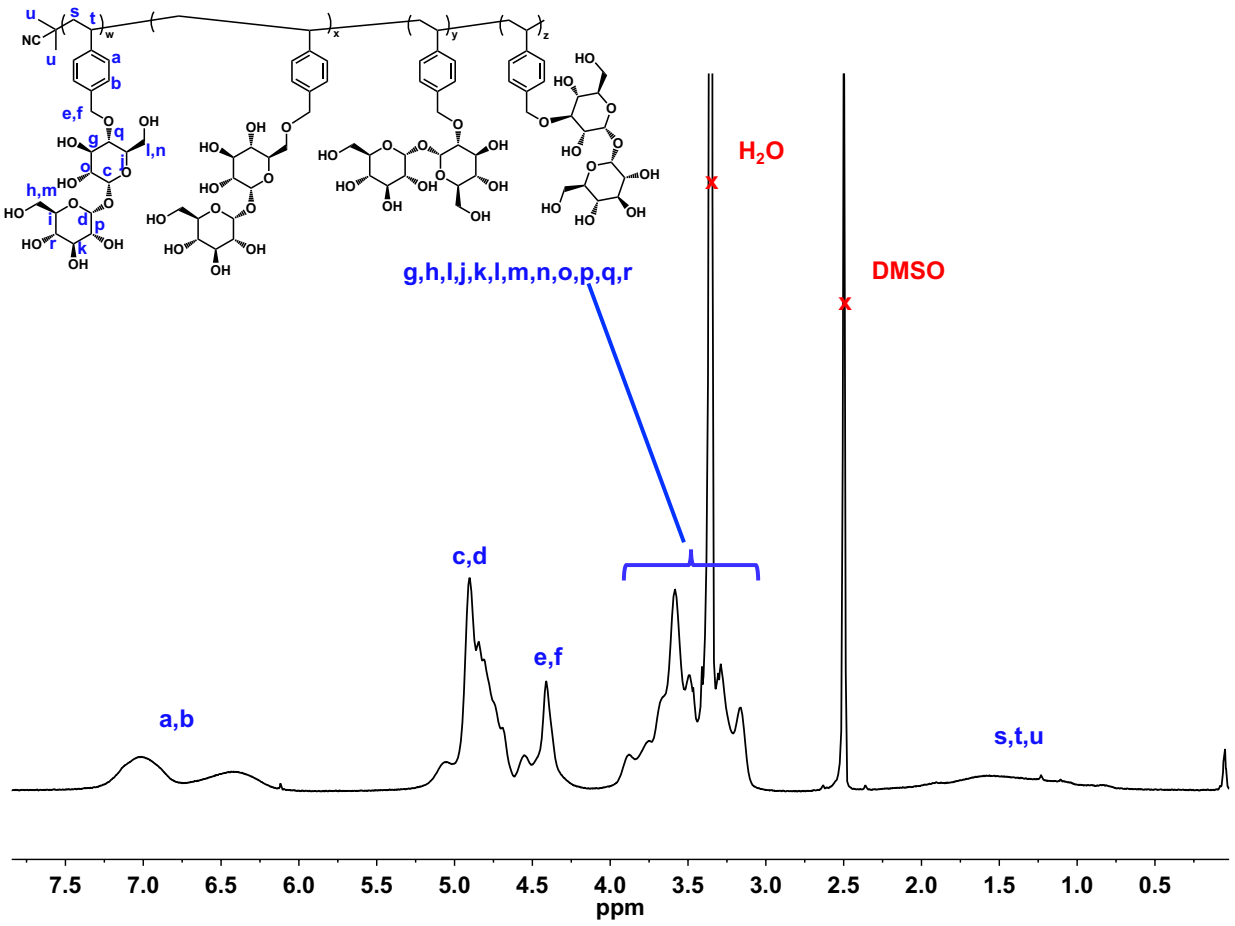


Figure S28. ^{1}H NMR spectrum of **PA** in DMSO-d_6 at 298K.

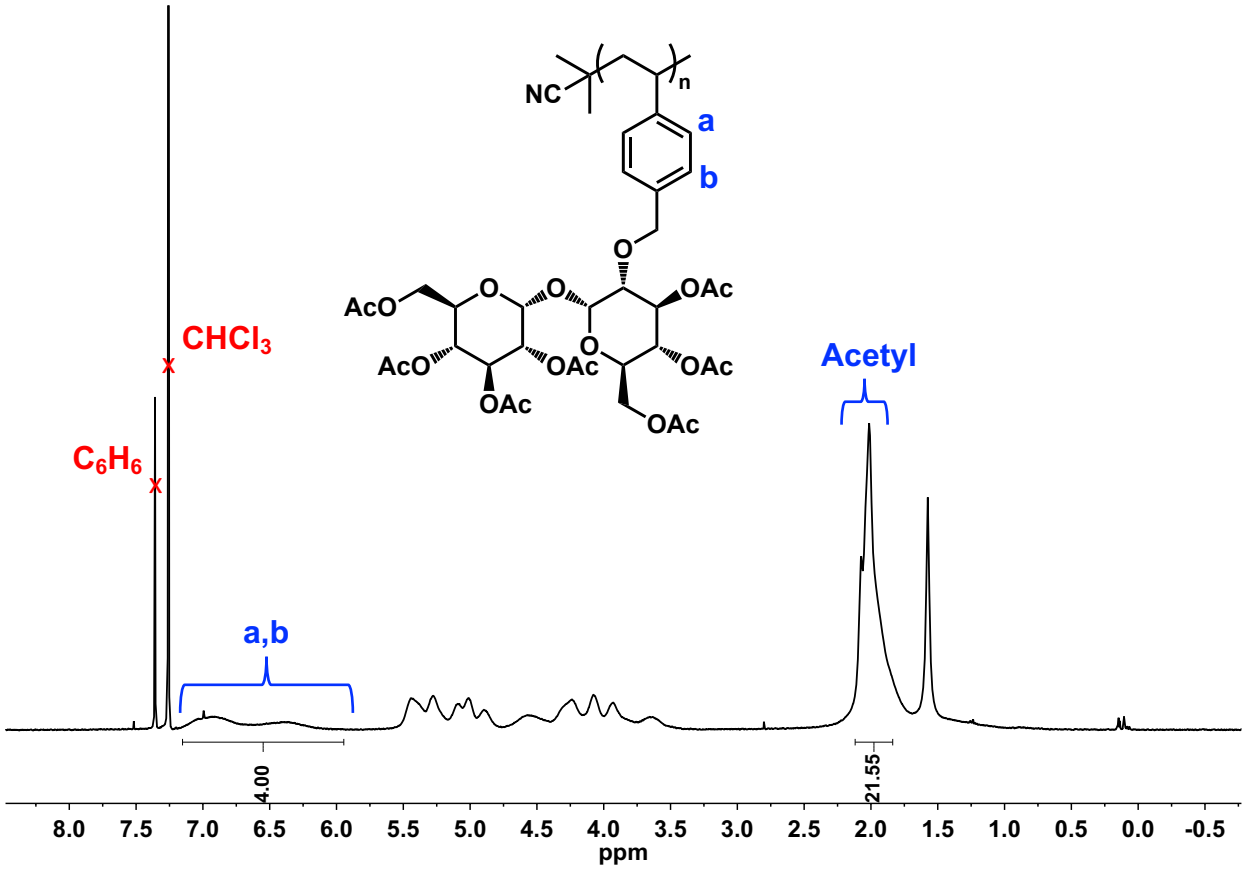


Figure S29. ^{1}H NMR spectrum of acetylated **P2-OAc** in $CDCl_3$ at 298 K.

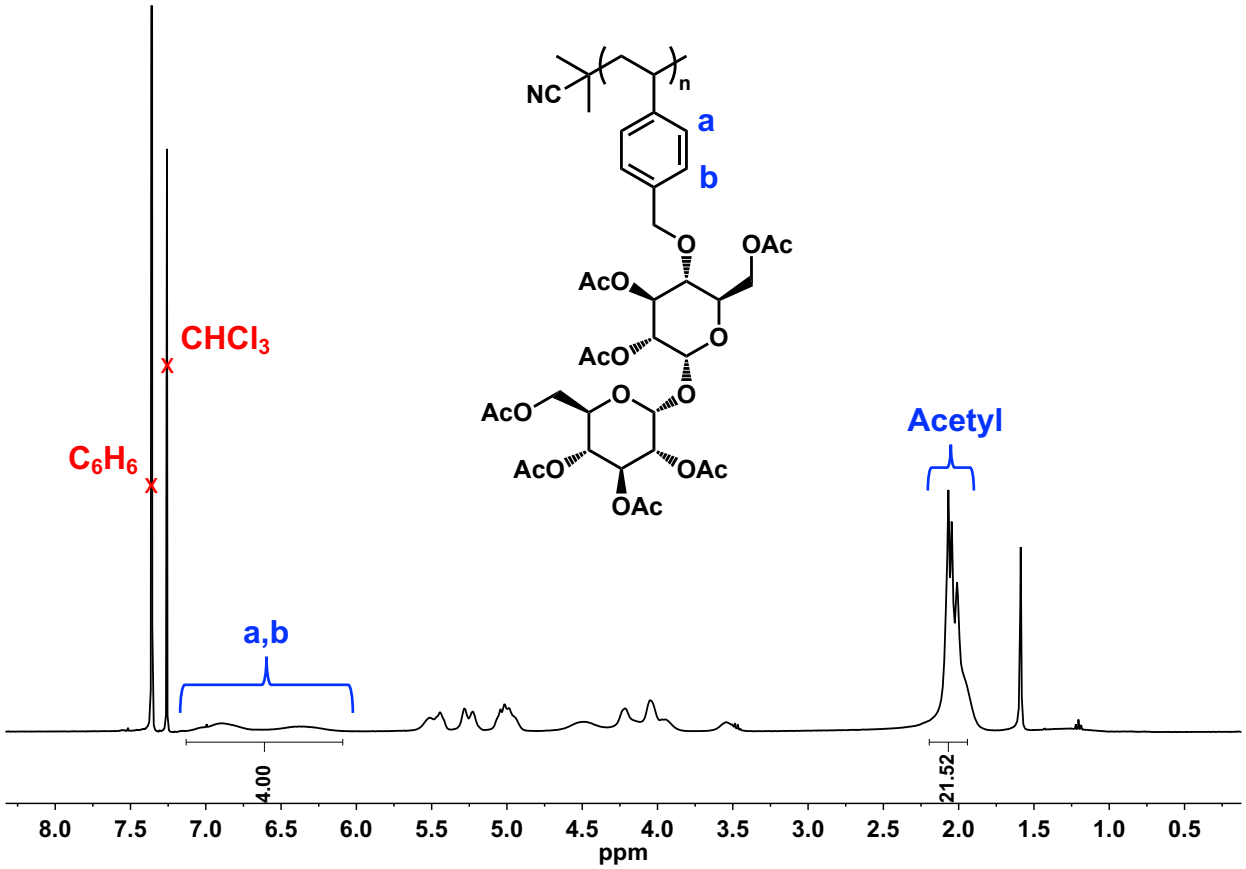


Figure S30. ^{1}H NMR spectrum of acetylated **P4-OAc** in $CDCl_3$ at 298 K.

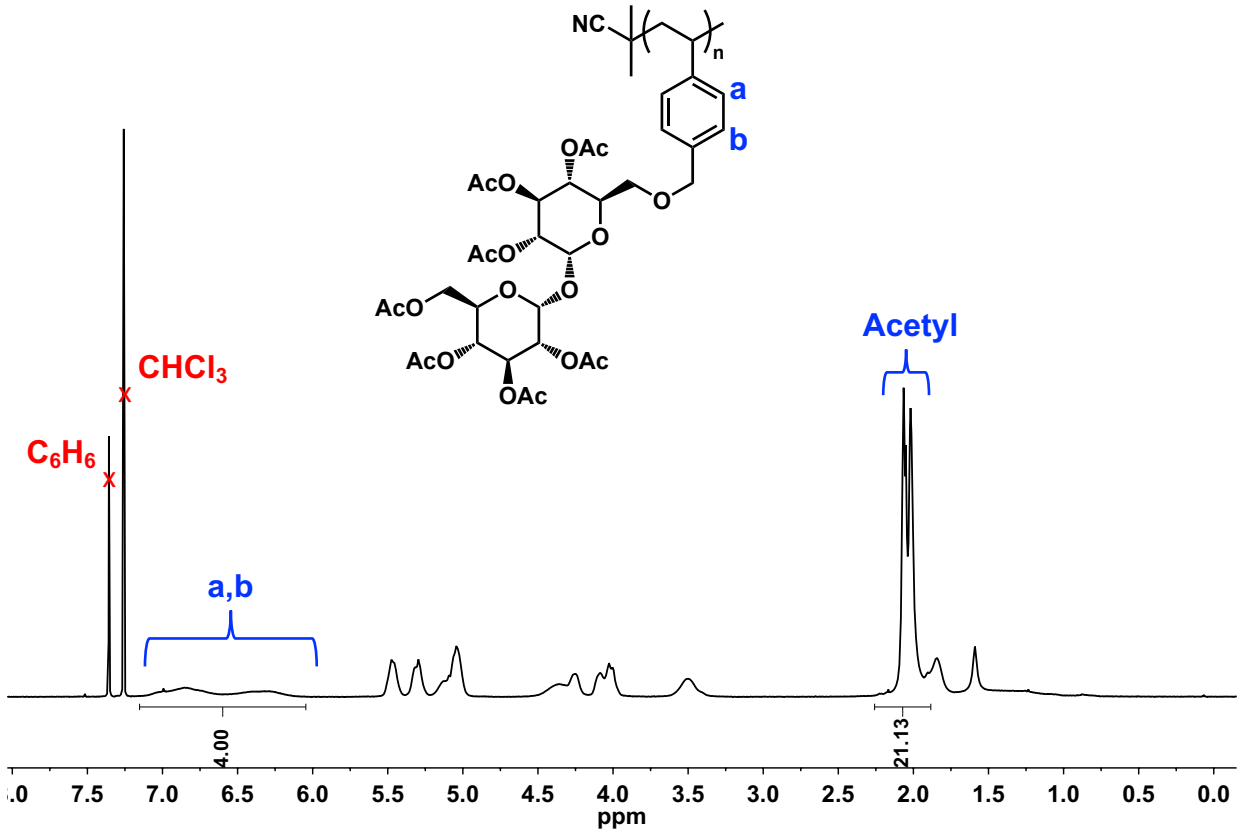


Figure S31. ^{1}H NMR spectrum of acetylated **P6-OAc** in $CDCl_3$ at 298 K.

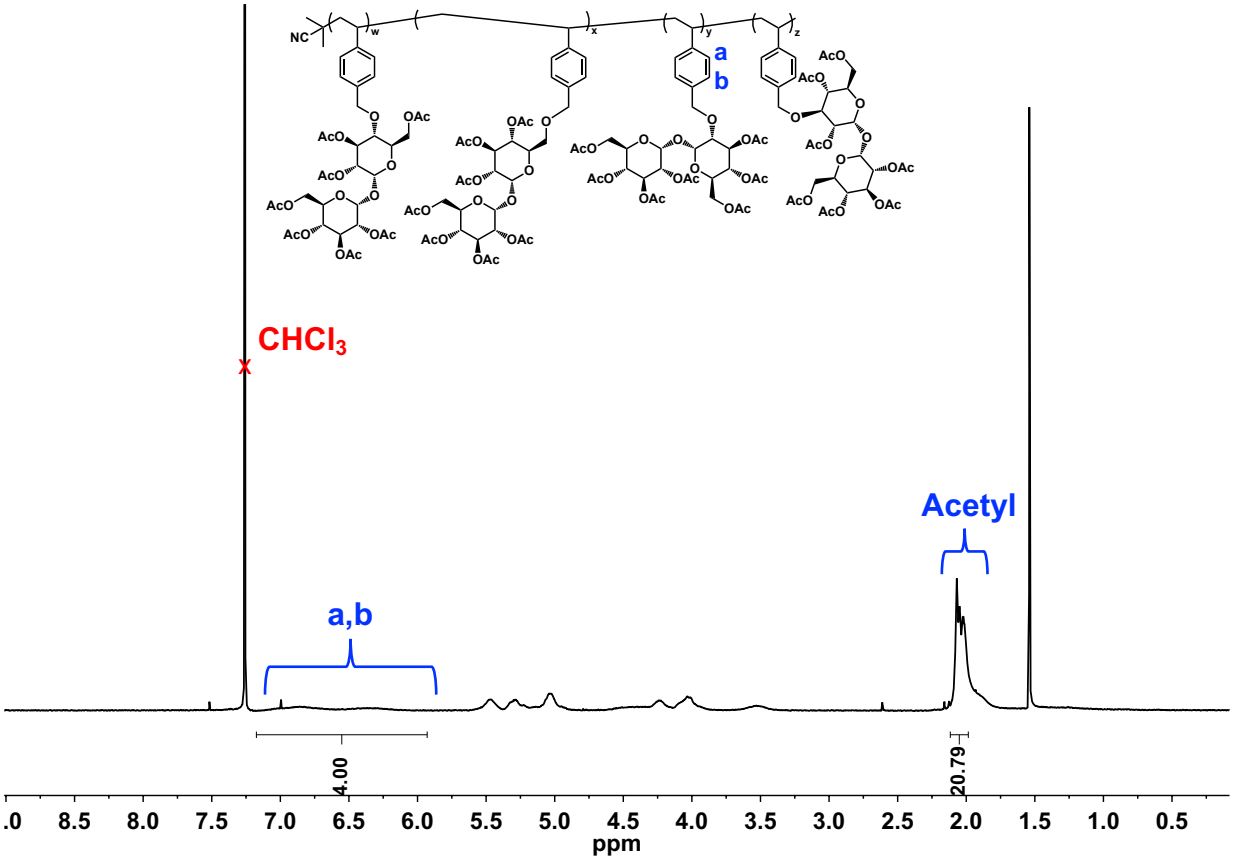


Figure S32. ^{1}H NMR spectrum of acetylated **PA-OAc** in $CDCl_3$ at 298 K.

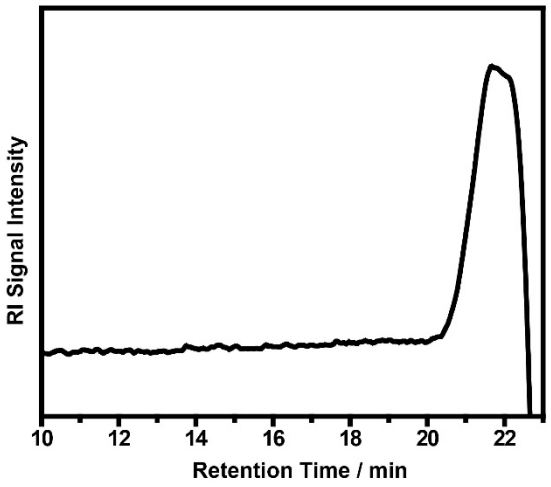


Figure S33. GPC trace of **P2**. M_n= 1.9 kDa; M_w= 2.1 kDa; $Đ$= 1.09.

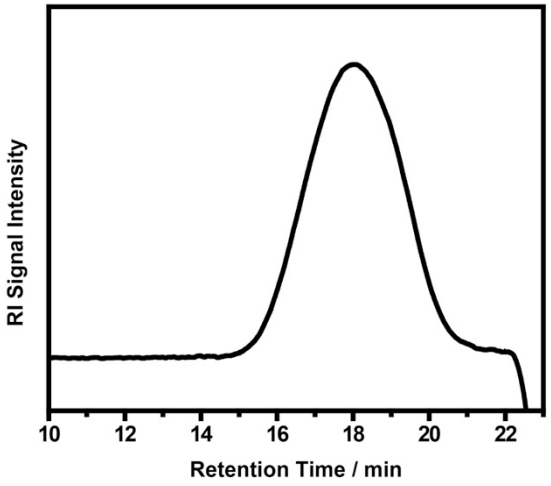


Figure S34. GPC trace of **P2-OAc**. M_n= 15.7 kDa; M_w= 25.0 kDa; $Đ$= 1.59.

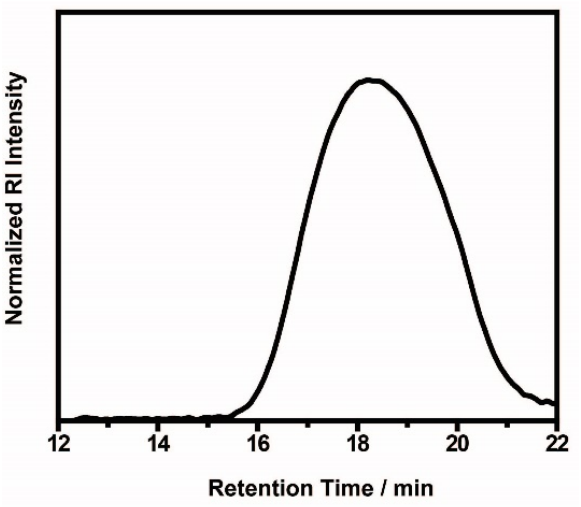


Figure S35. GPC trace of **P4**. M_n= 14.8 kDa; M_w= 23.2 kDa; $Đ$= 1.56.

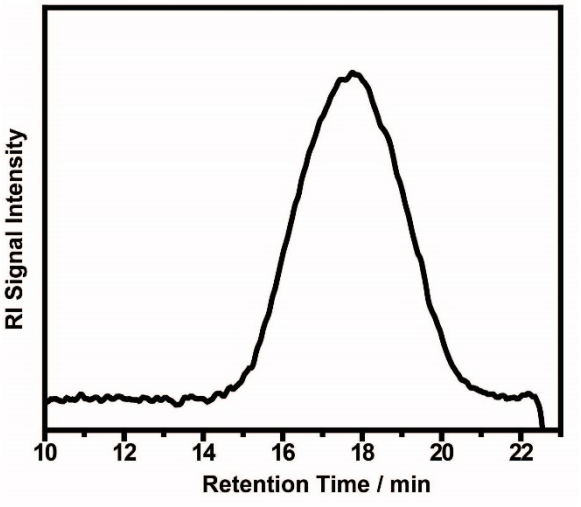


Figure S36. GPC trace of **P4-OAc**. M_n=19.6 kDa; M_w= 31.7 kDa; $Đ$= 1.62.

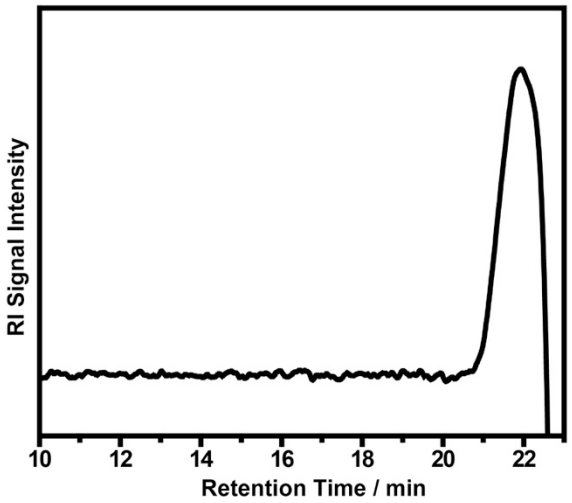


Figure S37. GPC trace of **P6**. M_n=1.8 kDa; M_w= 1.9 kDa; $Đ$= 1.05.

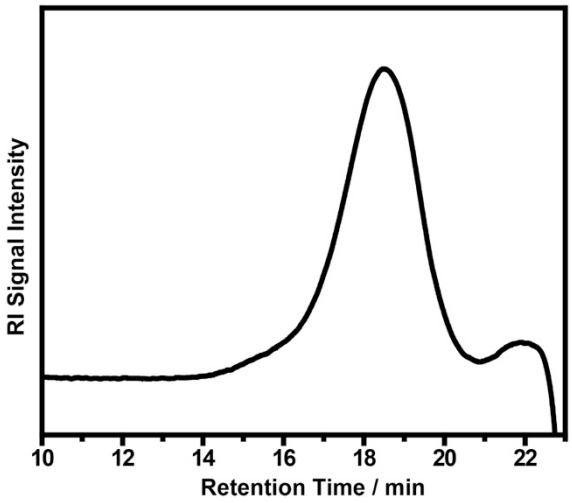


Figure S38. GPC trace of **P6-OAc**. M_n=15.4 kDa; M_w= 21.2 kDa; $Đ$= 1.37.

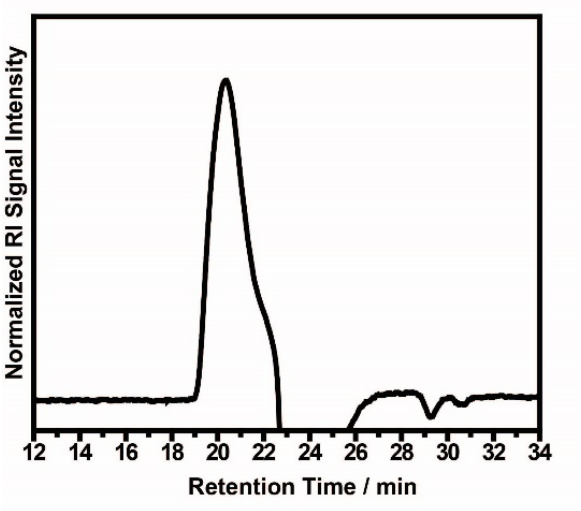


Figure S39. GPC trace of **PA**. M_n=4.4 kDa; M_w= 5.4 kDa; $Đ$= 1.21.

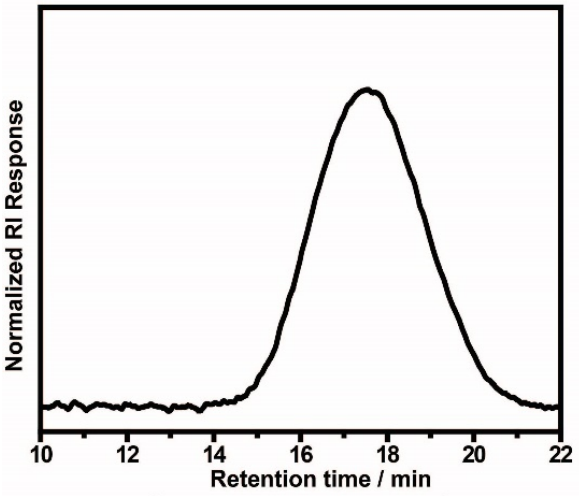


Figure S40. GPC trace of **PA-OAc**. M_n=19.6 kDa; M_w= 35.0 kDa; $Đ$= 1.62.

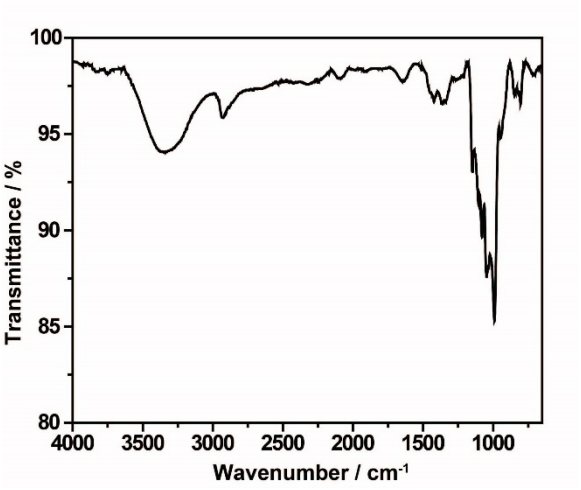


Figure S41. IR spectrum of **P2**.

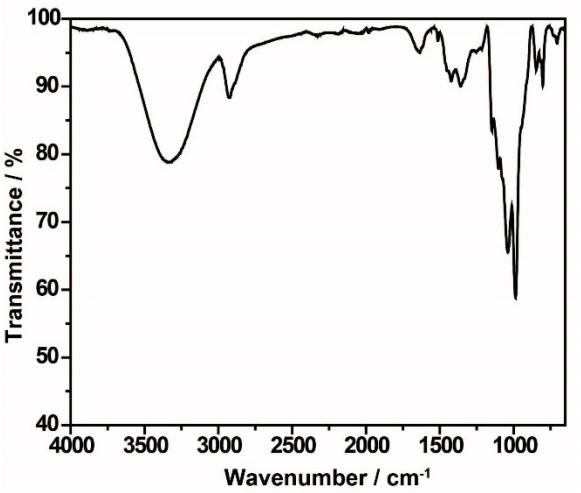


Figure S42. IR spectrum of **P4**.

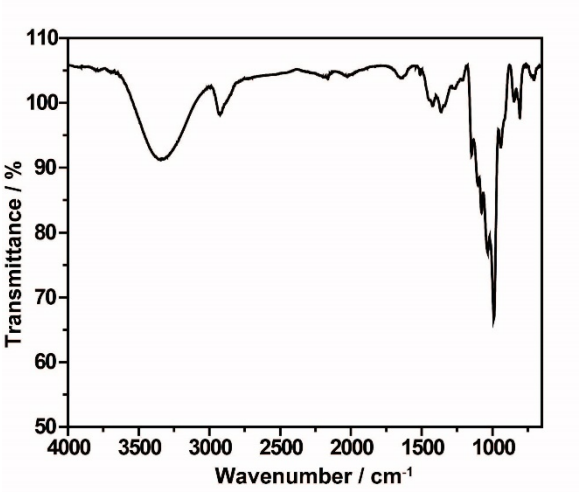


Figure S43. IR spectrum of **P6**.

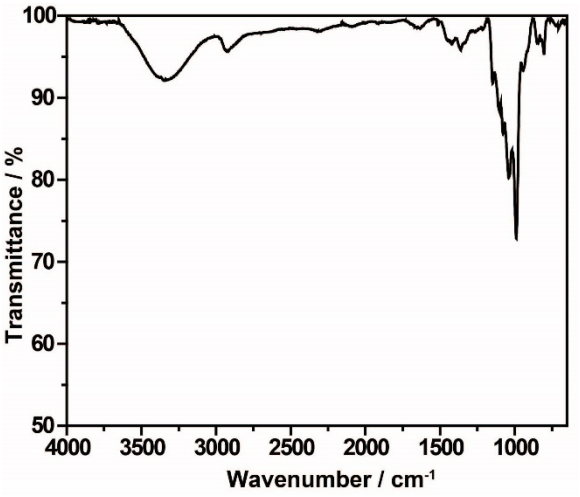


Figure S44. IR spectrum of **PA**.

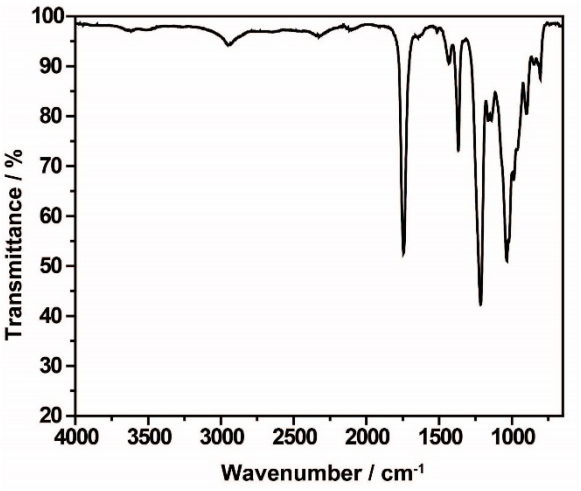


Figure S45. IR spectrum of **PA-OAc**.

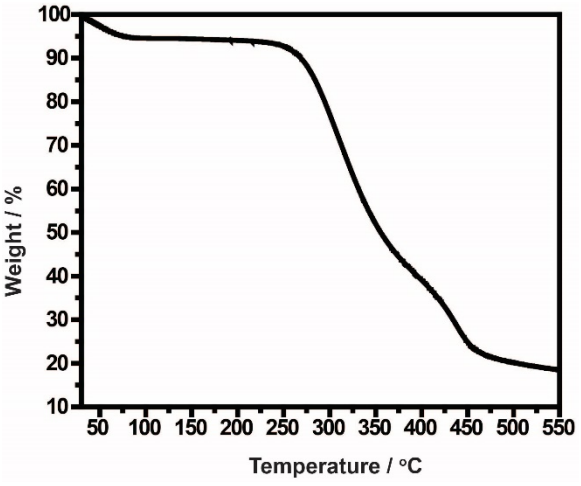


Figure S46. TGA of **P2**.

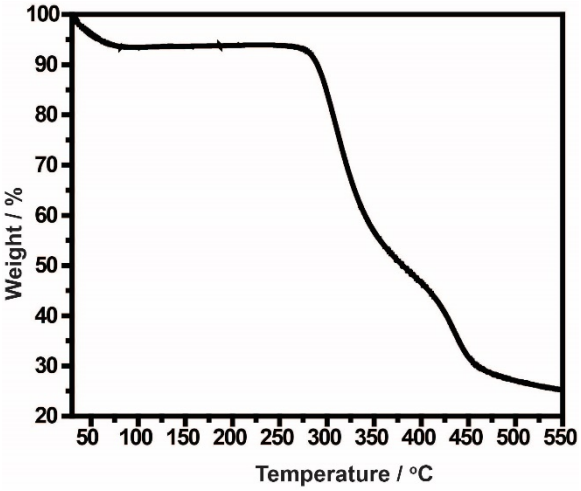


Figure S47. TGA of **P4**.

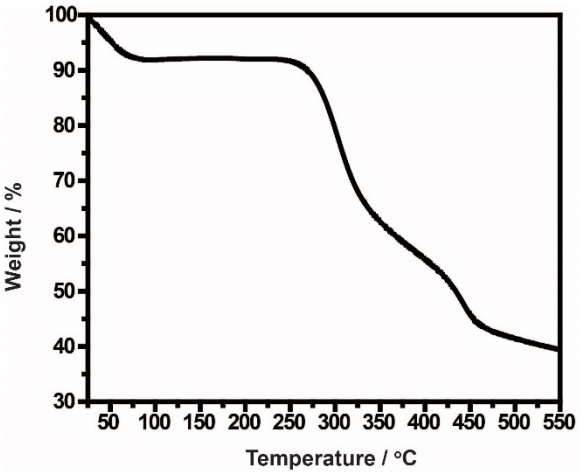


Figure S48. TGA of **P6**.

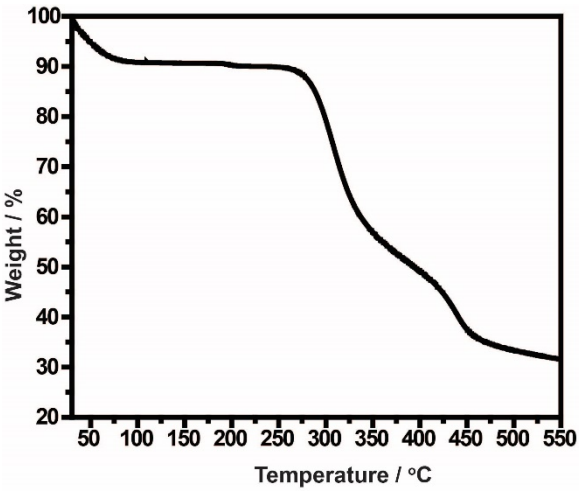


Figure S49. TGA of **PA**.

IV. Insulin Assay Data

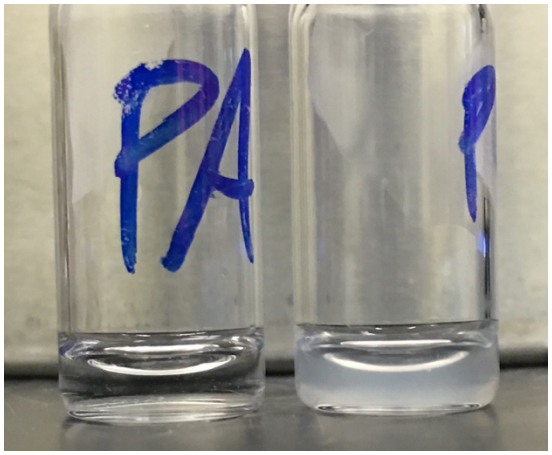


Figure S50. Non-aggregated (left) and aggregated (right) insulin samples.

A.

	Intact insulin (%)
DPBS	0%
P2	0%
P4	0%
P6	0%
PA	0%

B.

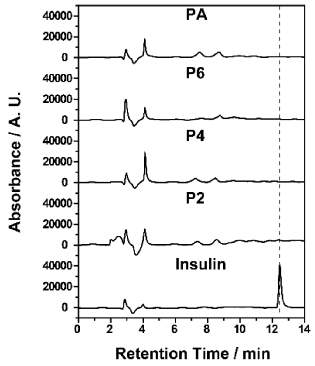


Figure S51. A) Insulin agitation assay using 1 wt. equiv. of polymer shows no stabilization. Samples were heated to 37 °C with 250 rpm agitation for 3 hours. B) Intact insulin quantified by HPLC, representative traces for 1 wt. equiv. polymer assay shown. Insulin data on bottom panel is an unstressed insulin stock solution with the protein eluting at 12 minutes. (n=3)

V. Computational Methods, Coordinates, and Energies

Computational Methods

Conformers for regioisomer **O2**, **O4**, and **O6** were searched by using Maestro 9.4. with OPLS_2015 force field in implicit water. For each regioisomer, the ensemble of conformers consist of those whose energies are within 10 kcal/mol from the lowest one. This ensemble typically include ~400 structures. The structures were then clustered to 25 representatives for **O2**, 33 for **O4**, and 42 for **O6** using the chemical informatics tool in Maestro 9.4. These structures were then optimized using B3LYP/6-31g(d) with SMD water model in Gaussian 09.

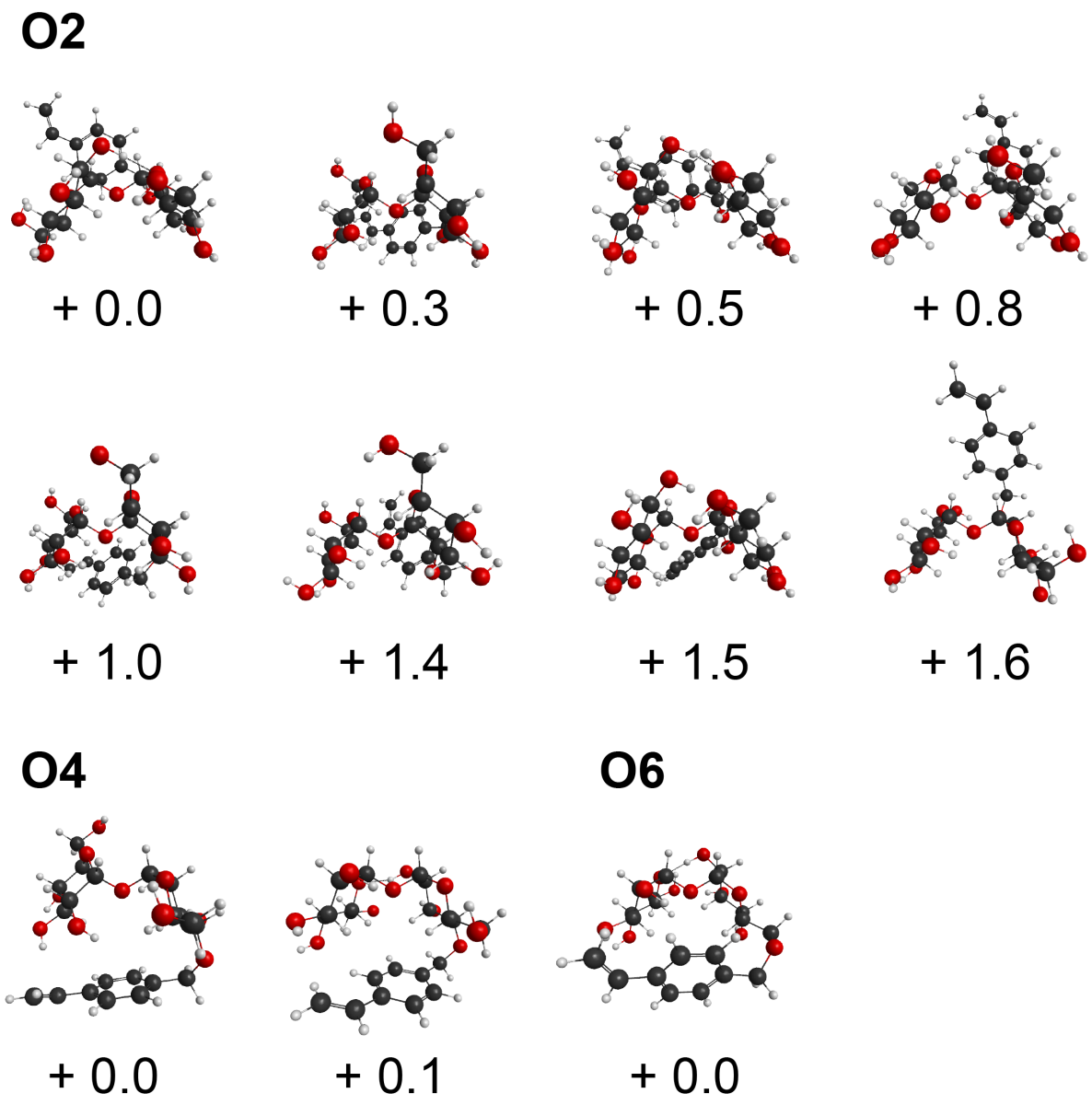


Figure S52. Conformers for the regioisomers within 2 kcal/mol of the most stable conformer (energy difference in kcal/mol shown below the structures)

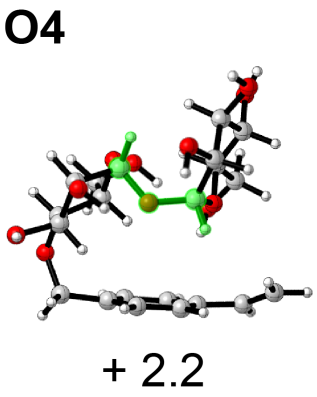


Figure S53. Example of conformer with disrupted clam shell conformation (**O4** conformer with 2.2 kcal/mol higher energy than the most stable conformation)

Coordinates and Energies

Conformations for **O2** (Energies in Hartree)

S0.out

O	2.153843	-0.842051	1.315374
C	3.591569	-0.943768	1.219514
C	4.017428	-1.497666	-0.155945
C	2.860805	-2.295295	-0.762233
C	1.642046	-1.393909	-1.010260
C	1.588606	-0.331550	0.107513
C	4.233175	0.400282	1.558667
H	3.868972	-1.678074	1.980728
O	5.164105	-2.318540	0.053858
H	5.376618	-2.714801	-0.809138
H	4.271055	-0.674043	-0.841736
O	3.332999	-2.892583	-1.967371
H	2.653276	-3.524396	-2.256016
H	2.564607	-3.069566	-0.041740
O	0.504421	-2.246321	-1.074785
H	1.779895	-0.877356	-1.968061
O	0.269178	0.048728	0.368775
H	2.171859	0.535521	-0.220751
C	0.146499	1.207204	1.200900
O	0.880707	2.298490	0.695811
C	0.491104	2.710665	-0.631085
C	-0.968868	3.165657	-0.602634
C	-1.849782	2.021233	-0.082348
C	-1.350072	1.537531	1.285136
H	0.562693	0.998782	2.189518
C	1.483890	3.778273	-1.056527
H	0.573363	1.862479	-1.324596
O	2.815781	3.258667	-1.129570
H	2.820147	2.577630	-1.823641
H	1.505571	4.581082	-0.313052
H	1.166486	4.201891	-2.017401
O	-1.357560	3.530558	-1.925097
H	-2.330034	3.583089	-1.907343
H	-1.063953	4.025006	0.081203
O	-3.225172	2.404235	-0.063675
H	-3.325941	3.112005	0.597676
H	-1.796553	1.195472	-0.797577
O	-2.104092	0.453889	1.805842
H	-1.980376	-0.308082	1.211397
H	-1.454642	2.355000	2.006925
O	3.843843	0.843218	2.858137
H	2.872213	0.892611	2.841037
H	3.975913	1.152859	0.798677
H	5.321590	0.285732	1.565043
C	-0.603292	-1.744994	-1.830983
H	-0.709295	-2.372654	-2.727582
H	-0.405665	-0.723689	-2.174223
C	-1.891014	-1.767416	-1.040635
C	-3.001693	-1.058039	-1.524072
C	-2.021290	-2.476562	0.156514
C	-4.202286	-1.041288	-0.823776
H	-2.914391	-0.496579	-2.451483
C	-3.230737	-2.467168	0.856103
H	-1.170293	-3.020567	0.551816
C	-4.342934	-1.746596	0.387856
H	-5.034123	-0.465860	-1.218434
H	-3.309524	-3.016847	1.790901
C	-5.582580	-1.750657	1.181791
H	-5.539344	-2.360416	2.084427
C	-6.719683	-1.094053	0.913084
H	-6.844591	-0.461826	0.037412
H	-7.575294	-1.172009	1.578117

Sum of electronic and thermal Free Energies= -1645.320765

SCF Energies= -1645.771012

S1.out

O	-2.522781	-0.121056	-1.329860
C	-3.859802	0.145321	-0.857712
C	-4.148671	-0.604019	0.461448
C	-3.291384	-1.870038	0.531736
C	-1.774495	-1.572945	0.450518
C	-1.602936	-0.220200	-0.245659
C	-4.103927	1.642176	-0.740635
H	-4.519152	-0.268064	-1.626890
O	-5.537834	-0.927517	0.468845
H	-5.680746	-1.477069	1.259462
H	-3.913540	0.032358	1.328266
O	-3.646403	-2.555343	1.733055
H	-3.321359	-3.467670	1.653311
H	-3.542866	-2.482615	-0.343838
O	-1.155439	-2.638406	-0.271148
H	-1.360657	-1.495644	1.461740
O	-0.299136	-0.058079	-0.732840
H	-1.818500	0.566752	0.486974
C	-0.061921	1.213511	-1.345076
O	-0.446860	2.292132	-0.516427
C	0.267241	2.390350	0.729781
C	1.755530	2.580178	0.436190
C	2.275787	1.429341	-0.415500
C	1.434462	1.276747	-1.687594
H	-0.681236	1.309504	-2.238865
C	-0.356135	3.563614	1.485088
H	0.133397	1.475322	1.320306
O	0.126658	3.649627	2.823771
H	1.100271	3.610487	2.763737
H	-1.439054	3.412392	1.540757
H	-0.170572	4.493462	0.926024
O	2.449265	2.634101	1.688332
H	3.396748	2.698132	1.475415
H	1.890098	3.522861	-0.114845
O	3.641934	1.717142	-0.719149
H	4.094910	0.874760	-0.900297
H	2.202196	0.509241	0.175107
O	1.846854	0.166160	-2.475621
H	1.710695	-0.635363	-1.938235
H	1.584037	2.164657	-2.309428
O	-3.970002	2.213647	-2.043356
H	-3.999659	3.178256	-1.938419
H	-3.380481	2.086389	-0.043056
H	-5.112356	1.800669	-0.330322
C	-0.216100	-3.432656	0.476580
H	-0.218689	-4.409755	-0.016435
H	-0.570842	-3.568542	1.505197
C	1.172167	-2.843155	0.452785
C	1.919648	-2.883875	-0.736184
C	1.731201	-2.223365	1.572629
C	3.188016	-2.320412	-0.805183
H	1.497094	-3.366941	-1.613909
C	3.008124	-1.661124	1.509092
H	1.168405	-2.182574	2.501698
C	3.756630	-1.691180	0.321229
H	3.740493	-2.371260	-1.738239
H	3.425649	-1.174901	2.387217
C	5.071522	-1.029979	0.289382
H	5.410212	-0.644191	1.250517
C	5.851842	-0.834630	-0.785381
H	5.582789	-1.175284	-1.782076
H	6.801884	-0.316612	-0.690894

Sum of electronic and thermal Free Energies= -1645.319787

SCF Energies= -1645.771574

S10.out

O	2.591188	-0.374530	-1.049595
C	3.777475	-0.647799	-0.279294
C	4.158748	0.575227	0.587501
C	3.388711	1.803602	0.098879
C	1.868005	1.601297	0.187143
C	1.542390	0.149474	-0.238510
C	3.598476	-1.923697	0.553604
H	4.555682	-0.797112	-1.031103
O	5.567519	0.771308	0.474771
H	5.765934	1.590636	0.961119
H	3.891610	0.398206	1.640957
O	3.807719	2.915323	0.888987
H	3.423943	3.710541	0.481787
H	3.643340	1.968964	-0.956337
O	1.253364	2.589055	-0.637787
H	1.562320	1.730807	1.229997
O	0.349364	0.100357	-0.966962
H	1.452487	-0.466006	0.663291
C	0.067417	-1.141497	-1.612445
O	0.227515	-2.261078	-0.762771
C	-0.637319	-2.303566	0.398176
C	-2.105247	-2.256464	-0.040458
C	-2.334004	-1.044571	-0.934800
C	-1.373052	-1.030506	-2.121432
H	0.770822	-1.300493	-2.430563
C	-0.293822	-3.578409	1.156965
H	-0.438120	-1.435006	1.037159
O	0.991000	-3.541704	1.771592
H	1.669827	-3.585218	1.067979
H	-0.386534	-4.433632	0.471920
H	-1.024661	-3.704892	1.960424
O	-2.903379	-2.164529	1.141273
H	-3.766879	-1.805173	0.867714
H	-2.350539	-3.170725	-0.603031
O	-3.696610	-1.071996	-1.360967
H	-3.905552	-0.182154	-1.691681
H	-2.147096	-0.150362	-0.332932
O	-1.557206	0.127369	-2.930702
H	-1.362971	0.899569	-2.368539
H	-1.571984	-1.892965	-2.763957
O	3.025961	-2.989185	-0.212261
H	2.205395	-2.635628	-0.614666
H	2.980648	-1.725209	1.438806
H	4.579356	-2.258282	0.903051
C	0.308667	3.450998	0.030038
H	0.199334	4.307599	-0.640732
H	0.745643	3.805714	0.971827
C	-1.040153	2.815044	0.280572
C	-1.315473	2.148033	1.484320
C	-2.050822	2.879494	-0.687430
C	-2.556118	1.560157	1.714069
H	-0.551807	2.101368	2.256480
C	-3.300170	2.304359	-0.455290
H	-1.862086	3.396928	-1.625256
C	-3.576245	1.625164	0.745389
H	-2.734329	1.054758	2.658193
H	-4.072391	2.368729	-1.218313
C	-4.889552	0.982262	0.917148
H	-5.616074	1.219820	0.140521

```
 C  -5.250850 0.137275 1.894080
 H  -4.577101 -0.165609 2.691254
 H  -6.252074 -0.283538 1.920682
Sum of electronic and thermal Free
Energies= -1645.328155
SCF Energies= -1645.784182
S11.out
 O  2.469595 -0.334960 1.322108
 C  3.911920 -0.287803 1.332037
 C  4.494949 -0.593172 -0.062240
 C  3.567352 -1.565972 -0.786375
 C  2.183623 -0.943550 -1.032849
 C  1.893594 0.082543 0.081862
 C  4.417747 1.010106 1.940833
 H  4.223387 -1.105565 1.990721
 O  5.784412 -1.166039 0.145788
 H  6.091001 -1.461609 -0.729103
 H  4.588083 0.326272 -0.656956
 O  4.204432 -1.951948 -2.002775
 H  3.700036 -2.699975 -2.364682
 H  3.425792 -2.440764 -0.136819
 O  1.264529 -2.030439 -1.096400
 H  2.202790 -0.407628 -1.989623
 O  0.518547 0.215634 0.300807
 H  2.320355 1.046951 -0.212673
 C  0.158663 1.456209 0.908173
 O  0.055879 2.479863 -0.059213
 C  -0.950868 2.254869 -1.070619
 C  -2.324478 2.115196 -0.410647
 C  -2.298269 1.014755 0.642822
 C  -1.168982 1.238053 1.647351
 H  0.944442 1.772916 1.597962
 C  -0.853474 3.437967 -2.022436
 H  -0.724275 1.334542 -1.624033
 O  -1.162698 4.679891 -1.388414
 H  -0.567528 4.752567 -0.622482
 H  -1.572728 3.306422 -2.834831
 H  0.157123 3.458379 -2.454274
 O  -3.270314 1.801059 -1.434630
 H  -4.057918 1.463685 -0.971646
 H  -2.582638 3.067561 0.074506
 O  -3.584857 1.001893 1.270906
 H  -3.741742 0.103255 1.605512
 H  -2.124829 0.065344 0.134016
 O  -1.068068 0.169906 2.584233
 H  -0.801355 -0.618853 2.077936
 H  -1.377740 2.141032 2.228660
 O  4.019076 2.114409 1.124088
 H  4.337659 2.923086 1.556836
 H  5.512877 0.949676 2.022608
 H  4.003850 1.106179 2.953772
 C  0.096254 -1.839676 -1.898437
 H  0.147149 -2.550399 -2.735626
 H  0.085687 -0.833059 -2.331969
 C  -1.177718 -2.057153 -1.112877
 C  -1.170663 -2.563027 0.190183
 C  -2.406710 -1.716981 -1.696427
 C  -2.359469 -2.677390 0.911241
 H  -0.227707 -2.830296 0.654533
 C  -3.593511 -1.829614 -0.977927
 H  -2.429328 -1.329882 -2.712506
 C  -3.587971 -2.285157 0.353897
 H  -2.331992 -3.042481 1.935012
 H  -4.530568 -1.542764 -1.446109
 C  -4.797622 -2.297010 1.195125
 H  -4.761361 -2.964733 2.055858
 C  -5.879713 -1.525182 1.017863
 H  -5.953802 -0.807011 0.204588
 H  -6.726927 -1.585068 1.695486
Sum of electronic and thermal Free
Energies= -1645.322083
SCF Energies= -1645.77311
S12.out
 O  3.271032 0.769312 0.278203
 C  4.487258 0.030165 0.075926
 C  4.396231 -1.393118 0.669546
 C  2.947090 -1.733353 1.014113
 C  2.036800 -1.318959 -0.140367
 C  2.089904 0.228131 -0.313469
 C  4.913527 0.010002 -1.388593
 H  5.231855 0.592940 0.644773
 O  5.235216 -1.454237 1.825152
 H  5.168308 -2.361002 2.171128
 H  4.735028 -2.129029 -0.074844
 O  2.876354 -3.136994 1.247516
 H  1.930255 -3.349604 1.334060
 H  2.656872 -1.176413 1.915974
 O  0.734694 -1.793478 0.157935
 H  2.402457 -1.793944 -1.060232
 O  1.015283 0.805588 0.385838
 H  2.038877 0.514702 -1.370449
 C  0.702989 2.137056 -0.015199
 O  -0.061650 2.156747 -1.201100
 C  -1.338281 1.486918 -1.083214
 C  -2.187577 2.191976 -0.024398
 C  -1.438386 2.171120 1.314800
 C  -0.047102 2.787155 1.157730
 H  1.619348 2.688394 -0.238327
 C  -1.941077 1.459341 -2.473066
 H  -1.170508 0.457791 -0.760640
 O  -1.159682 0.650349 -3.358094
 H  -0.245724 0.977401 -3.293862
 H  -2.934380 1.007918 -2.422778
 H  -2.039818 2.484932 -2.858060
 O  -3.480916 1.600516 0.116489
 H  -3.355437 0.664460 0.362551
 H  -2.364413 3.231717 -0.320138
 O  -2.149363 2.906612 2.307880
 H  -3.064681 2.576162 2.271822
 H  -1.328814 1.119755 1.627385
 O  0.726521 2.717689 2.349822
 H  0.994796 1.786277 2.447338
 H  -0.165492 3.850261 0.926553
 O  4.977900 1.358605 -1.849138
 H  5.225191 1.329009 -2.787541
 H  4.208599 -0.578881 -1.993041
 H  5.893318 -0.486257 -1.447744
 C  -0.090099 -2.013362 -0.988218
 H  0.163854 -2.984016 -1.439839
 H  0.094848 -1.243404 -1.748889
 C  -1.547723 -1.965260 -0.596909
 C  -1.962777 -1.801432 0.730264
 C  -2.521789 -2.018860 -1.602121
 C  -3.316248 -1.684474 1.045269
 H  -1.222966 -1.743323 1.520418
 C  -3.872349 -1.900047 -1.288848
```

```
 H  -2.216402 -2.124889 -2.639937
 C  -4.302442 -1.726666 0.041088
 H  -3.601699 -1.550077 2.084256
 H  -4.611615 -1.930860 -2.085537
 C  -5.742365 -1.580620 0.312565
 H  -6.375599 -1.626128 -0.573357
 C  -6.327793 -1.399994 1.504318
 H  -5.768987 -1.342052 2.435146
 H  -7.406922 -1.301838 1.582495
Sum of electronic and thermal Free
Energies= -1645.319371
SCF Energies= -1645.770576
S13.out
 O  -3.012181 -0.694234 1.346100
 C  -3.761815 -1.191162 0.215214
 C  -3.249628 -2.583850 -0.151266
 C  -1.747155 -2.533349 -0.444068
 C  -1.004682 -1.878763 0.724885
 C  -1.631804 -0.522914 1.082342
 C  -5.218854 -1.163896 0.645149
 H  -3.630545 -0.512253 -0.635748
 O  -3.979484 -3.031852 -1.292230
 H  -3.616814 -3.902071 -1.530727
 H  -3.411602 -3.259274 0.702169
 O  -1.317726 -3.882381 -0.639772
 H  -0.347546 -3.881688 -0.696989
 H  -1.605395 -1.947469 -1.362260
 O  0.412813 -1.823693 0.572031
 H  -1.155012 -2.513056 1.604664
 O  -1.421148 0.382895 0.013654
 H  -1.196783 -0.123968 2.002584
 C  -1.829837 1.718766 0.282312
 O  -1.011136 2.333624 1.253128
 C  0.384522 2.405284 0.888080
 C  0.525591 3.254662 -0.379600
 C  -0.313165 2.644698 -1.500390
 C  -1.766842 2.461789 -1.055413
 H  -2.843026 1.726783 0.692603
 C  1.121909 2.983144 2.077950
 H  0.763297 1.394490 0.697217
 O  1.027639 2.041062 3.149416
 H  1.483166 2.430408 3.913223
 H  0.670593 3.947572 2.352210
 H  2.166890 3.160017 1.793198
 O  1.906397 3.305064 -0.740666
 H  1.944655 3.679121 -1.638115
 H  0.148241 4.267654 -0.172137
 O  -0.224381 3.519323 -2.626072
 H  -0.732220 3.100681 -3.342213
 H  0.109695 1.662397 -1.754920
 O  -2.543202 1.807751 -2.056818
 H  -2.231693 0.885192 -2.091142
 H  -2.214831 3.449324 -0.913002
 O  -5.648200 0.170198 0.920389
 H  -5.049545 0.511632 1.606572
 H  -5.353282 -1.814869 1.521622
 H  -5.845302 -1.541583 -0.166145
 C  0.954684 -1.351251 -0.684766
 H  0.519968 -0.388700 -0.956152
 H  0.726460 -2.069270 -1.483906
 C  2.444586 -1.235631 -0.505615
 C  3.208641 -2.378359 -0.218766
 C  3.094369 -0.002687 -0.606921
 C  4.582966 -2.291039 -0.034161
 H  2.713263 -3.342987 -0.138878
 C  4.475564 0.085675 -0.426771
 H  2.525494 0.896349 -0.825480
 C  5.247713 -1.050978 -0.133947
 H  5.145621 -3.193730 0.184692
 H  4.964028 1.053746 -0.509792
 C  6.700411 -0.896757 0.051952
 H  7.066185 0.122412 -0.073615
 C  7.586597 -1.856698 0.351615
 H  7.306919 -2.897423 0.495772
 H  8.641364 -1.621597 0.464541
Sum of electronic and thermal Free
Energies= -1645.328191
SCF Energies= -1645.776811
S14.out
 O  -2.657111 0.062454 1.517002
 C  -3.715482 0.429822 0.603455
 C  -4.274763 -0.827655 -0.064362
 C  -3.140738 -1.587473 -0.747274
 C  -2.009232 -1.874515 0.240055
 C  -1.546028 -0.573586 0.917948
 C  -4.747192 1.184902 1.414931
 H  -3.321288 1.095434 -0.173817
 O  -5.258845 -0.420714 -1.013837
 H  -5.505420 -1.217499 -1.514241
 H  -4.720190 -1.479082 0.702725
 O  -3.692134 -2.799316 -1.261673
 H  -2.961920 -3.272835 -1.696048
 H  -2.750278 -0.967585 -1.567029
 O  -0.994676 -2.541808 -0.495529
 H  -2.397179 -2.526382 1.034357
 O  -0.921953 0.236499 -0.069705
 H  -0.847295 -0.766807 1.737565
 C  -0.595003 1.561539 0.334084
 O  0.553354 1.613893 1.152487
 C  1.793278 1.206380 0.529019
 C  2.048174 2.046169 -0.726683
 C  0.864671 1.925903 -1.678622
 C  -0.415969 2.357897 -0.963666
 H  -1.397976 1.981782 0.941761
 C  2.860452 1.388045 1.599556
 H  1.732987 0.150274 0.252164
 O  2.972122 2.747482 2.027035
 H  2.078568 3.020968 2.297171
 H  3.834331 1.098235 1.199781
 H  2.624256 0.727447 2.445455
 O  3.251476 1.572579 -1.332236
 H  3.325905 2.027856 -2.188415
 H  2.156786 3.099792 -0.432738
 O  1.130502 2.758630 -2.808062
 H  0.352900 2.691578 -3.388446
 H  0.769698 0.875647 -1.992872
 O  -1.558199 2.240690 -1.810068
 H  -1.728810 1.286296 -1.911603
 H  -0.332702 3.417205 -0.704317
 O  -4.163675 2.425665 1.820036
 H  -4.819899 2.888463 2.365630
 H  -5.041143 0.578670 2.283782
 H  -5.635371 1.347208 0.791196
 C  -0.025421 -3.265462 0.284931
 H  -0.008938 -4.287965 -0.112850
 H  -0.339139 -3.323334 1.332786
```

```
 C  1.347925 -2.648980 0.173165
 C  1.857298 -2.284597 -1.080259
 C  2.155779 -2.471519 1.303080
 C  3.140531 -1.758170 -1.196671
 H  1.240061 -2.408843 -1.965575
 C  3.443272 -1.951483 1.187191
 H  1.773968 -2.746686 2.283223
 C  3.959384 -1.576456 -0.066106
 H  3.514459 -1.465270 -2.174207
 H  4.046093 -1.828531 2.081827
 C  5.289766 -0.971039 -0.241692
 H  5.589538 -0.827250 -1.279514
 C  6.126143 -0.568312 0.725512
 H  5.893523 -0.661901 1.783420
 H  7.086503 -0.123783 0.479664
Sum of electronic and thermal Free
Energies= -1645.330685
SCF Energies= -1645.784222
S15.out
 O  2.770132 0.353966 -1.484314
 C  3.724483 0.564340 -0.417260
 C  4.270811 -0.782656 0.052502
 C  3.111067 -1.701898 0.465485
 C  2.117093 -1.817172 -0.696400
 C  1.640266 -0.417687 -1.126631
 C  4.776251 1.496037 -0.994756
 H  3.232762 1.067314 0.423204
 O  5.144020 -0.533047 1.155978
 H  5.675901 -1.334758 1.291003
 H  4.817906 -1.261620 -0.771529
 O  3.568230 -3.018527 0.770930
 H  4.038575 -2.970756 1.619420
 H  2.629858 -1.252986 1.344098
 O  1.086969 -2.774152 -0.497277
 H  2.664130 -2.207181 -1.561210
 O  0.899277 0.179896 -0.067533
 H  1.022467 -0.474084 -2.027255
 C  0.556344 1.550493 -0.260025
 O  -0.546839 1.717669 -1.123252
 C  -1.817012 1.241483 -0.619900
 C  -2.148423 1.982155 0.677613
 C  -1.051343 1.694942 1.696061
 C  0.301499 2.138449 1.136947
 H  1.381039 2.074132 -0.745390
 C  -2.822394 1.474735 -1.735674
 H  -1.753009 0.169186 -0.419796
 O  -2.968861 2.858442 -2.060703
 H  -2.078006 3.183082 -2.276768
 H  -3.804036 1.113411 -1.420504
 H  -2.508936 0.893764 -2.614803
 O  -3.423596 1.537955 1.139214
 H  -3.524749 1.881461 2.043489
 H  -2.172354 3.061975 0.472498
 O  -1.365676 2.405631 2.894445
 H  -0.652167 2.210335 3.525768
 H  -1.026864 0.612845 1.893097
 O  1.364082 1.826477 2.036009
 H  1.491971 0.861103 1.984108
 H  0.289910 3.228031 1.040435
 O  4.204749 2.754032 -1.360144
 H  3.505873 2.557924 -2.007362
 H  5.261710 1.014881 -1.856557
 H  5.536330 1.697869 -0.236794
 C  0.245225 -2.665160 0.653557
 H  0.602758 -1.898947 1.346184
 H  0.301938 -3.626177 1.181906
 C  -1.189927 -2.369305 0.278478
 C  -1.648382 -2.441240 -1.039530
 C  -2.100588 -2.025895 1.289057
 C  -2.978359 -2.144645 -1.342892
 H  -0.960342 -2.713910 -1.832222
 C  -3.424265 -1.728424 0.987486
 H  -1.761186 -1.978945 2.321468
 C  -3.885969 -1.758745 -0.342901
 H  -3.313880 -2.188405 -2.376357
 H  -4.103412 -1.458945 1.790291
 C  -5.253738 -1.368533 -0.723056
 H  -5.559646 -1.678270 -1.722527
 C  -6.111387 -0.649696 0.015479
 H  -5.861371 -0.274167 1.004573
 H  -7.100578 -0.404353 -0.361154
Sum of electronic and thermal Free
Energies= -1645.330224
SCF Energies= -1645.783447
S16.out
 O  3.310748 -0.164560 -1.304701
 C  4.159179 -0.253405 -0.137670
 C  3.898569 -1.584277 0.577096
 C  2.415344 -1.739641 0.930519
 C  1.551530 -1.549921 -0.314277
 C  1.928269 -0.245465 -1.030678
 C  5.586579 -0.112777 -0.644360
 H  3.940725 0.581246 0.543261
 O  4.712335 -1.731200 1.743278
 H  4.490187 -1.002538 2.350109
 H  4.187694 -2.401842 -0.089576
 O  2.160130 -3.034189 1.473505
 H  2.805748 -3.153843 2.192330
 H  2.146646 -0.960901 1.661152
 O  0.168710 -1.437884 -0.004768
 H  1.731964 -2.382413 -1.006508
 O  1.505803 0.820177 -0.198251
 H  1.425437 -0.187906 -1.998576
 C  1.225657 2.039472 -0.867585
 O  0.059496 1.953979 -1.659756
 C  -1.150145 1.607619 -0.945045
 C  -1.416328 2.649637 0.148489
 C  -0.189912 2.798974 1.049276
 C  1.069154 3.093338 0.230171
 H  2.035883 2.291263 -1.558059
 C  -2.219547 1.530232 -2.038559
 H  -1.034508 0.622173 -0.481122
 O  -3.469273 1.023567 -1.583183
 H  -3.331015 0.103470 -1.300886
 H  -1.814323 0.916126 -2.855438
 H  -2.413153 2.532452 -2.434895
 O  -2.543130 2.226036 0.918503
 H  -2.587559 2.823274 1.685180
 H  -1.617451 3.621950 -0.327848
 O  -0.464177 3.855787 1.970668
 H  0.317050 3.930555 2.545369
 H  -0.046353 1.852733 1.591058
 O  2.228381 3.167304 1.057781
 H  2.392092 2.264827 1.386709
 H  0.964635 4.072257 -0.246013
 O  5.952195 -1.155766 -1.548869
```

```
 H  5.299968 -1.134674 -2.270087
 H  6.273127 -0.171532 0.203884
 H  5.700141 0.873827 -1.115229
 C  -0.607609 -2.644651 -0.029660
 H  -0.294095 -3.304951 0.788131
 H  -0.452757 -3.178110 -0.976996
 C  -2.048696 -2.231116 0.125566
 C  -2.435862 -1.444535 1.218823
 C  -3.014799 -2.571979 -0.829598
 C  -3.752178 -1.012057 1.351298
 H  -1.695210 -1.154244 1.958566
 C  -4.336750 -2.150398 -0.692961
 H  -2.728460 -3.167462 -1.692787
 C  -4.732839 -1.359319 0.402941
 H  -4.029880 -0.390280 2.198532
 H  -5.060036 -2.427229 -1.453783
 C  -6.108775 -0.868732 0.588213
 H  -6.249733 -0.239419 1.466717
 C  -7.166801 -1.115256 -0.196392
 H  -7.109890 -1.734248 -1.088433
 H  -8.140855 -0.695023 0.037961
Sum of electronic and thermal Free
Energies= -1645.330838
SCF Energies= -1645.781727
S17.out
 O  3.196827 -0.811012 -1.184764
 C  3.864383 -0.744210 0.093350
 C  3.615692 -2.043912 0.853995
 C  2.110065 -2.197690 1.058311
 C  1.364196 -2.117795 -0.273058
 C  1.786507 -0.881652 -1.094155
 C  5.317348 -0.436018 -0.214031
 H  3.455267 0.087420 0.681613
 O  4.296053 -1.965061 2.104490
 H  3.997589 -2.727680 2.629738
 H  3.987297 -2.891984 0.259460
 O  1.886843 -3.453681 1.698121
 H  0.935190 -3.504602 1.891340
 H  1.766648 -1.376034 1.703100
 O  -0.021297 -2.089539 0.037769
 H  1.613269 -3.009076 -0.864721
 O  1.260588 0.279141 -0.486378
 H  1.436440 -0.961606 -2.126406
 C  0.781251 1.305615 -1.343729
 O  -0.629114 1.365339 -1.312093
 C  -1.206011 1.663789 -0.019620
 C  -0.633304 2.975274 0.557354
 C  0.895332 2.979657 0.513839
 C  1.381092 2.638371 -0.894678
 H  1.050066 1.091250 -2.381607
 C  -2.708191 1.711492 -0.294657
 H  -0.989475 0.838620 0.672039
 O  -3.435834 1.763866 0.933627
 H  -4.341502 1.472695 0.735878
 H  -2.968810 0.813416 -0.864167
 H  -2.929081 2.587595 -0.922999
 O  -1.111180 3.216474 1.880126
 H  -0.832656 2.463470 2.430812
 H  -0.994442 3.815723 -0.046356
 O  1.359723 4.269767 0.907628
 H  2.309843 4.281461 0.695527
 H  1.269750 2.212680 1.210569
 O  2.802571 2.656259 -0.986484
 H  3.151669 1.938858 -0.428734
 H  1.028864 3.410591 -1.585078
 O  5.440810 0.858093 -0.809281
 H  4.859093 0.859450 -1.589288
 H  5.732094 -1.217422 -0.867184
 H  5.892864 -0.416865 0.714101
 C  -0.883902 -2.489909 -1.031462
 H  -0.827983 -3.582951 -1.151550
 H  -0.563629 -2.042905 -1.980210
 C  -2.292794 -2.046461 -0.723307
 C  -2.715653 -1.816454 0.592955
 C  -3.207355 -1.853334 -1.764949
 C  -4.003813 -1.363330 0.857161
 H  -2.024738 -1.973821 1.414197
 C  -4.501601 -1.409720 -1.499714
 H  -2.898741 -2.030363 -2.792452
 C  -4.916649 -1.125942 -0.186294
 H  -4.298117 -1.181716 1.886303
 H  -5.191736 -1.243780 -2.323426
 C  -6.251890 -0.546635 0.038009
 H  -6.923561 -0.593339 -0.819220
 C  -6.682022 0.055070 1.157216
 H  -6.059262 0.161514 2.042594
 H  -7.686218 0.465018 1.218803
Sum of electronic and thermal Free
Energies= -1645.326103
SCF Energies= -1645.779522
S18.out
 O  2.737252 -1.553723 -1.420039
 C  3.561708 -1.516815 -0.232349
 C  2.938053 -2.359133 0.889402
 C  1.490793 -1.935857 1.124151
 C  0.719469 -2.000999 -0.190337
 C  1.415291 -1.109251 -1.235422
 C  4.929604 -2.027694 -0.637820
 H  3.653706 -0.480879 0.114722
 O  3.724263 -2.161471 2.063613
 H  3.255267 -2.612181 2.786992
 H  2.945317 -3.419133 0.592704
 O  0.935523 -2.806936 2.109261
 H  0.053222 -2.454743 2.318243
 H  1.484694 -0.904037 1.494269
 O  -0.617722 -1.611158 0.072229
 H  0.746110 -3.031307 -0.572191
 O  1.480015 0.262116 -0.840352
 H  0.928195 -1.183018 -2.212268
 C  0.335406 1.081148 -1.017525
 O  -0.368435 1.287325 0.189410
 C  0.406358 1.897781 1.236124
 C  0.825150 3.302837 0.793492
 C  1.619061 3.190733 -0.506662
 C  0.830206 2.423591 -1.572653
 H  -0.372359 0.609026 -1.703806
 C  -0.445592 1.874988 2.494844
 H  1.313101 1.305861 1.417741
 O  -0.733517 0.543666 2.933393
 H  0.113802 0.090820 3.084348
 H  -1.412480 2.347140 2.295531
 H  0.066234 2.446340 3.279171
 O  1.619146 3.883530 1.827982
 H  1.994196 4.701417 1.458283
 H  -0.076902 3.906420 0.610098
 O  1.925929 4.514159 -0.946824
```

```
 H  2.430698 4.417837 -1.772955
 H  2.547024 2.640394 -0.290553
 O  1.603621 2.240072 -2.755584
 H  2.273086 1.565884 -2.534991
 H  -0.043102 3.016860 -1.859162
 O  5.508464 -1.087668 -1.545339
 H  6.384421 -1.429144 -1.787666
 H  4.818789 -3.017311 -1.104539
 H  5.542216 -2.140488 0.265712
 C  -1.571029 -2.069256 -0.883059
 H  -1.629572 -3.168520 -0.847285
 H  -1.259655 -1.799534 -1.901512
 C  -2.922816 -1.461847 -0.594751
 C  -3.163008 -0.647620 0.514973
 C  -3.982457 -1.725621 -1.477829
 C  -4.433807 -0.111342 0.731632
 H  -2.361607 -0.424538 1.208907
 C  -5.246525 -1.192450 -1.259724
 H  -3.808852 -2.354703 -2.348269
 C  -5.501239 -0.369590 -0.143511
 H  -4.601080 0.522247 1.599724
 H  -6.042310 -1.415164 -1.964540
 C  -6.818747 0.223110 0.139655
 H  -6.852641 0.840741 1.037495
 C  -7.943629 0.081609 -0.575615
 H  -7.996367 -0.516524 -1.482310
 H  -8.862948 0.571006 -0.266006
Sum of electronic and thermal Free
Energies= -1645.323113
SCF Energies= -1645.772156
S19.out
 O  2.465537 -1.522843 -1.050564
 C  3.061645 -1.656275 0.257159
 C  2.444407 -2.864024 0.959765
 C  0.939234 -2.641693 1.068793
 C  0.312274 -2.352448 -0.295872
 C  1.069869 -1.237503 -1.049147
 C  4.562995 -1.757953 0.045573
 H  2.847574 -0.758139 0.849508
 O  3.037838 -2.977208 2.251541
 H  2.531357 -3.655867 2.730318
 H  2.632731 -3.767894 0.361405
 O  0.369314 -3.812538 1.652842
 H  -0.577299 -3.627113 1.776899
 H  0.769666 -1.771670 1.719233
 O  -1.038152 -2.011237 -0.022916
 H  0.371051 -3.260828 -0.911415
 O  0.779560 -0.003425 -0.440033
 H  0.798042 -1.214944 -2.107536
 C  0.747709 1.160005 -1.275521
 O  -0.065313 2.113045 -0.635329
 C  0.423381 2.568542 0.647977
 C  1.819406 3.186614 0.504512
 C  2.754499 2.203745 -0.195130
 C  2.139493 1.764538 -1.525700
 H  0.257128 0.913009 -2.222705
 C  -0.612326 3.562884 1.150706
 H  0.474553 1.718418 1.337941
 O  -1.896479 2.957474 1.308111
 H  -2.178402 2.676787 0.421934
 H  -0.662918 4.415980 0.458828
 H  -0.309260 3.931541 2.133375
 O  2.279027 3.504577 1.818389
 H  3.177518 3.863105 1.719700
 H  1.750448 4.096425 -0.111029
 O  4.015383 2.844876 -0.394793
 H  4.524687 2.257131 -0.980737
 H  2.881858 1.326640 0.452944
 O  3.006801 0.923192 -2.270768
 H  3.143968 0.092884 -1.765717
 H  1.981734 2.652805 -2.146425
 O  5.095767 -0.578578 -0.562809
 H  4.939834 0.162938 0.046841
 H  4.784240 -2.583727 -0.637546
 H  5.044939 -1.963514 1.008707
 C  -1.907510 -1.945007 -1.162403
 H  -2.109233 -2.955592 -1.542783
 H  -1.430274 -1.375427 -1.970974
 C  -3.176946 -1.253947 -0.736394
 C  -3.110953 -0.051873 -0.020292
 C  -4.435345 -1.778175 -1.055030
 C  -4.275870 0.605019 0.366749
 H  -2.142801 0.366726 0.236390
 C  -5.601443 -1.116203 -0.677445
 H  -4.502973 -2.716187 -1.600591
 C  -5.545947 0.091761 0.042300
 H  -4.204404 1.532974 0.929214
 H  -6.562449 -1.551755 -0.934829
 C  -6.744428 0.832829 0.470542
 H  -6.537715 1.718457 1.071573
 C  -8.021816 0.536068 0.193562
 H  -8.312325 -0.323541 -0.405743
 H  -8.829524 1.160258 0.565638
Sum of electronic and thermal Free
Energies= -1645.330951
SCF Energies= -1645.784379
S2.out
 O  2.758442 1.711829 -0.514422
 C  3.060819 0.786516 0.556973
 C  3.515994 -0.517864 -0.083445
 C  2.355179 -1.088927 -0.914891
 C  1.807988 -0.051424 -1.908453
 C  1.609374 1.321926 -1.234791
 C  4.022287 1.501115 1.481976
 H  2.153819 0.585135 1.131248
 O  3.821926 -1.515657 0.896082
 H  4.725516 -1.352761 1.211991
 H  4.376713 -0.337480 -0.740280
 O  2.814908 -2.221211 -1.654369
 H  3.081552 -2.882441 -0.992953
 H  1.562120 -1.381285 -0.215605
 O  0.554736 -0.330662 -2.537368
 H  2.578660 0.079702 -2.681632
 O  0.490725 1.237041 -0.369857
 H  1.447300 2.094277 -1.992388
 C  0.061204 2.477151 0.162668
 O  -0.950843 3.057199 -0.643185
 C  -2.094729 2.203482 -0.820659
 C  -2.713089 1.865563 0.543601
 C  -1.677873 1.307077 1.515813
 C  -0.468918 2.238222 1.583836
 H  0.883068 3.197980 0.172015
 C  -3.063899 2.954465 -1.733097
 H  -1.787046 1.280064 -1.320740
 O  -4.133425 2.117235 -2.168530
 H  -4.476542 1.678347 -1.366336
```

```
 H  -2.525096 3.283482 -2.627050
 H  -3.436012 3.849446 -1.211116
 O  -3.764302 0.916178 0.310996
 H  -4.195624 0.750399 1.166959
 H  -3.130257 2.786446 0.976540
 O  -2.324962 1.175339 2.783778
 H  -1.697199 0.726862 3.374835
 H  -1.344819 0.324790 1.158157
 O  0.489739 1.642945 2.450357
 H  1.333009 2.139831 2.401272
 H  -0.790775 3.214595 1.972614
 O  3.357094 2.607247 2.117421
 H  3.102829 3.219351 1.404711
 H  4.911586 1.844233 0.936620
 H  4.336723 0.823772 2.279456
 C  0.146593 -1.686132 -2.799439
 H  0.979745 -2.284010 -3.175089
 H  -0.591106 -1.584244 -3.602866
 C  -0.497485 -2.337212 -1.592791
 C  -0.029599 -3.548725 -1.066402
 C  -1.573378 -1.707380 -0.955163
 C  -0.608221 -4.107244 0.070811
 H  0.810157 -4.048050 -1.540586
 C  -2.147507 -2.256970 0.187715
 H  -1.968273 -0.778603 -1.353678
 C  -1.673183 -3.465573 0.730945
 H  -0.219619 -5.047153 0.451798
 H  -2.969280 -1.735594 0.672269
 C  -2.305637 -3.993593 1.951516
 H  -3.153639 -3.409837 2.310426
 C  -1.945027 -5.082175 2.645304
 H  -1.106565 -5.713819 2.361319
 H  -2.488601 -5.377070 3.538706
Sum of electronic and thermal Free
Energies= -1645.326224
SCF Energies= -1645.779371
S20.out
 O  -1.985583 -0.675940 1.370973
 C  -3.117591 -0.180917 0.624408
 C  -3.730421 -1.334688 -0.168298
 C  -2.663711 -1.927409 -1.085359
 C  -1.420178 -2.332895 -0.293255
 C  -0.907170 -1.166715 0.572906
 C  -4.063181 0.449651 1.634190
 H  -2.783020 0.588876 -0.081132
 O  -4.824772 -0.819724 -0.924070
 H  -5.114855 -1.537245 -1.513240
 H  -4.070654 -2.114484 0.529591
 O  -3.241374 -3.056905 -1.738823
 H  -2.547972 -3.427783 -2.311743
 H  -2.378976 -1.163416 -1.822775
 O  -0.476954 -2.798763 -1.249653
 H  -1.693995 -3.144161 0.395062
 O  -0.368206 -0.167878 -0.256863
 H  -0.165809 -1.510533 1.297848
 C  0.721727 0.606040 0.267577
 O  1.390224 1.169305 -0.831727
 C  0.643023 2.140247 -1.599080
 C  0.156602 3.284748 -0.701989
 C  -0.604867 2.721845 0.492134
 C  0.281309 1.719113 1.232269
 H  1.434506 -0.063213 0.756823
 C  1.597645 2.596992 -2.694038
 H  -0.226243 1.657965 -2.063315
 O  2.772893 3.214347 -2.168264
 H  3.168176 2.570553 -1.555234
 H  1.098777 3.339176 -3.321990
 H  1.856106 1.730171 -3.318486
 O  -0.672515 4.122297 -1.509024
 H  -0.990463 4.837880 -0.932711
 H  1.027789 3.842931 -0.332524
 O  -0.985695 3.803847 1.343565
 H  -1.296129 3.395156 2.171377
 H  -1.501125 2.210161 0.119109
 O  -0.320110 1.243429 2.427485
 H  -1.137417 0.754463 2.186028
 H  1.198523 2.230099 1.544670
 O  -3.462252 1.553980 2.315473
 H  -3.292475 2.250171 1.658378
 H  -4.319077 -0.284697 2.404091
 H  -4.983919 0.750623 1.120405
 C  0.585860 -3.626742 -0.740207
 H  0.860384 -4.274279 -1.579361
 H  0.210608 -4.262012 0.071805
 C  1.785496 -2.826457 -0.285996
 C  2.448935 -1.987552 -1.189300
 C  2.245902 -2.884706 1.036070
 C  3.539375 -1.225616 -0.779364
 H  2.096849 -1.919187 -2.215201
 C  3.337278 -2.123883 1.449336
 H  1.738026 -3.528342 1.750385
 C  4.004016 -1.271843 0.548582
 H  4.034733 -0.570267 -1.491540
 H  3.666839 -2.190268 2.481881
 C  5.147206 -0.425172 0.929201
 H  5.572031 0.154295 0.109483
 C  5.691508 -0.297134 2.147147
 H  5.324279 -0.833982 3.018447
 H  6.536681 0.365947 2.309704
Sum of electronic and thermal Free
Energies= -1645.333857
SCF Energies= -1645.786289
S21.out
 O  1.960739 0.718328 1.444637
 C  3.093679 0.357840 0.614203
 C  3.584334 1.618452 -0.096633
 C  2.441642 2.172772 -0.945057
 C  1.191680 2.414853 -0.097935
 C  0.808640 1.167038 0.720775
 C  4.125087 -0.298921 1.520163
 H  2.777824 -0.369490 -0.141072
 O  4.696128 1.260920 -0.914027
 H  4.910528 2.045758 -1.446977
 H  3.873869 2.372034 0.650801
 O  2.895953 3.388500 -1.537395
 H  2.160030 3.722644 -2.078856
 H  2.203100 1.434612 -1.724147
 O  0.182562 2.844842 -1.001125
 H  1.414461 3.208937 0.627903
 O  0.314836 0.166715 -0.130645
 H  0.076611 1.415838 1.493121
 C  -0.657351 -0.746025 0.406335
 O  -1.336967 -1.305023 -0.685978
 C  -0.512061 -2.081350 -1.583332
 C  0.084480 -3.264074 -0.821727
 C  0.855696 -2.765234 0.407152
```

```
 C  -0.049833 -1.875495 1.265971
 H  -1.395288 -0.182956 0.985116
 C  -1.436638 -2.475366 -2.723353
 H  0.295825 -1.452833 -1.974794
 O  -1.931412 -1.324242 -3.409093
 H  -2.315668 -0.746665 -2.727026
 H  -0.885223 -3.074007 -3.452535
 H  -2.261093 -3.084499 -2.323463
 O  0.943999 -3.980400 -1.705041
 H  1.439136 -4.603454 -1.143892
 H  -0.737824 -3.910898 -0.473577
 O  1.398292 -3.864141 1.141582
 H  0.650299 -4.367512 1.509728
 H  1.724430 -2.195669 0.069576
 O  0.576862 -1.402557 2.451128
 H  1.191533 -0.678659 2.198131
 H  -0.902287 -2.478998 1.600500
 O  3.795684 -1.649769 1.848827
 H  2.964945 -1.657806 2.353423
 H  4.258784 0.316174 2.421090
 H  5.078522 -0.341387 0.988796
 C  -0.947309 3.519379 -0.416129
 H  -1.283163 4.221313 -1.186580
 H  -0.628222 4.101247 0.457515
 C  -2.066661 2.570817 -0.053573
 C  -2.546913 2.474246 1.258923
 C  -2.640422 1.756766 -1.037883
 C  -3.572561 1.589215 1.584171
 H  -2.107040 3.095357 2.035440
 C  -3.665990 0.872763 -0.715646
 H  -2.268625 1.802213 -2.058393
 C  -4.151890 0.765235 0.601070
 H  -3.918502 1.536453 2.612107
 H  -4.093682 0.242414 -1.492265
 C  -5.226817 -0.200666 0.883771
 H  -5.573588 -0.757598 0.013268
 C  -5.798323 -0.454733 2.069066
 H  -5.510206 0.053241 2.986195
 H  -6.587692 -1.196268 2.155900
Sum of electronic and thermal Free
Energies= -1645.332179
SCF Energies= -1645.785776
S22.out
 O  2.009635 0.698814 1.440795
 C  3.143128 0.307425 0.632714
 C  3.630553 1.527200 -0.151762
 C  2.487452 2.078796 -1.011355
 C  1.263899 2.375674 -0.150319
 C  0.875362 1.146487 0.700698
 C  4.179529 -0.262724 1.575646
 H  2.836646 -0.474593 -0.073263
 O  4.770353 1.240971 -0.963485
 H  4.519958 0.534245 -1.585678
 H  3.953028 2.305256 0.548039
 O  2.884894 3.284157 -1.659127
 H  3.752753 3.093171 -2.057205
 H  2.216054 1.314475 -1.756897
 O  0.229563 2.806763 -1.022170
 H  1.523153 3.177290 0.555444
 O  0.370680 0.137585 -0.138527
 H  0.139423 1.421754 1.459913
 C  -0.657790 -0.716512 0.383378
 O  -1.357209 -1.238317 -0.716333
 C  -0.571834 -2.064288 -1.602454
 C  -0.043359 -3.272666 -0.831017
 C  0.741336 -2.815320 0.405918
 C  -0.121010 -1.871363 1.252279
 H  -1.372049 -0.115535 0.953261
 C  -1.513603 -2.419260 -2.742040
 H  0.270032 -1.482982 -1.995906
 O  -1.956650 -1.248955 -3.430769
 H  -2.319729 -0.656257 -2.749850
 H  -2.365020 -2.988523 -2.339841
 H  -0.990921 -3.044569 -3.469988
 O  0.784445 -4.036370 -1.705424
 H  1.246074 -4.679165 -1.137975
 H  -0.901241 -3.874280 -0.487443
 O  1.207181 -3.945391 1.146648
 H  0.423849 -4.402277 1.502372
 H  1.646353 -2.297775 0.075456
 O  0.514366 -1.422110 2.436974
 H  1.287373 -0.876152 2.182035
 H  -1.007662 -2.426488 1.582507
 O  3.668753 -1.493222 2.096035
 H  4.267138 -1.781884 2.804176
 H  4.375348 0.460050 2.379547
 H  5.111107 -0.421455 1.017649
 C  -0.862765 3.511590 -0.404899
 H  -1.189200 4.239640 -1.155560
 H  -0.508507 4.066426 0.472765
 C  -2.010316 2.599236 -0.037228
 C  -2.614185 1.805388 -1.019763
 C  -2.487275 2.516021 1.277440
 C  -3.664560 0.952343 -0.693911
 H  -2.245943 1.840945 -2.041963
 C  -3.537964 1.662378 1.606278
 H  -2.024424 3.121758 2.052778
 C  -4.146891 0.857622 0.625047
 H  -4.113207 0.335504 -1.469523
 H  -3.879997 1.618012 2.635918
 C  -5.249144 -0.075467 0.912847
 H  -5.616371 -0.621892 0.044066
 C  -5.822741 -0.311731 2.100822
 H  -5.515411 0.188046 3.016251
 H  -6.633622 -1.029124 2.192056
Sum of electronic and thermal Free
Energies= -1645.329115
SCF Energies= -1645.782608
S23.out
 O  -1.180106 1.842854 -1.145552
 C  -2.571322 1.785568 -0.767615
 C  -2.780039 2.578702 0.520372
 C  -1.901108 1.966643 1.607735
 C  -0.442272 1.903378 1.155280
 C  -0.302010 1.223187 -0.220683
 C  -3.349710 2.294960 -1.966781
 H  -2.861800 0.742891 -0.584637
 O  -4.161903 2.502931 0.865715
 H  -4.252405 2.920228 1.739379
 H  -2.474172 3.623300 0.359582
 O  -2.028456 2.769001 2.780993
 H  -1.441499 2.370469 3.447292
 H  -2.257686 0.945189 1.804522
 O  0.282224 1.227001 2.180688
 H  -0.075432 2.931021 1.040830
 O  -0.589082 -0.152541 -0.095693
```

H 0.700027 1.370004 -0.628210
C 0.143937 -1.063309 -0.902297
O 0.935390 -1.903873 -0.085536
C 0.179524 -2.661532 0.876477
C -0.857522 -3.554363 0.165734
C -1.725758 -2.737821 -0.789079
C -0.822989 -1.922612 -1.722161
H 0.838743 -0.526186 -1.553692
C 1.201335 -3.475353 1.671289
H -0.338009 -1.977995 1.562272
O 0.605380 -4.126743 2.791035
H -0.199153 -4.562208 2.446605
H 1.970368 -2.799750 2.059666
H 1.690466 -4.195481 0.997239
O -1.640485 -4.287420 1.119495
H -2.139000 -3.641508 1.653122
H -0.327165 -4.315162 -0.417327
O -2.550839 -3.629004 -1.535812
H -2.944952 -3.091844 -2.245813
H -2.348626 -2.043488 -0.202798
O -1.572100 -1.174919 -2.672012
H -2.128748 -0.529920 -2.202048
H -0.216683 -2.617636 -2.311041
O -3.152439 1.440157 -3.096802
H -2.198665 1.451768 -3.288931
H -3.050914 3.328116 -2.193800
H -4.418316 2.282862 -1.741736
C 1.578924 1.786702 2.480048
H 1.903507 1.253335 3.377979
H 1.471790 2.851138 2.724336
C 2.554532 1.589935 1.347485
C 2.926700 2.648528 0.513633
C 3.014391 0.300001 1.042752
C 3.730141 2.421517 -0.604194
H 2.573505 3.653499 0.731020
C 3.810080 0.069056 -0.072319
H 2.723720 -0.532501 1.677363
C 4.183812 1.129578 -0.923271
H 4.006680 3.255044 -1.245287
H 4.133338 -0.944343 -0.290346
C 5.021023 0.944670 -2.120379
H 5.166032 1.846520 -2.715127
C 5.606711 -0.189176 -2.529901
H 5.518717 -1.128218 -1.988911
H 6.205388 -0.208270 -3.436391

Sum of electronic and thermal Free Energies= -1645.330646

SCF Energies= -1645.782774

S24.out

O -0.346789 2.107526 -1.129002
C -1.697701 2.581536 -0.936353
C -1.889358 3.036148 0.512772
C -1.486420 1.937781 1.501862
C -0.062159 1.476520 1.197083
C 0.032597 1.043825 -0.278969
C -1.887865 3.702305 -1.949456
H -2.412120 1.778414 -1.157899
O -3.260208 3.390785 0.679210
H -3.381054 3.543969 1.633070
H -1.240936 3.908190 0.688965
O -1.644049 2.390267 2.847453
H -1.036616 3.140383 2.977087
H -2.172861 1.091662 1.397962
O 0.298115 0.418633 2.081874
H 0.617305 2.328524 1.330107
O -0.823640 -0.063808 -0.500758
H 1.059555 0.793249 -0.550168
C -0.274098 -1.258333 -1.026170
O 0.019363 -2.182646 0.000701
C -1.122888 -2.542528 0.801169
C -2.151737 -3.253389 -0.083417
C -2.546119 -2.322687 -1.229369
C -1.309217 -1.842931 -1.994406
H 0.673876 -1.056387 -1.532782
C -0.615818 -3.382322 1.958970
H -1.581952 -1.632633 1.210066
O 0.304230 -2.656277 2.780226
H -0.017006 -1.739190 2.836856
H -0.082124 -4.261387 1.583088
H -1.478694 -3.725908 2.543968
O -3.283928 -3.584290 0.719909
H -3.970072 -3.901877 0.107822
H -1.695370 -4.161941 -0.504983
O -3.436680 -3.040258 -2.084625
H -3.696054 -2.423798 -2.790949
H -3.058708 -1.448914 -0.800866
O -1.653578 -0.908454 -3.013064
H -1.869385 -0.073775 -2.557658
H -0.854207 -2.700418 -2.498685
O -0.990056 4.791189 -1.733392
H -0.094087 4.412900 -1.745485
H -2.901599 4.100922 -1.860966
H -1.765744 3.286303 -2.959634
C 1.643141 0.509436 2.607029
H 1.696760 -0.283375 3.357691
H 1.769968 1.475777 3.111046
C 2.688490 0.316684 1.537666
C 3.411659 1.396958 1.024144
C 2.872211 -0.951007 0.962336
C 4.285113 1.219461 -0.049632
H 3.282060 2.385640 1.457366
C 3.736395 -1.129191 -0.110615
H 2.308760 -1.792637 1.351961
C 4.457670 -0.041430 -0.645894
H 4.836088 2.071435 -0.440532
H 3.854526 -2.121935 -0.534942
C 5.375814 -0.166537 -1.790231
H 5.902815 0.751723 -2.049791
C 5.609160 -1.262849 -2.524986
H 5.119782 -2.215538 -2.337774
H 6.311629 -1.235394 -3.353406

Sum of electronic and thermal Free Energies= -1645.331440

SCF Energies= -1645.782633

S3.out

O -1.561522 2.522839 -0.861306
C -0.814654 3.089268 0.235148
C 0.661160 3.155479 -0.156119
C 1.185106 1.767285 -0.544274
C 0.278608 1.138980 -1.612758
C -1.191512 1.192083 -1.163628
C -1.431005 4.446467 0.533399
H -0.923614 2.452430 1.122154
O 1.398865 3.669281 0.950841
H 2.337770 3.563387 0.716279
H 0.764662 3.816142 -1.030844

```
 O  2.516572 1.972247 -1.022463
 H  2.990843 1.125557 -0.955564
 H  1.197200 1.147408 0.360384
 O  0.661794 -0.154788 -2.082378
 H  0.337063 1.772675 -2.503592
 O  -1.355359 0.349949 -0.033511
 H  -1.854821 0.869642 -1.971458
 C  -2.693563 0.215261 0.421520
 O  -3.471318 -0.560798 -0.464974
 C  -2.969180 -1.899397 -0.672643
 C  -2.973780 -2.642672 0.663059
 C  -2.136599 -1.881089 1.698829
 C  -2.608041 -0.426375 1.814123
 H  -3.176053 1.194694 0.468517
 C  -3.870455 -2.517869 -1.728250
 H  -1.945598 -1.850590 -1.062602
 O  -3.783500 -1.805407 -2.963136
 H  -4.017676 -0.883124 -2.762448
 H  -4.905238 -2.544212 -1.355619
 H  -3.547657 -3.542589 -1.927243
 O  -2.445008 -3.949730 0.452635
 H  -2.289921 -4.319560 1.340032
 H  -4.011422 -2.699343 1.031446
 O  -2.151019 -2.560380 2.955628
 H  -3.068543 -2.548089 3.282567
 H  -1.090213 -1.896856 1.376046
 O  -1.789008 0.348608 2.683233
 H  -0.913956 0.410283 2.260123
 H  -3.614208 -0.412609 2.246046
 O  -2.790191 4.328912 0.960178
 H  -2.785259 3.846094 1.804027
 H  -1.444148 5.054489 -0.376886
 H  -0.816921 4.960088 1.283664
 C  0.971423 -1.185174 -1.123540
 H  0.727779 -2.118925 -1.642668
 H  0.326523 -1.116693 -0.247330
 C  2.425243 -1.190223 -0.708553
 C  2.783849 -1.309508 0.641391
 C  3.443378 -1.069089 -1.664115
 C  4.120580 -1.315109 1.029442
 H  2.003325 -1.389315 1.394566
 C  4.782117 -1.067351 -1.275886
 H  3.181574 -0.957359 -2.712461
 C  5.149854 -1.193136 0.076909
 H  4.363723 -1.402977 2.084163
 H  5.558840 -0.967258 -2.030067
 C  6.579632 -1.184552 0.429389
 H  7.254236 -1.070445 -0.419103
 C  7.111441 -1.302466 1.653823
 H  6.509132 -1.420629 2.551205
 H  8.188527 -1.283039 1.795084
Sum of electronic and thermal Free
Energies= -1645.329128
SCF Energies= -1645.77857
S4.out
 O  0.446947 1.843539 1.289919
 C  0.762422 3.109352 0.670871
 C  -0.401544 3.530383 -0.225320
 C  -0.657483 2.444981 -1.269251
 C  -0.844823 1.080157 -0.608791
 C  0.289001 0.773918 0.380200
 C  1.042543 4.065127 1.818038
 H  1.670467 3.004125 0.065088
 O  -0.054664 4.766831 -0.845907
 H  -0.755747 4.958951 -1.492061
 H  -1.305817 3.643690 0.391573
 O  -1.827386 2.821819 -1.998363
 H  -1.959543 2.146463 -2.685560
 H  0.211638 2.400640 -1.940244
 O  -0.931616 0.134712 -1.669791
 H  -1.775281 1.102896 -0.028134
 O  1.464114 0.536209 -0.371679
 H  0.057577 -0.094953 0.999857
 C  2.581467 0.065068 0.372827
 O  2.287551 -1.140786 1.039795
 C  2.371565 -2.300206 0.187423
 C  3.838264 -2.549595 -0.230393
 C  4.646300 -1.225416 -0.239824
 C  3.734560 -0.070827 -0.654412
 H  2.839195 0.779838 1.157119
 C  1.760787 -3.451440 0.961632
 H  1.776052 -2.123560 -0.715711
 O  0.361624 -3.265594 1.189500
 H  0.258465 -2.406478 1.633077
 H  1.869935 -4.370832 0.379390
 H  2.299609 -3.575602 1.912388
 O  3.875678 -3.189668 -1.506838
 H  3.545902 -2.518931 -2.134951
 H  4.324528 -3.235799 0.472021
 O  5.184030 -0.893081 1.037273
 H  5.811013 -1.594802 1.279617
 H  5.443252 -1.335385 -0.987322
 O  3.258486 -0.388647 -1.966849
 H  2.341266 -0.059575 -2.017054
 H  4.290438 0.874080 -0.673380
 O  2.177951 3.641276 2.573833
 H  1.983615 2.736036 2.871614
 H  0.147857 4.144513 2.453187
 H  1.273839 5.055824 1.420036
 C  -1.333743 -1.191229 -1.289019
 H  -0.591534 -1.647481 -0.624079
 H  -1.318260 -1.752067 -2.229881
 C  -2.707169 -1.253137 -0.659873
 C  -3.762297 -0.477128 -1.165377
 C  -2.953987 -2.093409 0.429483
 C  -5.030868 -0.546125 -0.602240
 H  -3.573496 0.202066 -1.992593
 C  -4.229884 -2.170879 0.988675
 H  -2.144486 -2.691283 0.840540
 C  -5.293816 -1.401155 0.487600
 H  -5.824469 0.072616 -1.010702
 H  -4.404752 -2.830964 1.834977
 C  -6.617674 -1.515607 1.122417
 H  -6.654293 -2.197312 1.972281
 C  -7.745670 -0.885692 0.765345
 H  -7.796517 -0.192303 -0.070708
 H  -8.669886 -1.050116 1.312405
Sum of electronic and thermal Free
Energies= -1645.324988
SCF Energies= -1645.776064
S5.out
 O  0.695027 2.008441 1.423695
 C  0.940287 3.003029 0.408606
 C  -0.298236 3.117018 -0.483912
 C  -0.597211 1.753716 -1.110686
 C  -0.697036 0.670497 -0.037480
```

```
 C  0.520630 0.707372 0.894635
 C  1.318675 4.288246 1.124769
 H  1.791246 2.689591 -0.209137
 O  -0.037273 4.090978 -1.493401
 H  -0.778332 4.039489 -2.121717
 H  -1.159644 3.416548 0.132363
 O  -1.821215 1.879807 -1.835630
 H  -1.972501 1.031157 -2.285600
 H  0.225756 1.501182 -1.793742
 O  -0.812470 -0.586146 -0.702228
 H  -1.586594 0.870720 0.572139
 O  1.657734 0.306103 0.154675
 H  0.378332 0.051145 1.757264
 C  2.730733 -0.149552 0.959318
 O  2.518735 -1.482588 1.379191
 C  2.359611 -2.413379 0.287344
 C  3.615463 -2.423690 -0.604032
 C  3.953669 -1.001972 -1.061831
 C  4.013818 -0.052239 0.139770
 H  2.804419 0.451286 1.869976
 C  2.068652 -3.770825 0.907003
 H  1.500119 -2.107191 -0.324850
 O  0.821448 -3.792622 1.605912
 H  0.118918 -3.722108 0.938614
 H  2.098715 -4.533224 0.119480
 H  2.842154 -4.005949 1.645304
 O  3.446967 -3.306009 -1.713796
 H  2.720707 -2.951762 -2.257617
 H  4.462129 -2.821019 -0.032502
 O  5.206952 -1.040464 -1.747450
 H  5.302156 -0.196016 -2.218696
 H  3.160327 -0.657537 -1.740774
 O  4.188525 1.307955 -0.259511
 H  5.119169 1.416528 -0.515948
 H  4.838172 -0.369268 0.790936
 O  2.519149 4.130801 1.885295
 H  3.213741 3.839863 1.269364
 H  0.534499 4.564505 1.836911
 H  1.413492 5.093607 0.385067
 C  -1.532055 -1.588070 0.038920
 H  -1.106237 -1.709972 1.042453
 H  -1.352447 -2.516001 -0.515067
 C  -3.010634 -1.289962 0.114136
 C  -3.727902 -1.008387 -1.060145
 C  -3.690902 -1.275741 1.333679
 C  -5.087778 -0.729595 -1.016566
 H  -3.206897 -1.010196 -2.014322
 C  -5.059117 -1.002382 1.379573
 H  -3.148626 -1.479319 2.253802
 C  -5.785171 -0.723615 0.209528
 H  -5.613765 -0.516622 -1.942431
 H  -5.573695 -0.996857 2.337398
 C  -7.226143 -0.439945 0.315963
 H  -7.618458 -0.468274 1.332553
 C  -8.073687 -0.162145 -0.684552
 H  -7.765527 -0.114977 -1.726095
 H  -9.123939 0.030361 -0.483390
Sum of electronic and thermal Free
Energies= -1645.325808
SCF Energies= -1645.778104
S6.out
 O  -0.804714 -1.728973 1.369902
 C  -2.023543 -2.354886 0.907846
 C  -1.640145 -3.415547 -0.116876
 C  -0.980218 -2.691377 -1.300105
 C  0.185749 -1.810326 -0.833644
 C  -0.190363 -0.935235 0.371476
 C  -2.762811 -2.809719 2.148612
 H  -2.649825 -1.607796 0.414073
 O  -2.815364 -4.103744 -0.535829
 H  -2.564972 -4.602261 -1.333889
 H  -0.915857 -4.115222 0.329798
 O  -0.571648 -3.615003 -2.311390
 H  0.120867 -4.182532 -1.928455
 H  -1.736508 -2.058753 -1.776201
 O  0.636376 -0.995457 -1.912419
 H  0.989714 -2.470045 -0.483120
 O  -1.061986 0.100406 -0.049422
 H  0.706743 -0.510609 0.831675
 C  -1.306056 1.070203 0.957808
 O  -0.429954 2.174334 0.827340
 C  -0.558366 2.890937 -0.419383
 C  -1.982664 3.433156 -0.565563
 C  -2.999615 2.303289 -0.422406
 C  -2.767778 1.539599 0.878480
 H  -1.101783 0.648379 1.945081
 C  0.486071 3.995068 -0.369972
 H  -0.338563 2.212380 -1.252740
 O  1.811691 3.469399 -0.288791
 H  1.815754 2.842835 0.455019
 H  0.433037 4.588458 -1.285665
 H  0.271354 4.653009 0.485109
 O  -2.081361 4.053279 -1.846689
 H  -3.018104 4.286618 -1.966660
 H  -2.168907 4.166785 0.233935
 O  -4.297204 2.901762 -0.459280
 H  -4.943873 2.175918 -0.448648
 H  -2.877737 1.609717 -1.266089
 O  -3.706489 0.472788 0.925713
 H  -3.537737 -0.084377 1.715322
 H  -2.920401 2.229681 1.720354
 O  -3.140712 -1.665713 2.936000
 H  -2.310822 -1.242479 3.218473
 H  -2.148429 -3.500109 2.741347
 H  -3.687641 -3.315476 1.863713
 C  1.980231 -1.275068 -2.340157
 H  2.105537 -0.682555 -3.252064
 H  2.077354 -2.335515 -2.605716
 C  3.005603 -0.884566 -1.301926
 C  3.926492 -1.805810 -0.797976
 C  3.022029 0.426606 -0.799282
 C  4.851435 -1.424436 0.176218
 H  3.920914 -2.828506 -1.167044
 C  3.939156 0.807884 0.171667
 H  2.304949 1.152906 -1.169659
 C  4.876343 -0.114407 0.682968
 H  5.560866 -2.155241 0.557020
 H  3.933407 1.833308 0.529728
 C  5.869520 0.233277 1.712992
 H  6.548841 -0.576830 1.978444
 C  6.012337 1.411651 2.335637
 H  5.373869 2.268480 2.134546
 H  6.788416 1.553430 3.082737
Sum of electronic and thermal Free
Energies= -1645.332045
SCF Energies= -1645.785849
```

S7.out

```
 O  -2.002016 -0.734996 1.509999
 C  -3.336226 -0.330381 1.139934
 C  -3.893320 -1.348466 0.147272
 C  -2.971573 -1.437790 -1.073732
 C  -1.524163 -1.722277 -0.658479
 C  -1.078439 -0.740424 0.440856
 C  -4.132877 -0.221096 2.429313
 H  -3.306916 0.657033 0.660212
 O  -5.202043 -0.940649 -0.244236
 H  -5.432608 -1.492708 -1.012676
 H  -3.923995 -2.336813 0.634677
 O  -3.461871 -2.406069 -2.002789
 H  -3.436035 -3.273445 -1.560015
 H  -3.006707 -0.480280 -1.604150
 O  -0.707184 -1.628926 -1.819977
 H  -1.473036 -2.730618 -0.227007
 O  -0.962824 0.536889 -0.165503
 H  -0.123199 -1.035427 0.882239
 C  -0.606775 1.601506 0.705457
 O  0.733722 1.510830 1.136829
 C  1.719446 1.554398 0.080835
 C  1.546142 2.838822 -0.732630
 C  0.114638 2.972649 -1.259708
 C  -0.879379 2.880931 -0.097215
 H  -1.210628 1.570292 1.615722
 C  3.068335 1.465757 0.781916
 H  1.596329 0.687454 -0.578929
 O  3.310327 2.584304 1.638229
 H  2.557135 2.623308 2.252631
 H  3.866567 1.454215 0.036058
 H  3.111816 0.525625 1.346099
 O  2.480427 2.801884 -1.810057
 H  2.238742 3.543994 -2.392227
 H  1.751105 3.696908 -0.074176
 O  -0.032553 4.175624 -2.017335
 H  0.111060 4.921773 -1.407973
 H  -0.080684 2.159318 -1.966549
 O  -2.237925 2.928338 -0.521403
 H  -2.401211 2.102495 -1.011839
 H  -0.733748 3.738015 0.568576
 O  -3.612910 0.795659 3.289711
 H  -3.728743 1.644882 2.830824
 H  -4.064315 -1.162003 2.984560
 H  -5.186869 -0.038941 2.184711
 C  0.252668 -2.687224 -2.001996
 H  0.475232 -2.681193 -3.072900
 H  -0.210951 -3.649677 -1.751406
 C  1.516015 -2.474287 -1.204448
 C  1.665471 -3.020489 0.079325
 C  2.549255 -1.680444 -1.715910
 C  2.806004 -2.771222 0.836509
 H  0.875953 -3.646968 0.487105
 C  3.697201 -1.437268 -0.964713
 H  2.452981 -1.248982 -2.709264
 C  3.846901 -1.970001 0.328393
 H  2.888471 -3.207115 1.827651
 H  4.489030 -0.817561 -1.377963
 C  5.068009 -1.652404 1.087950
 H  5.793542 -1.048055 0.543674
 C  5.355250 -2.010720 2.346999
 H  4.683673 -2.606735 2.960183
 H  6.291311 -1.709320 2.808853
```

Sum of electronic and thermal Free Energies= -1645.331508

SCF Energies= -1645.783907

S8.out

```
 O  1.621677 -0.422565 1.329609
 C  2.664577 -1.378828 1.054707
 C  3.930047 -0.628629 0.635126
 C  3.615700 0.247241 -0.576744
 C  2.429589 1.172986 -0.300104
 C  1.231165 0.365264 0.224900
 C  2.831102 -2.206677 2.311859
 H  2.354376 -2.039050 0.235081
 O  4.936418 -1.590195 0.322348
 H  5.684738 -1.093989 -0.051923
 H  4.255493 0.019318 1.462967
 O  4.789489 1.000735 -0.878608
 H  4.574690 1.538193 -1.660782
 H  3.359391 -0.410630 -1.419036
 O  2.156029 1.864530 -1.516600
 H  2.712991 1.880860 0.489205
 O  0.739903 -0.427802 -0.854823
 H  0.435010 1.002746 0.607840
 C  -0.351550 -1.238729 -0.510641
 O  -1.456792 -0.394230 -0.216743
 C  -2.516588 -1.105275 0.445445
 C  -2.653257 -2.538568 -0.108641
 C  -2.170364 -2.582722 -1.562800
 C  -0.696180 -2.150625 -1.694866
 H  -0.103285 -1.851187 0.364257
 C  -2.326943 -1.063259 1.960256
 H  -3.428817 -0.560423 0.180264
 O  -2.228805 0.272053 2.454624
 H  -3.021695 0.760994 2.165959
 H  -1.390173 -1.558079 2.239083
 H  -3.154763 -1.613723 2.431920
 O  -4.029187 -2.901386 -0.019633
 H  -4.113694 -3.745416 -0.497605
 H  -2.045197 -3.240443 0.483110
 O  -2.397945 -3.912938 -2.031869
 H  -2.379238 -3.888305 -3.002807
 H  -2.775124 -1.867856 -2.136003
 O  -0.556950 -1.484025 -2.948133
 H  0.341782 -1.112166 -2.970573
 H  -0.054356 -3.041332 -1.649877
 O  1.624887 -2.953400 2.501414
 H  1.713248 -3.437906 3.338084
 H  3.023600 -1.539039 3.163593
 H  3.696323 -2.870351 2.189404
 C  1.681930 3.217432 -1.362663
 H  1.681918 3.619777 -2.379953
 H  2.397421 3.792822 -0.760858
 C  0.301531 3.280466 -0.755209
 C  -0.789225 2.722277 -1.439514
 C  0.095102 3.801204 0.525899
 C  -2.046019 2.663583 -0.850395
 H  -0.639719 2.304631 -2.431855
 C  -1.165346 3.741250 1.120711
 H  0.929571 4.236231 1.070108
 C  -2.252344 3.149630 0.455443
 H  -2.870052 2.217711 -1.399065
 H  -1.305711 4.133052 2.125111
 C  -3.541152 3.033398 1.158228
 H  -3.623058 3.629101 2.067205
```

```
 C  -4.573295 2.247432 0.813785
 H  -4.555377 1.607200 -0.064721
 H  -5.480975 2.227926 1.410504
Sum of electronic and thermal Free
Energies= -1645.320206
SCF Energies= -1645.770135
S9.out
 O  2.882640 -0.945919 -0.432787
 C  4.067278 -0.612356 0.318607
 C  4.147500 0.904987 0.591690
 C  3.355141 1.651883 -0.482320
 C  1.864996 1.268963 -0.450668
 C  1.742525 -0.200326 -0.009783
 C  4.160222 -1.432648 1.596071
 H  4.898434 -0.876878 -0.341730
 O  5.524233 1.274334 0.569238
 H  5.539221 2.247502 0.598057
 H  3.713793 1.142432 1.576146
 O  3.548498 3.052137 -0.265711
 H  3.370975 3.505379 -1.106338
 H  3.754784 1.362402 -1.462275
 O  1.293529 1.484379 -1.740128
 H  1.359906 1.881108 0.302639
 O  0.614665 -0.803920 -0.578676
 H  1.665121 -0.232016 1.085225
 C  0.243263 -2.014510 0.080363
 O  -0.521491 -1.759014 1.237902
 C  -1.794655 -1.116430 0.985699
 C  -2.649776 -2.046510 0.122192
 C  -1.922594 -2.275843 -1.199671
 C  -0.531359 -2.860877 -0.937508
 H  1.139357 -2.540211 0.419605
 C  -2.388153 -0.809619 2.348525
 H  -1.623382 -0.174200 0.455256
 O  -1.621329 0.179642 3.038673
 H  -0.705632 -0.147603 3.059558
 H  -2.457270 -1.739161 2.933145
 H  -3.392496 -0.399425 2.226388
 O  -3.927044 -1.445395 -0.082398
 H  -4.356159 -1.948907 -0.795650
 H  -2.760835 -3.011924 0.639729
 O  -2.713045 -3.168015 -1.985528
 H  -2.242309 -3.283446 -2.828822
 H  -1.819442 -1.308387 -1.712959
 O  0.207644 -3.023797 -2.143568
 H  0.501378 -2.131580 -2.403671
 H  -0.656790 -3.861135 -0.512074
 O  4.187272 -2.815335 1.237244
 H  4.187621 -3.324672 2.063572
 H  3.303237 -1.212794 2.247921
 H  5.074046 -1.134354 2.130932
 C  0.459047 2.659848 -1.825509
 H  0.348135 2.841876 -2.898117
 H  0.979884 3.516807 -1.382085
 C  -0.889412 2.457533 -1.178665
 C  -1.148909 2.920945 0.119081
 C  -1.901906 1.763170 -1.853719
 C  -2.379666 2.694139 0.730014
 H  -0.380821 3.476679 0.651352
 C  -3.140044 1.551578 -1.253364
 H  -1.719709 1.396002 -2.860876
 C  -3.401266 2.003281 0.053893
 H  -2.550168 3.070010 1.734035
 H  -3.914817 1.013956 -1.792912
 C  -4.714342 1.721688 0.657781
 H  -5.465247 1.346147 -0.036742
 C  -5.045693 1.852821 1.949941
 H  -4.341563 2.192442 2.705562
 H  -6.047021 1.610867 2.295129
Sum of electronic and thermal Free
Energies= -1645.320512
SCF Energies= -1645.771496
```

Conformations for **O4** (Energies in Hartree)

```
S0.out
 O  -0.166743 -0.365657 -1.198435
 C  -0.949840 -0.355273 0.017440
 C  -1.395358 1.078596 0.330712
 C  -0.178667 1.999678 0.416702
 C  0.685932 1.878225 -0.844717
 C  1.009368 0.411612 -1.137179
 C  -2.101479 -1.317232 -0.231208
 H  -0.338608 -0.741634 0.841560
 O  -2.090197 1.075154 1.580368
 H  -2.046624 1.428092 -0.479591
 O  -0.635782 3.341204 0.582705
 H  0.158417 3.903197 0.563602
 H  0.422529 1.693418 1.286352
 O  1.871625 2.664153 -0.739674
 H  0.124599 2.278374 -1.693720
 O  1.873271 -0.014440 -0.094808
 H  1.500240 0.293329 -2.106558
 C  2.507505 -1.265745 -0.304667
 O  3.515427 -1.183643 -1.292621
 C  4.565792 -0.244981 -0.991188
 C  5.245745 -0.644519 0.324712
 C  4.223060 -0.734052 1.452277
 C  3.084140 -1.678092 1.053280
 H  1.784590 -1.998686 -0.672383
 C  5.521228 -0.280965 -2.184314
 H  4.149382 0.765749 -0.896693
 O  6.503243 0.749028 -2.109502
 H  6.863283 0.706296 -1.201936
 H  4.946627 -0.118857 -3.101546
 H  5.983160 -1.278560 -2.245837
 O  6.247987 0.341008 0.609580
 H  6.770641 0.011883 1.360259
 H  5.712304 -1.631121 0.192505
 O  4.893734 -1.204004 2.620562
 H  4.211247 -1.303302 3.307022
 H  3.809269 0.270168 1.627650
 O  2.074969 -1.734983 2.058349
 H  1.652239 -0.857522 2.081512
 H  3.482780 -2.692138 0.960114
 O  -1.621676 -2.635082 -0.502922
 H  -1.036673 -2.558435 -1.275891
 H  -2.727584 -0.942869 -1.054438
 H  -2.718918 -1.381856 0.665695
 C  -3.327335 1.820153 1.588434
 H  -3.168360 2.813113 1.154311
```

```
 C  -4.427708 1.082335 0.866578
 C  -4.819947 1.443051 -0.426093
 C  -5.018505 -0.048846 1.453068
 C  -5.766823 0.687942 -1.119638
 H  -4.379956 2.318664 -0.896738
 C  -5.960908 -0.803529 0.765638
 H  -4.724821 -0.341861 2.458268
 C  -6.351019 -0.452898 -0.543493
 H  -6.055472 0.982548 -2.125676
 H  -6.397870 -1.672142 1.249148
 C  -7.334497 -1.220679 -1.325585
 H  -7.549255 -0.808366 -2.311587
 C  -7.965156 -2.344117 -0.956172
 H  -7.807171 -2.823376 0.006919
 H  -8.674441 -2.825947 -1.623400
 H  2.423059 2.245383 -0.053794
 H  -3.568631 1.940577 2.648529
Sum of electronic and thermal Free
Energies= -1645.330357
SCF Energies= -1645.782249
S1.out
 O  1.064853 -2.434617 0.106257
 C  -0.180647 -1.926642 0.633897
 C  -1.137147 -1.577126 -0.512648
 C  -0.471686 -0.620393 -1.500111
 C  0.880849 -1.170387 -1.950928
 C  1.745072 -1.522205 -0.734241
 C  -0.722297 -3.014440 1.545846
 H  0.018653 -1.030063 1.232350
 O  -2.294641 -0.946591 0.034350
 H  -1.409553 -2.498052 -1.044033
 O  -1.351077 -0.450344 -2.612927
 H  -0.903312 0.155018 -3.228941
 H  -0.309567 0.341588 -0.994056
 O  1.492380 -0.179079 -2.773664
 H  0.712643 -2.096860 -2.514532
 O  2.042487 -0.311602 -0.065568
 H  2.668236 -2.027194 -1.033872
 C  3.057665 -0.404620 0.920899
 O  4.335972 -0.558830 0.339016
 C  4.715254 0.518777 -0.545489
 C  4.741148 1.837942 0.236175
 C  3.382344 2.084625 0.886043
 C  2.967790 0.885372 1.742850
 H  2.901623 -1.288490 1.545469
 C  6.051050 0.146347 -1.158351
 H  3.981463 0.600627 -1.357715
 O  7.034352 0.043297 -0.126357
 H  7.888896 -0.108283 -0.560872
 H  6.319025 0.916376 -1.892919
 H  5.936580 -0.809065 -1.690016
 O  5.067587 2.877711 -0.686376
 H  4.988708 3.715150 -0.198458
 H  5.501201 1.770069 1.026432
 O  3.487451 3.271021 1.674504
 H  2.617716 3.404555 2.089322
 H  2.637087 2.224007 0.088951
 O  1.666828 1.065023 2.299216
 H  1.040849 1.060305 1.552401
 H  3.655284 0.798856 2.588915
 O  0.143320 -3.241963 2.658415
 H  1.011352 -3.473492 2.286358
 H  -0.874749 -3.935699 0.964459
 H  -1.686466 -2.696113 1.950559
 C  -3.547314 -1.575164 -0.281851
 H  -3.732512 -2.414129 0.402447
 C  -4.640498 -0.542862 -0.182964
 C  -5.754070 -0.730438 0.644356
 C  -4.557739 0.630836 -0.944093
 C  -6.767888 0.223461 0.704990
 H  -5.828591 -1.633099 1.245815
 C  -5.566400 1.587359 -0.879941
 H  -3.697097 0.785909 -1.589275
 C  -6.692932 1.405459 -0.054368
 H  -7.621472 0.047150 1.352898
 H  -5.488047 2.491981 -1.478306
 C  -7.729597 2.451139 -0.024777
 H  -7.545128 3.290591 -0.695262
 C  -8.839704 2.469113 0.725823
 H  -9.094104 1.673777 1.422303
 H  -9.538880 3.298449 0.664111
 H  2.239744 -0.596560 -3.233562
 H  -3.505191 -1.976441 -1.302591
Sum of electronic and thermal Free
Energies= -1645.326229
SCF Energies= -1645.774157
S10.out
 O  1.985957 0.478074 2.162017
 C  2.345117 -0.427160 1.086689
 C  3.097814 0.346359 -0.016419
 C  2.210612 1.486831 -0.517018
 C  1.815762 2.367524 0.677339
 C  1.143260 1.533606 1.780205
 C  3.182219 -1.510806 1.742447
 H  1.432158 -0.875606 0.687806
 O  3.621825 -0.518878 -1.031659
 H  3.991331 0.791338 0.438572
 O  2.929746 2.252852 -1.481819
 H  2.357849 3.013673 -1.688533
 H  1.294139 1.082743 -0.963925
 O  1.047557 3.490969 0.272839
 H  2.731814 2.776626 1.116173
 O  -0.105773 0.963706 1.362987
 H  0.980526 2.145061 2.673643
 C  -1.266538 1.759554 1.498337
 O  -1.559566 2.456061 0.297027
 C  -1.880040 1.596995 -0.821914
 C  -3.179259 0.862919 -0.492062
 C  -2.916623 -0.018308 0.730122
 C  -2.426578 0.832903 1.907296
 H  -1.111673 2.534758 2.253383
 C  -1.928810 2.470327 -2.054851
 H  -1.077915 0.863998 -0.952360
 O  -0.583329 2.876751 -2.335066
 H  -0.617634 3.548871 -3.035034
 H  -2.577624 3.337096 -1.871083
 H  -2.346427 1.891222 -2.887334
 O  -3.583098 0.084170 -1.616084
 H  -4.261417 -0.531267 -1.285726
 H  -3.955388 1.602867 -0.244006
 O  -4.135596 -0.693877 1.048610
 H  -3.894858 -1.509429 1.518060
 H  -2.142793 -0.751448 0.472232
 O  -2.054638 0.033293 3.023849
 H  -1.196376 -0.368031 2.792941
 H  -3.255734 1.465653 2.237722
```

```
 O  2.404146 -2.292957 2.649231
 H  2.017177 -1.668419 3.286563
 H  4.039633 -1.045752 2.251714
 H  3.563004 -2.191516 0.980291
 C  2.791069 -0.877004 -2.154915
 H  3.471341 -1.441697 -2.800303
 C  1.588118 -1.712631 -1.787263
 C  0.290640 -1.247305 -2.032299
 C  1.745215 -2.934146 -1.119905
 C  -0.821806 -1.951996 -1.581014
 H  0.150534 -0.306742 -2.560433
 C  0.636614 -3.630103 -0.645675
 H  2.744276 -3.321675 -0.939293
 C  -0.669323 -3.142597 -0.846087
 H  -1.809451 -1.548181 -1.773099
 H  0.778738 -4.559326 -0.099217
 C  -1.804451 -3.877109 -0.262762
 H  -1.530253 -4.789000 0.267808
 C  -3.098833 -3.528300 -0.304252
 H  -3.452284 -2.635433 -0.809744
 H  -3.855082 -4.144841 0.173742
 H  0.187033 3.173363 -0.073677
 H  2.482447 0.022485 -2.698348
Sum of electronic and thermal Free
Energies= -1645.334552
SCF Energies= -1645.790379
S12.out
 O  -3.581032 0.074211 0.237935
 C  -2.993790 -0.892116 -0.660163
 C  -2.230927 -2.013079 0.075266
 C  -1.291643 -1.425660 1.136981
 C  -2.040514 -0.399898 1.997291
 C  -2.667011 0.680158 1.114928
 C  -4.154347 -1.420849 -1.490089
 H  -2.284958 -0.378236 -1.318767
 O  -1.598109 -2.718915 -0.997549
 H  -2.937172 -2.681470 0.590970
 O  -0.811039 -2.470771 1.984208
 H  -0.332356 -2.019710 2.702829
 H  -0.455561 -0.924673 0.635719
 O  -1.207466 0.117790 3.027696
 H  -2.865627 -0.910478 2.504382
 O  -1.682003 1.363088 0.327917
 H  -3.226518 1.405801 1.713681
 C  -1.099916 2.532052 0.857879
 O  0.036793 2.241004 1.667373
 C  1.162604 1.646864 0.980780
 C  1.622188 2.571096 -0.149565
 C  0.464554 2.835427 -1.103439
 C  -0.718772 3.424933 -0.328806
 H  -1.801373 3.040933 1.524890
 C  2.227595 1.423825 2.054930
 H  0.876577 0.676945 0.557710
 O  3.295875 0.603669 1.594764
 H  3.574583 0.956705 0.728364
 H  1.764987 0.900801 2.898309
 H  2.588017 2.399499 2.414983
 O  2.712316 1.918370 -0.807200
 H  3.087466 2.541476 -1.451894
 H  1.955195 3.525889 0.281586
 O  0.912148 3.741731 -2.108722
 H  0.132096 3.954418 -2.650356
 H  0.157311 1.880500 -1.556433
 O  -1.836416 3.648963 -1.180644
 H  -2.195295 2.768031 -1.395141
 H  -0.424977 4.402658 0.063633
 O  -4.763922 -0.384840 -2.259187
 H  -5.031926 0.301860 -1.625106
 H  -4.883620 -1.900654 -0.820303
 H  -3.785802 -2.168387 -2.195487
 C  -0.558583 -3.654426 -0.692780
 H  -0.592239 -4.382925 -1.512131
 C  0.812232 -3.010042 -0.648702
 C  1.120149 -1.936475 -1.497814
 C  1.804575 -3.483704 0.213773
 C  2.383552 -1.355756 -1.489736
 H  0.352811 -1.547383 -2.160304
 C  3.074206 -2.906037 0.220167
 H  1.581726 -4.304143 0.891431
 C  3.391576 -1.830910 -0.627972
 H  2.581899 -0.517470 -2.149031
 H  3.831011 -3.283828 0.903669
 C  4.742178 -1.248127 -0.564946
 H  5.402618 -1.718452 0.163722
 C  5.221178 -0.223880 -1.286198
 H  4.630542 0.301721 -2.031726
 H  6.241303 0.122835 -1.146092
 H  -0.614732 0.793897 2.636148
 H  -0.769642 -4.190924 0.237288
Sum of electronic and thermal Free
Energies= -1645.329926
SCF Energies= -1645.785069
S13.out
 O  -0.508454 -1.560550 1.666700
 C  0.248013 -2.130051 0.579075
 C  1.374766 -1.172177 0.148540
 C  0.792907 0.200952 -0.189227
 C  -0.080653 0.709206 0.957623
 C  -1.134189 -0.336812 1.342562
 C  0.760944 -3.478374 1.064194
 H  -0.418541 -2.292888 -0.279046
 O  2.016060 -1.708174 -1.013476
 H  2.089361 -1.056630 0.972755
 O  1.866955 1.107543 -0.434812
 H  1.459015 1.978312 -0.580528
 H  0.166300 0.100227 -1.087622
 O  -0.637145 1.950990 0.544471
 H  0.559260 0.845142 1.841120
 O  -2.058658 -0.502758 0.275267
 H  -1.662868 -0.020107 2.245011
 C  -3.397049 -0.681924 0.711865
 O  -3.904275 0.509984 1.274293
 C  -3.895360 1.608996 0.335814
 C  -4.921862 1.325271 -0.766582
 C  -4.470397 0.046216 -1.482221
 C  -4.247189 -1.106184 -0.489320
 H  -3.438773 -1.435638 1.504074
 C  -4.088368 2.876756 1.133903
 H  -2.908256 1.672473 -0.131990
 O  -2.933268 3.010471 1.984574
 H  -2.880972 3.936138 2.272635
 H  -5.005355 2.823646 1.736468
 H  -4.169213 3.722135 0.442660
 O  -5.056860 2.420602 -1.670760
 H  -4.187106 2.567396 -2.083497
 H  -5.912640 1.172998 -0.325994
```

```
 O  -5.449593 -0.323893 -2.449568
 H  -5.164212 -1.186968 -2.797756
 H  -3.510859 0.264196 -1.980013
 O  -3.713477 -2.254223 -1.145030
 H  -2.796714 -2.036125 -1.392504
 H  -5.225193 -1.404949 -0.100196
 O  -0.303034 -4.366767 1.410242
 H  -0.795455 -4.556392 0.593596
 H  1.354616 -3.338931 1.973329
 H  1.404867 -3.915534 0.291391
 C  3.375052 -2.153472 -0.823463
 H  3.590229 -2.754274 -1.712117
 C  4.347281 -1.006104 -0.705451
 C  4.942962 -0.682411 0.520523
 C  4.627161 -0.202693 -1.818223
 C  5.796750 0.411832 0.636918
 H  4.734168 -1.296567 1.393193
 C  5.478897 0.891930 -1.705404
 H  4.167014 -0.435103 -2.775503
 C  6.080555 1.224486 -0.476181
 H  6.243235 0.634553 1.601476
 H  5.686896 1.504386 -2.579552
 C  6.972084 2.395254 -0.417086
 H  7.106931 2.908689 -1.369207
 C  7.610906 2.874598 0.659325
 H  7.527697 2.424812 1.645742
 H  8.246360 3.752434 0.581411
 H  -1.286849 2.272372 1.207802
 H  3.441768 -2.807372 0.054570
Sum of electronic and thermal Free
Energies= -1645.322992
SCF Energies= -1645.775476
S14.out
 O  0.089512 0.231236 -1.516072
 C  -0.405337 0.089547 -0.162707
 C  -1.068293 1.404482 0.264328
 C  -0.042474 2.533022 0.158859
 C  0.563864 2.588200 -1.249008
 C  1.102675 1.222913 -1.687857
 C  -1.333804 -1.114967 -0.146881
 H  0.432285 -0.108542 0.512669
 O  -1.505262 1.273189 1.617963
 H  -1.910359 1.615551 -0.405303
 O  -0.686971 3.767152 0.467484
 H  -0.030079 4.465649 0.300133
 H  0.762172 2.332917 0.883035
 O  1.564950 3.595903 -1.342665
 H  -0.226151 2.871961 -1.950377
 O  2.259456 0.942029 -0.932703
 H  1.329306 1.218765 -2.757824
 C  3.276577 0.113641 -1.531048
 O  4.441950 0.281021 -0.765070
 C  4.377404 -0.188493 0.602402
 C  3.948112 -1.664551 0.656249
 C  2.663450 -1.854164 -0.148453
 C  2.889899 -1.376112 -1.584216
 H  3.499529 0.494434 -2.533376
 C  5.777790 0.089519 1.154035
 H  3.641449 0.405154 1.161114
 O  5.893512 -0.161068 2.550503
 H  5.267886 0.429349 3.002858
 H  6.038495 1.129450 0.910930
 H  6.501267 -0.565078 0.657565
 O  3.722143 -2.028959 2.017312
 H  3.196725 -2.848639 1.976194
 H  4.743614 -2.287152 0.216900
 O  2.262524 -3.222155 -0.077403
 H  1.286906 -3.202815 -0.088188
 H  1.894980 -1.238337 0.322597
 O  1.809103 -1.642370 -2.464613
 H  1.034330 -1.135850 -2.137616
 H  3.753035 -1.903494 -2.004195
 O  -0.643159 -2.349528 -0.393882
 H  -0.449152 -2.401838 -1.343598
 H  -2.146967 -0.975407 -0.870126
 H  -1.769253 -1.199536 0.849231
 C  -2.836744 1.769930 1.877295
 H  -2.944820 2.779884 1.467305
 C  -3.898448 0.847697 1.330298
 C  -4.578905 1.145903 0.141426
 C  -4.162094 -0.375228 1.960586
 C  -5.491066 0.248462 -0.408644
 H  -4.389938 2.092505 -0.359021
 C  -5.072366 -1.275035 1.413470
 H  -3.641593 -0.626068 2.881832
 C  -5.755099 -0.984318 0.216694
 H  -5.997498 0.510878 -1.332815
 H  -5.263937 -2.219732 1.916649
 C  -6.706592 -1.974757 -0.314782
 H  -6.777267 -2.891559 0.270520
 C  -7.469930 -1.860631 -1.410477
 H  -7.463940 -0.979125 -2.047054
 H  -8.138866 -2.664280 -1.705607
 H  2.332130 3.268373 -0.838209
 H  -2.898061 1.830634 2.967545
Sum of electronic and thermal Free
Energies= -1645.324660
SCF Energies= -1645.77889
S15.out
 O  -0.529265 -1.284857 -1.255071
 C  0.561898 -2.167226 -0.940297
 C  1.266113 -1.807873 0.387042
 C  0.329556 -1.033500 1.327657
 C  -1.121706 -1.479943 1.128527
 C  -1.572908 -1.141816 -0.303390
 C  0.150068 -3.643279 -1.008590
 H  1.275859 -1.983965 -1.748387
 O  2.429711 -1.059045 0.036231
 H  1.568117 -2.731984 0.903226
 O  0.725558 -1.258924 2.679455
 H  0.003541 -0.901357 3.228071
 H  0.403510 0.034650 1.074465
 O  -1.979245 -0.883422 2.097297
 H  -1.192501 -2.556978 1.297327
 O  -1.929389 0.228495 -0.287466
 H  -2.440486 -1.738512 -0.603435
 C  -2.834045 0.643356 -1.305352
 O  -4.098696 0.031717 -1.181275
 C  -4.780517 0.292859 0.065677
 C  -4.997822 1.800702 0.231546
 C  -3.660850 2.531168 0.124904
 C  -2.944865 2.165414 -1.178447
 H  -2.454414 0.348362 -2.287374
 C  -6.077965 -0.488101 0.021672
 H  -4.172246 -0.078736 0.898022
 O  -5.753541 -1.880801 0.032859
```

```
 H  -6.590616 -2.369507 -0.021687
 H  -6.635282 -0.215173 -0.886111
 H  -6.684744 -0.212870 0.893782
 O  -5.600002 2.020143 1.506976
 H  -5.635126 2.983998 1.632508
 H  -5.655882 2.159161 -0.574771
 O  -3.928022 3.931849 0.187546
 H  -3.068484 4.379408 0.101018
 H  -3.032099 2.227162 0.975546
 O  -1.675824 2.805160 -1.275368
 H  -1.097770 2.379250 -0.617030
 H  -3.538993 2.529712 -2.021368
 O  -0.544331 -3.951279 -2.213053
 H  0.060706 -3.764504 -2.950958
 H  -0.528367 -3.908780 -0.193053
 H  1.058330 -4.253411 -0.896209
 C  3.345690 -0.837229 1.111081
 H  3.618282 -1.795345 1.578090
 C  4.573660 -0.138450 0.582408
 C  5.815290 -0.339317 1.202915
 C  4.500894 0.753947 -0.492733
 C  6.952524 0.331857 0.765096
 H  5.890240 -1.032518 2.037549
 C  5.642101 1.419956 -0.937725
 H  3.549766 0.922189 -0.987822
 C  6.890777 1.226840 -0.320606
 H  7.897929 0.151274 1.268263
 H  5.566564 2.105014 -1.779069
 C  8.062281 1.956162 -0.834756
 H  7.848976 2.619726 -1.672958
 C  9.324105 1.883196 -0.388499
 H  9.623060 1.246184 0.440390
 H  10.110619 2.472800 -0.851412
 H  -2.103541 0.043454 1.819096
 H  2.873749 -0.223320 1.890466
Sum of electronic and thermal Free
Energies= -1645.311322
SCF Energies= -1645.759802
S16.out
 O  1.533050 -2.345528 -0.015236
 C  0.363568 -1.703814 0.545184
 C  -0.789663 -1.756769 -0.463154
 C  -0.348054 -1.098051 -1.768296
 C  0.945071 -1.735570 -2.286349
 C  2.029345 -1.742474 -1.202846
 C  0.059813 -2.415693 1.845564
 H  0.593797 -0.654420 0.759994
 O  -1.896975 -1.040168 0.080268
 H  -1.055889 -2.804421 -0.652740
 O  -1.396399 -1.236416 -2.726759
 H  -1.059071 -0.853771 -3.555658
 H  -0.160437 -0.033360 -1.564509
 O  1.403882 -1.087510 -3.468389
 H  0.736165 -2.773542 -2.561096
 O  2.425154 -0.405029 -0.989411
 H  2.883117 -2.354024 -1.507561
 C  3.795911 -0.152339 -0.648250
 O  4.068888 1.183732 -0.982158
 C  3.322722 2.163444 -0.220944
 C  3.586730 2.013013 1.291777
 C  3.315265 0.577219 1.721865
 C  4.104340 -0.392827 0.837318
 H  4.441831 -0.773219 -1.277955
 C  3.741430 3.520908 -0.748688
 H  2.250027 2.024819 -0.401948
 O  3.295109 3.635594 -2.101473
 H  3.566006 4.513187 -2.416003
 H  4.835375 3.611348 -0.679869
 H  3.291182 4.299384 -0.118673
 O  2.714515 2.864770 2.038542
 H  3.124098 3.743088 2.087971
 H  4.637748 2.250998 1.504818
 O  3.692995 0.421411 3.088656
 H  3.605270 -0.530461 3.273832
 H  2.240406 0.380034 1.606812
 O  3.932668 -1.743255 1.245659
 H  2.991714 -1.990379 1.114936
 H  5.170876 -0.178157 0.963770
 O  1.132292 -2.140910 2.752501
 H  0.991986 -2.684809 3.544482
 H  -0.035838 -3.493891 1.657510
 H  -0.896385 -2.043633 2.234740
 C  -3.159533 -1.725849 0.002158
 H  -3.240498 -2.455169 0.819369
 C  -4.259716 -0.700186 0.075445
 C  -4.342075 0.297145 -0.905606
 C  -5.207682 -0.710142 1.105382
 C  -5.349944 1.255341 -0.856489
 H  -3.609354 0.313583 -1.708389
 C  -6.220910 0.245029 1.153094
 H  -5.150740 -1.472742 1.878235
 C  -6.312437 1.249372 0.172068
 H  -5.400915 2.021919 -1.626064
 H  -6.940187 0.212507 1.966198
 C  -7.358228 2.286595 0.173207
 H  -7.279142 3.009313 -0.639012
 C  -8.364750 2.421550 1.047888
 H  -8.517611 1.741563 1.882614
 H  -9.080814 3.232694 0.948942
 H  1.737781 -0.215664 -3.186975
 H  -3.219130 -2.271698 -0.947334
Sum of electronic and thermal Free
Energies= -1645.325465
SCF Energies= -1645.77314
S17.out
 O  -0.274726 1.497877 -1.373878
 C  -1.352616 1.388681 -0.408640
 C  -0.901573 1.221825 1.052020
 C  0.266710 2.148724 1.460652
 C  1.013629 2.756443 0.260894
 C  1.022024 1.776917 -0.904862
 C  -2.300650 2.582367 -0.565372
 H  -1.897228 0.485621 -0.697317
 O  -0.524971 -0.143267 1.319067
 H  -1.749113 1.480612 1.693285
 O  -0.266351 3.179349 2.296747
 H  0.472409 3.776953 2.506697
 H  0.979812 1.532936 2.022352
 O  2.330142 3.166734 0.616410
 H  0.491158 3.659728 -0.064052
 O  1.668470 0.607689 -0.418944
 H  1.572596 2.179344 -1.760765
 C  2.115142 -0.326519 -1.387589
 O  3.519074 -0.260081 -1.542041
 C  4.263702 -0.541923 -0.338630
 C  3.925350 -1.947888 0.178520
```

```
 C  2.417431 -2.081297 0.370791
 C  1.683149 -1.721085 -0.922215
 H  1.688368 -0.095426 -2.366827
 C  5.732549 -0.393973 -0.682900
 H  4.002094 0.193157 0.433783
 O  5.984571 0.978615 -0.991573
 H  6.925013 1.049623 -1.221759
 H  5.968561 -1.045088 -1.537161
 H  6.328720 -0.725275 0.176832
 O  4.619453 -2.139081 1.412178
 H  4.307150 -2.986496 1.773053
 H  4.249224 -2.690839 -0.566506
 O  2.138783 -3.425884 0.764956
 H  1.169767 -3.489973 0.831054
 H  2.104761 -1.386395 1.163347
 O  0.274131 -1.810516 -0.770751
 H  0.006879 -1.151360 -0.087695
 H  1.963852 -2.438969 -1.699389
 O  -2.723587 2.757384 -1.915858
 H  -3.237716 1.968315 -2.158232
 H  -1.808199 3.514254 -0.272741
 H  -3.160098 2.427593 0.102587
 C  -1.514720 -0.923566 2.034467
 H  -1.712391 -0.443736 3.000514
 C  -2.792365 -1.110698 1.253877
 C  -3.913452 -0.306491 1.504673
 C  -2.854161 -2.035289 0.203406
 C  -5.058671 -0.406628 0.719639
 H  -3.885512 0.409174 2.322490
 C  -3.999549 -2.139479 -0.581558
 H  -1.992254 -2.660743 -0.010492
 C  -5.122222 -1.322973 -0.347029
 H  -5.908926 0.231285 0.941352
 H  -4.029515 -2.861171 -1.394263
 C  -6.301015 -1.467434 -1.217903
 H  -6.216054 -2.253358 -1.968323
 C  -7.426950 -0.741582 -1.180984
 H  -7.587978 0.064676 -0.469299
 H  -8.236354 -0.937633 -1.878739
 H  2.837002 2.354458 0.797466
 H  -1.016393 -1.880633 2.210698
Sum of electronic and thermal Free
Energies= -1645.320633
SCF Energies= -1645.77265
S18.out
 O  0.589965 1.714573 1.472446
 C  -0.215279 2.119635 0.343662
 C  -1.457608 1.220586 0.229807
 C  -1.050451 -0.257290 0.193497
 C  -0.115211 -0.587507 1.355575
 C  1.061177 0.384781 1.387629
 C  -0.568885 3.577249 0.555820
 H  0.375701 2.025696 -0.574766
 O  -2.138977 1.549324 -0.986236
 H  -2.108300 1.383616 1.097763
 O  -2.169487 -1.134575 0.325684
 H  -2.750071 -0.995969 -0.442837
 H  -0.523724 -0.448264 -0.751216
 O  0.391043 -1.915310 1.268834
 H  -0.671279 -0.445589 2.293317
 O  1.830601 0.176444 0.216205
 H  1.675157 0.227520 2.278680
 C  3.113066 0.774765 0.246538
 O  3.998280 0.046527 1.077121
 C  4.196615 -1.330837 0.681299
 C  4.750952 -1.381143 -0.746118
 C  3.841633 -0.604703 -1.700363
 C  3.642213 0.817686 -1.187360
 H  3.054055 1.777840 0.677557
 C  5.138688 -1.925959 1.717105
 H  3.240508 -1.867494 0.721055
 O  6.416059 -1.287703 1.730846
 H  6.247623 -0.340036 1.870369
 H  5.311723 -2.979191 1.483066
 H  4.658410 -1.864518 2.703964
 O  4.843121 -2.756297 -1.122418
 H  5.327365 -2.785127 -1.964596
 H  5.744012 -0.912546 -0.751359
 O  4.416298 -0.505616 -3.009547
 H  4.203725 -1.325596 -3.484971
 H  2.867405 -1.105453 -1.754832
 O  2.732380 1.553539 -1.996643
 H  3.007008 1.396222 -2.917117
 H  4.620961 1.317876 -1.154116
 O  0.637546 4.342060 0.485589
 H  0.392821 5.272390 0.617207
 H  -1.058433 3.694524 1.533501
 H  -1.277706 3.882480 -0.224659
 C  -3.483572 2.045536 -0.830079
 H  -3.716644 2.516841 -1.789572
 C  -4.456616 0.933043 -0.528887
 C  -5.044549 0.793881 0.730775
 C  -4.716709 -0.045774 -1.504018
 C  -5.873481 -0.293051 1.011277
 H  -4.848378 1.537081 1.499366
 C  -5.534561 -1.134310 -1.223566
 H  -4.263451 0.048970 -2.487905
 C  -6.131416 -1.280790 0.045932
 H  -6.320719 -0.385329 1.998053
 H  -5.714719 -1.874038 -1.997674
 C  -7.005918 -2.412037 0.398570
 H  -7.400135 -2.380107 1.414209
 C  -7.348528 -3.443871 -0.385050
 H  -6.997629 -3.551811 -1.408467
 H  -8.004170 -4.227297 -0.015185
 H  -0.380219 -2.492724 1.134670
 H  -3.514887 2.816952 -0.050821
Sum of electronic and thermal Free
Energies= -1645.326391
SCF Energies= -1645.775127
S19.out
 O  -0.674970 -1.065969 1.531786
 C  -0.184399 -1.320469 0.192697
 C  1.170824 -0.620020 0.010491
 C  0.982554 0.877575 0.256114
 C  0.342011 1.118364 1.624377
 C  -0.951728 0.313667 1.807084
 C  -0.147219 -2.829567 -0.000657
 H  -0.882449 -0.896975 -0.535049
 O  1.625187 -0.819627 -1.329079
 H  1.895178 -1.011950 0.734554
 O  2.252405 1.521634 0.195963
 H  2.098363 2.441951 0.472682
 H  0.315826 1.274938 -0.523723
 O  0.121938 2.519706 1.745111
 H  1.044920 0.766434 2.390138
```

```
 O  -1.953596 0.831249 0.968629
 H  -1.275743 0.332187 2.852464
 C  -3.325196 0.677894 1.380515
 O  -4.085311 1.601823 0.642925
 C  -4.125813 1.376373 -0.785649
 C  -4.621176 -0.042284 -1.107770
 C  -3.784384 -1.061078 -0.339569
 C  -3.870388 -0.745775 1.157061
 H  -3.416728 0.964303 2.433823
 C  -5.035226 2.440053 -1.367037
 H  -3.117524 1.497056 -1.200063
 O  -4.421667 3.716737 -1.177734
 H  -5.019407 4.378236 -1.562410
 H  -6.011825 2.388505 -0.863915
 H  -5.186509 2.223565 -2.432633
 O  -4.491445 -0.242849 -2.514452
 H  -4.562903 -1.205106 -2.647692
 H  -5.674564 -0.139250 -0.801039
 O  -4.242237 -2.375723 -0.652332
 H  -3.450255 -2.941688 -0.587833
 H  -2.751813 -0.955733 -0.678999
 O  -3.261216 -1.716421 1.995133
 H  -2.292755 -1.674786 1.836064
 H  -4.925186 -0.721608 1.450884
 O  -1.454303 -3.423134 -0.025001
 H  -1.799161 -3.440145 0.882859
 H  0.297553 -3.041881 -0.974922
 H  0.470924 -3.293177 0.778298
 C  2.773020 -1.683946 -1.463153
 H  2.818646 -1.908241 -2.532941
 C  4.046574 -1.021975 -0.999213
 C  4.571672 0.067583 -1.712969
 C  4.699275 -1.435050 0.165238
 C  5.715434 0.723600 -1.276776
 H  4.068694 0.402832 -2.616762
 C  5.850233 -0.779608 0.605475
 H  4.305369 -2.275780 0.731100
 C  6.379171 0.313484 -0.101387
 H  6.099247 1.560043 -1.853237
 H  6.345513 -1.114932 1.513706
 C  7.590719 0.973470 0.413348
 H  8.009127 0.512914 1.308212
 C  8.205580 2.052643 -0.090589
 H  7.852768 2.576699 -0.975457
 H  9.099239 2.450592 0.382173
 H  0.030098 2.726564 2.689968
 H  2.607839 -2.624570 -0.923642
Sum of electronic and thermal Free
Energies= -1645.321230
SCF Energies= -1645.774803
S2.out
 O  0.227890 1.218691 -1.392108
 C  0.766200 0.820181 -0.106481
 C  1.092326 -0.681157 -0.092291
 C  -0.137873 -1.478362 -0.510657
 C  -0.642548 -0.971216 -1.864344
 C  -0.932518 0.536983 -1.795654
 C  1.990120 1.698732 0.104907
 H  0.027665 1.037059 0.674429
 O  1.484054 -1.033097 1.237142
 H  1.903727 -0.876045 -0.803933
 O  0.188977 -2.865783 -0.587855
 H  -0.562222 -3.283256 -1.047335
 H  -0.914961 -1.324098 0.248474
 O  -1.727482 -1.746898 -2.353161
 H  0.162324 -1.091226 -2.597336
 O  -1.970965 0.879574 -0.866304
 H  -1.195341 0.922596 -2.786278
 C  -3.309986 0.681598 -1.268430
 O  -3.787338 -0.610160 -0.913540
 C  -3.788261 -0.887664 0.503672
 C  -4.731887 0.089078 1.207403
 C  -4.272256 1.516095 0.914693
 C  -4.165986 1.760680 -0.593595
 H  -3.397261 0.736043 -2.357167
 C  -4.174665 -2.349762 0.656819
 H  -2.778252 -0.742808 0.904216
 O  -3.237531 -3.220052 0.016777
 H  -2.387793 -3.135032 0.481622
 H  -5.139661 -2.527485 0.172146
 H  -4.272869 -2.582561 1.723661
 O  -4.686347 -0.188839 2.606334
 H  -5.187163 0.520449 3.044655
 H  -5.751881 -0.044314 0.816267
 O  -5.213458 2.408151 1.510642
 H  -4.906942 3.308146 1.304064
 H  -3.278875 1.655724 1.367383
 O  -3.671125 3.065543 -0.873953
 H  -2.728254 3.058215 -0.626324
 H  -5.169182 1.709318 -1.026374
 O  1.641016 3.082362 0.138077
 H  1.170316 3.263868 -0.693303
 H  2.727167 1.491376 -0.685247
 H  2.444351 1.459941 1.067893
 C  2.634010 -1.904504 1.315228
 H  2.499993 -2.759270 0.643710
 C  3.916245 -1.169714 1.010016
 C  4.556162 -1.305553 -0.229909
 C  4.444686 -0.262299 1.937065
 C  5.686007 -0.553023 -0.540879
 H  4.161967 -2.008370 -0.959751
 C  5.574224 0.491362 1.630058
 H  3.960085 -0.141060 2.902876
 C  6.217411 0.365036 0.383783
 H  6.155052 -0.680335 -1.511940
 H  5.969811 1.190570 2.362828
 C  7.406860 1.189161 0.109377
 H  7.684952 1.866283 0.916979
 C  8.155578 1.183414 -1.002161
 H  7.948745 0.536282 -1.851165
 H  9.016358 1.839771 -1.095118
 H  -2.477465 -1.660307 -1.724211
 H  2.630994 -2.269817 2.346155
Sum of electronic and thermal Free
Energies= -1645.330351
SCF Energies= -1645.782891
S20.out
 O  0.276144 -0.012513 -1.423099
 C  -1.148696 0.020894 -1.227469
 C  -1.619183 -0.887517 -0.062879
 C  -0.430119 -1.333582 0.784461
 C  0.475909 -0.121843 1.028543
 C  1.100465 0.320104 -0.314504
 C  -1.676067 1.452294 -1.079759
 H  -1.541459 -0.398857 -2.157506
 O  -2.322390 -2.009821 -0.608799
```

```
 H  -2.291926 -0.316667 0.589919
 O  -0.910764 -1.857346 2.019390
 H  -0.128885 -1.925567 2.596806
 H  0.134716 -2.100935 0.234902
 O  1.468958 -0.399243 2.011427
 H  -0.127411 0.693539 1.438256
 O  2.289883 -0.425952 -0.469498
 H  1.332540 1.390446 -0.317111
 C  3.295006 0.165011 -1.286940
 O  3.763908 1.387394 -0.764505
 C  4.338102 1.295335 0.560805
 C  5.535202 0.333106 0.562380
 C  5.106336 -1.023305 0.002080
 C  4.433426 -0.854416 -1.367518
 H  2.887272 0.397182 -2.274493
 C  4.701344 2.719049 0.944548
 H  3.575228 0.924523 1.256266
 O  3.540515 3.548252 1.019726
 H  3.101786 3.481332 0.154195
 H  5.429029 3.118214 0.222316
 H  5.161175 2.719478 1.935330
 O  6.097932 0.219140 1.868993
 H  5.418822 -0.173808 2.445798
 H  6.331016 0.740263 -0.071261
 O  6.253937 -1.860987 -0.108152
 H  5.958071 -2.654548 -0.588338
 H  4.376441 -1.469397 0.697868
 O  3.997662 -2.107107 -1.887035
 H  3.261643 -2.405250 -1.322665
 H  5.173919 -0.469875 -2.074756
 O  -1.214949 2.311584 -2.118158
 H  -1.556453 1.958258 -2.957016
 H  -1.331561 1.898277 -0.141261
 H  -2.774555 1.407550 -1.045606
 C  -3.476936 -2.411142 0.142291
 H  -3.203076 -2.647361 1.177065
 C  -4.583729 -1.377874 0.111526
 C  -5.339677 -1.098576 1.257397
 C  -4.869823 -0.676144 -1.065968
 C  -6.358554 -0.149456 1.230986
 H  -5.120955 -1.625529 2.183209
 C  -5.883221 0.278882 -1.092866
 H  -4.284070 -0.870465 -1.959799
 C  -6.649592 0.563825 0.053107
 H  -6.923008 0.044790 2.138333
 H  -6.088371 0.817478 -2.015096
 C  -7.703014 1.589201 -0.033249
 H  -7.818811 2.035283 -1.021152
 C  -8.504750 2.014534 0.952939
 H  -8.452858 1.625077 1.966758
 H  -9.250223 2.783136 0.768505
 H  2.175834 -0.893849 1.555815
 H  -3.805129 -3.340206 -0.337065
Sum of electronic and thermal Free
Energies= -1645.316321
SCF Energies= -1645.766073
S21.out
 O  -0.594517 1.091852 -1.296798
 C  0.209461 1.803457 -0.328396
 C  1.523861 1.050761 -0.100071
 C  1.228808 -0.388496 0.335622
 C  0.273830 -1.065378 -0.647472
 C  -0.968291 -0.206935 -0.888767
 C  0.378171 3.204001 -0.890145
 H  -0.336438 1.868305 0.620602
 O  2.259692 1.708652 0.937577
 H  2.098994 1.025070 -1.033537
 O  2.403658 -1.198939 0.368038
 H  3.015959 -0.809089 1.016577
 H  0.755628 -0.359753 1.326967
 O  -0.144753 -2.344192 -0.182053
 H  0.788962 -1.153034 -1.614819
 O  -1.717696 -0.189909 0.312402
 H  -1.572337 -0.615701 -1.701261
 C  -2.952154 0.520396 0.276051
 O  -3.759542 0.119627 -0.806089
 C  -4.514312 -1.079017 -0.551420
 C  -5.617316 -0.760325 0.467108
 C  -5.133075 0.277478 1.510285
 C  -3.606750 0.260277 1.658751
 H  -2.766263 1.585041 0.119183
 C  -5.047675 -1.550140 -1.891858
 H  -3.853136 -1.847282 -0.136143
 O  -3.994415 -1.929601 -2.779280
 H  -3.477059 -1.124529 -2.949477
 H  -5.671431 -0.759877 -2.334332
 H  -5.671757 -2.434485 -1.735382
 O  -5.980946 -2.004620 1.063999
 H  -6.801602 -1.859177 1.563403
 H  -6.478109 -0.313963 -0.049816
 O  -5.570389 1.565935 1.071399
 H  -5.294368 2.212933 1.742740
 H  -5.583759 0.018088 2.477897
 O  -3.245795 -1.008088 2.201160
 H  -2.360396 -1.212246 1.845929
 H  -3.290877 1.066131 2.336682
 O  -0.884129 3.865254 -1.002594
 H  -1.438878 3.297198 -1.564618
 H  0.886811 3.151020 -1.863861
 H  0.991410 3.798919 -0.209122
 C  3.514990 2.291732 0.527583
 H  3.795129 2.949579 1.355381
 C  4.562877 1.232205 0.297097
 C  5.061063 0.496275 1.386338
 C  4.978449 0.883301 -0.990461
 C  5.935008 -0.566832 1.190746
 H  4.746747 0.757700 2.394082
 C  5.862234 -0.178122 -1.188612
 H  4.601011 1.439394 -1.844857
 C  6.351353 -0.929787 -0.107014
 H  6.300643 -1.116624 2.052742
 H  6.171437 -0.437325 -2.198265
 C  7.268081 -2.050640 -0.375103
 H  7.518906 -2.188292 -1.426831
 C  7.799802 -2.893293 0.521144
 H  7.597802 -2.828016 1.587541
 H  8.466604 -3.690614 0.204757
 H  0.668693 -2.839298 0.016638
 H  3.371843 2.906667 -0.369321
Sum of electronic and thermal Free
Energies= -1645.318390
SCF Energies= -1645.768515
S22.out
 O  -1.921553 -1.362127 1.661141
 C  -2.168264 -0.081067 1.033730
 C  -3.291440 -0.269456 -0.001176
```

```
 C  -2.774434 -1.252983 -1.056149
 C  -2.324666 -2.564938 -0.391659
 C  -1.372744 -2.321653 0.787567
 C  -2.438903 0.890108 2.167983
 H  -1.258328 0.251797 0.525936
 O  -3.802822 0.959445 -0.527911
 H  -4.151264 -0.721091 0.507301
 O  -3.808837 -1.508518 -2.003969
 H  -3.460654 -2.193170 -2.602143
 H  -1.897963 -0.818870 -1.557938
 O  -1.753291 -3.448689 -1.351321
 H  -3.213095 -3.067632 0.001825
 O  -0.124928 -1.908895 0.260734
 H  -1.248943 -3.234697 1.377550
 C  1.058608 -2.280521 0.967270
 O  2.042229 -2.621337 0.016695
 C  2.457947 -1.535214 -0.843722
 C  3.011073 -0.376089 -0.001937
 C  1.944110 0.059187 0.999465
 C  1.597698 -1.154629 1.860039
 H  0.868265 -3.182806 1.556768
 C  3.469480 -2.107869 -1.827879
 H  1.595884 -1.169280 -1.417057
 O  4.675161 -2.557971 -1.207566
 H  5.212942 -1.772882 -1.013923
 H  3.672545 -1.353758 -2.597771
 H  3.023743 -2.980657 -2.314757
 O  3.390227 0.668782 -0.891229
 H  3.379136 1.501391 -0.382596
 H  3.888409 -0.730222 0.560119
 O  2.455105 1.130416 1.797956
 H  1.698646 1.697867 2.022221
 H  1.056326 0.399566 0.456612
 O  0.675457 -0.846513 2.906759
 H  1.171238 -0.306625 3.547276
 H  2.520758 -1.540877 2.310128
 O  -1.214953 1.304610 2.780988
 H  -0.636993 0.513410 2.831294
 H  -3.110439 0.412279 2.897204
 H  -2.934293 1.784563 1.788527
 C  -3.114130 1.596628 -1.621276
 H  -3.800663 2.395909 -1.918625
 C  -1.768154 2.181308 -1.258524
 C  -0.600382 1.769429 -1.912625
 C  -1.661140 3.130238 -0.233826
 C  0.641681 2.292442 -1.560072
 H  -0.663821 1.022497 -2.700378
 C  -0.418534 3.627259 0.148111
 H  -2.557619 3.469316 0.277671
 C  0.756169 3.231274 -0.518357
 H  1.532212 1.931723 -2.061869
 H  -0.352599 4.347119 0.960186
 C  2.045405 3.809176 -0.101718
 H  2.050223 4.250947 0.894502
 C  3.169346 3.860253 -0.832727
 H  3.222273 3.477732 -1.849120
 H  4.073504 4.312274 -0.434719
 H  -0.865592 -3.096449 -1.548556
 H  -3.020559 0.909712 -2.468997
Sum of electronic and thermal Free
Energies= -1645.330492
SCF Energies= -1645.787558
S23.out
 O  0.153798 0.206650 0.756394
 C  1.490139 -0.064491 0.284084
 C  1.573205 -1.319402 -0.633426
 C  0.185020 -1.769400 -1.066463
 C  -0.628894 -0.533274 -1.458484
 C  -0.895566 0.308941 -0.193894
 C  2.127190 1.180240 -0.340225
 H  2.032790 -0.296498 1.201967
 O  2.213813 -2.414702 0.033707
 H  2.129552 -1.069656 -1.546073
 O  0.316741 -2.661869 -2.168116
 H  -0.573073 -2.722587 -2.560726
 H  -0.310869 -2.270497 -0.221584
 O  -1.839560 -0.892492 -2.116573
 H  -0.058667 0.057487 -2.181758
 O  -2.043501 -0.249733 0.416973
 H  -1.089924 1.358004 -0.441362
 C  -2.798740 0.632490 1.238044
 O  -3.411901 1.664363 0.496933
 C  -4.339489 1.215565 -0.518682
 C  -5.464954 0.377195 0.107733
 C  -4.866724 -0.770506 0.920435
 C  -3.850528 -0.232481 1.935935
 H  -2.143781 1.129942 1.958251
 C  -4.842845 2.477323 -1.199197
 H  -3.798919 0.607734 -1.254834
 O  -3.787252 3.171711 -1.863688
 H  -3.123357 3.375424 -1.183031
 H  -5.336000 3.120039 -0.454821
 H  -5.576783 2.204239 -1.960690
 O  -6.373550 -0.086752 -0.890264
 H  -5.876119 -0.669916 -1.490647
 H  -6.057511 1.009702 0.778459
 O  -5.918891 -1.461184 1.588820
 H  -5.482167 -2.078925 2.201564
 H  -4.344723 -1.451794 0.228086
 O  -3.261245 -1.289760 2.687322
 H  -2.682202 -1.779565 2.075679
 H  -4.379127 0.398173 2.656459
 O  2.231226 2.252734 0.597023
 H  2.909347 1.989855 1.243161
 H  1.514729 1.548621 -1.170010
 H  3.112081 0.914206 -0.742065
 C  3.576106 -2.645525 -0.362963
 H  3.616881 -2.878113 -1.435684
 C  4.490623 -1.483947 -0.045913
 C  5.186415 -0.813906 -1.060019
 C  4.596812 -1.004185 1.265720
 C  5.960236 0.310088 -0.779188
 H  5.107448 -1.168114 -2.084869
 C  5.355976 0.127998 1.548137
 H  4.061662 -1.509252 2.065644
 C  6.053802 0.810688 0.532477
 H  6.479251 0.810712 -1.591019
 H  5.418498 0.491952 2.570854
 C  6.840348 2.003247 0.890119
 H  6.773204 2.290566 1.939422
 C  7.608096 2.741017 0.076350
 H  7.734258 2.518619 -0.980584
 H  8.145115 3.606336 0.454831
 H  -2.450225 -1.192800 -1.417339
 H  3.873829 -3.541665 0.191004
Sum of electronic and thermal Free
```

Energies= -1645.316783
SCF Energies= -1645.767243
S24.out
O 2.765376 -1.621108 -0.309688
C 3.511193 -0.396977 -0.530123
C 2.750850 0.900942 -0.218832
C 1.908148 0.834505 1.082496
C 1.812435 -0.576835 1.674722
C 1.647662 -1.585928 0.545322
C 4.831028 -0.459665 0.238144
H 3.743322 -0.396463 -1.598995
O 1.972309 1.228175 -1.378155
H 3.499335 1.690157 -0.075191
O 2.474045 1.746272 2.026326
H 1.926317 1.684035 2.828260
H 0.888692 1.138825 0.829460
O 0.757031 -0.663046 2.628168
H 2.726713 -0.819012 2.220953
O 0.472690 -1.189296 -0.156911
H 1.520659 -2.602612 0.927865
C -0.080202 -2.164834 -1.023033
O -0.886659 -3.091604 -0.323521
C -2.003103 -2.505565 0.379131
C -2.907043 -1.754413 -0.605713
C -2.092961 -0.734489 -1.394467
C -0.887550 -1.393369 -2.070734
H 0.713777 -2.751511 -1.492458
C -2.728197 -3.637852 1.077778
H -1.632367 -1.800860 1.132985
O -1.865891 -4.165909 2.088287
H -2.342649 -4.895150 2.516972
H -2.992415 -4.406261 0.336922
H -3.656836 -3.244535 1.511186
O -3.934591 -1.102439 0.146945
H -4.386453 -0.500372 -0.469711
H -3.348424 -2.475563 -1.310469
O -2.982557 -0.143078 -2.345382
H -2.495620 0.567680 -2.794345
H -1.733877 0.026633 -0.692596
O -0.069113 -0.456127 -2.762774
H 0.466288 0.030255 -2.100517
H -1.248696 -2.107013 -2.817773
O 5.503922 -1.660003 -0.140979
H 6.323980 -1.700826 0.377029
H 4.653740 -0.431666 1.321550
H 5.424862 0.427058 -0.026764
C 1.646831 2.631097 -1.535330
H 1.530244 2.765144 -2.614655
C 0.373669 3.004199 -0.815886
C -0.842747 2.513634 -1.306227
C 0.370189 3.727242 0.382296
C -2.019462 2.656941 -0.581478
H -0.849258 1.975343 -2.249231
C -0.812155 3.890272 1.105502
H 1.303451 4.120806 0.775316
C -2.016961 3.316974 0.661076
H -2.942093 2.240764 -0.975181
H -0.796700 4.432802 2.047565
C -3.224282 3.387121 1.502561
H -3.270577 4.225399 2.197721
C -4.211766 2.480931 1.503220
H -4.182702 1.589823 0.878721
H -5.071190 2.589295 2.159379
H -0.070747 -0.471419 2.152629
H 2.493277 3.240976 -1.197697
Sum of electronic and thermal Free Energies= -1645.320461
SCF Energies= -1645.775585
S25.out
O 3.237422 -0.680864 0.578807
C 2.975249 0.326491 -0.429427
C 2.575315 1.645242 0.260638
C 1.377347 1.404048 1.196318
C 1.729801 0.283384 2.168593
C 2.136955 -0.980685 1.403946
C 4.241546 0.454326 -1.250245
H 2.164902 -0.030715 -1.073973
O 2.399433 2.747476 -0.636250
H 3.416302 1.961123 0.888908
O 1.077268 2.561839 1.976876
H 0.443420 3.091481 1.464571
H 0.495859 1.098778 0.627565
O 0.652661 0.001608 3.061871
H 2.612166 0.584216 2.750253
O 1.094229 -1.487680 0.576445
H 2.470370 -1.757229 2.098987
C 0.305184 -2.559555 1.059497
O -0.900430 -2.103390 1.627374
C -1.739854 -1.396355 0.684206
C -2.246840 -2.403348 -0.357901
C -1.016088 -2.918851 -1.102424
C 0.015100 -3.499005 -0.120574
H 0.835447 -3.092902 1.853628
C -2.765132 -0.664161 1.525691
H -1.146349 -0.634823 0.166951
O -2.144147 0.421317 2.219537
H -1.257858 0.115087 2.503144
H -3.238147 -1.370038 2.225100
H -3.543001 -0.231862 0.891724
O -3.116512 -1.810080 -1.323882
H -3.956797 -1.598505 -0.884601
H -2.748173 -3.238814 0.150204
O -1.411452 -3.918865 -2.039334
H -0.585549 -4.276236 -2.410386
H -0.559606 -2.065967 -1.630071
O 1.214939 -3.861530 -0.797469
H 1.693175 -3.027283 -0.962935
H -0.401634 -4.423135 0.291008
O 4.420067 -0.760107 -1.983129
H 5.245824 -0.671080 -2.486072
H 5.088179 0.641984 -0.574149
H 4.146698 1.315679 -1.923363
C 1.525692 2.598510 -1.772095
H 1.797009 1.721154 -2.369244
C 0.056774 2.556447 -1.422968
C -0.743863 1.473841 -1.806087
C -0.526528 3.591929 -0.679958
C -2.089509 1.417973 -1.453868
H -0.302792 0.655092 -2.370044
C -1.867986 3.528549 -0.308643
H 0.078901 4.445908 -0.383902
C -2.677481 2.440541 -0.687291
H -2.670206 0.550243 -1.744945
H -2.301666 4.334122 0.278810
C -4.087623 2.417434 -0.266096
H -4.387697 3.257125 0.360776

```
 C  -5.007636 1.490264 -0.571134
 H  -4.791492 0.625472 -1.194031
 H  -6.024386 1.574111 -0.197607
 H  0.473591 0.841745 3.521915
 H  1.743132 3.485365 -2.376057
Sum of electronic and thermal Free
Energies= -1645.328932
SCF Energies= -1645.782766
S26.out
 O  0.573489 0.117509 -0.598749
 C  -0.426972 0.224400 0.433103
 C  -1.156748 1.575228 0.322456
 C  -0.164391 2.737624 0.280359
 C  0.901489 2.497094 -0.795405
 C  1.556804 1.129763 -0.590716
 C  -1.381341 -0.945739 0.218773
 H  0.057576 0.133130 1.412482
 O  -2.025594 1.706063 1.450024
 H  -1.729298 1.580008 -0.613426
 O  -0.886755 3.938450 0.007726
 H  -0.218767 4.641042 -0.078244
 H  0.330862 2.808262 1.259004
 O  1.874402 3.539813 -0.812626
 H  0.422669 2.505250 -1.778288
 O  2.258893 1.246242 0.639893
 H  2.219072 0.889122 -1.422925
 C  3.406447 0.486067 1.024103
 O  3.086291 -0.788819 1.525922
 C  2.815314 -1.822151 0.556110
 C  4.054737 -2.041273 -0.312783
 C  4.400369 -0.734500 -1.025441
 C  4.552124 0.405187 -0.009982
 H  3.766524 1.046210 1.888425
 C  2.388525 -3.049263 1.351112
 H  1.985700 -1.509266 -0.084419
 O  1.233987 -2.795431 2.146410
 H  0.501326 -2.569126 1.529058
 H  3.193448 -3.334402 2.037890
 H  2.226410 -3.881377 0.652715
 O  3.761111 -3.073280 -1.254207
 H  4.507352 -3.099039 -1.877662
 H  4.901964 -2.328314 0.328699
 O  5.624833 -0.935590 -1.732615
 H  5.814463 -0.102878 -2.198363
 H  3.594894 -0.515839 -1.739107
 O  4.835558 1.660072 -0.621821
 H  4.021453 2.020205 -1.013284
 H  5.444148 0.165954 0.578366
 O  -0.716388 -2.215168 0.226284
 H  -0.116133 -2.231352 -0.539224
 H  -1.923106 -0.814966 -0.726749
 H  -2.106736 -0.968085 1.032034
 C  -3.354420 2.183136 1.141296
 H  -3.293038 3.084451 0.522598
 C  -4.190416 1.120521 0.472506
 C  -4.665115 0.029756 1.218608
 C  -4.438733 1.145593 -0.903340
 C  -5.355577 -1.009709 0.608426
 H  -4.479639 -0.001970 2.289671
 C  -5.133825 0.103929 -1.519884
 H  -4.084445 1.984632 -1.496882
 C  -5.598235 -0.997326 -0.780925
 H  -5.713081 -1.836775 1.214517
 H  -5.315265 0.139150 -2.591365
 C  -6.312654 -2.076951 -1.482800
 H  -6.472298 -1.898682 -2.546262
 C  -6.762037 -3.223941 -0.954956
 H  -6.636289 -3.480735 0.094046
 H  -7.276670 -3.955056 -1.572249
 H  2.384623 3.450161 0.013545
 H  -3.778382 2.456719 2.111776
Sum of electronic and thermal Free
Energies= -1645.322762
SCF Energies= -1645.77842
S27.out
 O  -0.042829 1.439435 1.398246
 C  1.181930 0.675426 1.380753
 C  2.373610 1.597348 1.025324
 C  2.101559 2.414144 -0.237754
 C  0.737524 3.108977 -0.144980
 C  -0.347626 2.077172 0.177005
 C  1.352916 0.076655 2.773721
 H  1.078444 -0.125918 0.645755
 O  3.620025 0.885130 1.008794
 H  2.488247 2.313227 1.849009
 O  3.154522 3.367592 -0.384398
 H  2.907627 3.923722 -1.144115
 H  2.066399 1.757756 -1.113233
 O  0.450145 3.826754 -1.342817
 H  0.759251 3.846735 0.661825
 O  -0.352519 1.196784 -0.940950
 H  -1.316719 2.554674 0.313836
 C  -1.438338 0.358591 -1.311354
 O  -1.456778 -0.876992 -0.628790
 C  -2.092788 -0.929716 0.666025
 C  -3.552322 -0.503252 0.532051
 C  -3.597724 0.924609 -0.001148
 C  -2.837348 1.027799 -1.323004
 H  -1.178891 0.090035 -2.337267
 C  -1.928039 -2.360515 1.149297
 H  -1.579217 -0.256799 1.358691
 O  -0.554573 -2.680064 1.407411
 H  -0.058005 -2.514713 0.586582
 H  -2.343214 -3.054634 0.405850
 H  -2.460269 -2.490356 2.093218
 O  -4.160931 -0.582755 1.818841
 H  -5.025072 -0.143008 1.737537
 H  -4.061655 -1.168043 -0.182335
 O  -4.973756 1.266634 -0.179460
 H  -5.005169 2.209290 -0.414144
 H  -3.144343 1.582708 0.751906
 O  -2.778337 2.404708 -1.679623
 H  -2.322018 2.477244 -2.534944
 H  -3.422098 0.463279 -2.062974
 O  0.244186 -0.704446 3.201446
 H  0.097212 -1.428164 2.550427
 H  1.458213 0.890425 3.500439
 H  2.284919 -0.504459 2.780930
 C  4.036679 0.229931 -0.207382
 H  5.051348 -0.107358 0.024435
 C  3.169489 -0.945305 -0.597241
 C  2.358186 -0.908032 -1.739140
 C  3.116827 -2.079289 0.223468
 C  1.481763 -1.949632 -2.030725
 H  2.403349 -0.047925 -2.401786
 C  2.253236 -3.130840 -0.071904
```

```
 H  3.746026 -2.130070 1.108451
 C  1.395449 -3.073076 -1.188577
 H  0.861696 -1.892772 -2.920460
 H  2.214258 -3.997426 0.583247
 C  0.420087 -4.157015 -1.407611
 H  0.656876 -5.101518 -0.918455
 C  -0.727234 -4.050117 -2.092338
 H  -1.043670 -3.120624 -2.558943
 H  -1.397058 -4.899386 -2.194769
 H  0.237268 3.156206 -2.017548
 H  4.106012 0.952450 -1.027665
Sum of electronic and thermal Free
Energies= -1645.329695
SCF Energies= -1645.787016
S28.out
 O  -0.043887 0.043750 -1.281421
 C  -0.817313 -0.352944 -0.123506
 C  -1.374396 0.891583 0.586615
 C  -0.248199 1.882380 0.888843
 C  0.515022 2.191530 -0.392135
 C  1.049175 0.890504 -1.010884
 C  -1.910910 -1.271946 -0.629203
 H  -0.175480 -0.906868 0.571291
 O  -1.993997 0.494548 1.812669
 H  -2.098515 1.379736 -0.076215
 O  -0.750772 3.127230 1.383534
 H  -0.999703 2.989311 2.312246
 H  0.431871 1.432725 1.623611
 O  1.574043 3.123262 -0.173682
 H  -0.189348 2.606340 -1.127133
 O  1.933948 0.137846 -0.180508
 H  1.521018 1.093345 -1.974134
 C  3.087839 0.700949 0.444985
 O  3.597114 -0.292033 1.305715
 C  4.071687 -1.491062 0.652406
 C  5.201546 -1.140996 -0.316461
 C  4.726986 -0.075470 -1.299654
 C  4.182337 1.136447 -0.549568
 H  2.803217 1.531531 1.092177
 C  4.509833 -2.421738 1.771455
 H  3.249617 -1.956897 0.097289
 O  3.412021 -2.800140 2.601185
 H  3.018724 -1.972298 2.926095
 H  5.303041 -1.933028 2.356843
 H  4.915764 -3.339780 1.339803
 O  5.578993 -2.336727 -0.997735
 H  6.191208 -2.065889 -1.703643
 H  6.051895 -0.735550 0.253345
 O  5.847845 0.268832 -2.117462
 H  5.519855 0.865686 -2.810766
 H  3.923839 -0.501596 -1.916679
 O  3.732098 2.078878 -1.516922
 H  3.157133 2.727563 -1.060962
 H  4.994190 1.565604 0.056873
 O  -1.297664 -2.448645 -1.163878
 H  -2.016473 -3.043479 -1.432270
 H  -2.503492 -0.748828 -1.394018
 H  -2.574189 -1.517003 0.207529
 C  -3.290584 1.086897 2.057480
 H  -3.240707 2.168329 1.889678
 C  -4.369117 0.457665 1.211221
 C  -4.841765 1.086024 0.050252
 C  -4.856799 -0.817139 1.526003
 C  -5.765322 0.457252 -0.781134
 H  -4.478986 2.078840 -0.203927
 C  -5.780601 -1.448530 0.697705
 H  -4.500410 -1.320044 2.421863
 C  -6.250488 -0.828100 -0.475851
 H  -6.107550 0.970103 -1.675010
 H  -6.148007 -2.438616 0.957037
 C  -7.220907 -1.547234 -1.318535
 H  -7.493996 -2.535637 -0.949131
 C  -7.780843 -1.118636 -2.458247
 H  -7.564306 -0.146892 -2.895304
 H  -8.487895 -1.743351 -2.996993
 H  1.233259 3.809314 0.427568
 H  -3.476586 0.908292 3.120277
Sum of electronic and thermal Free
Energies= -1645.313941
SCF Energies= -1645.763925
S29.out
 O  3.101848 -0.660001 -1.047149
 C  3.451520 0.737826 -0.887956
 C  2.676410 1.489001 0.200867
 C  2.489352 0.689710 1.515452
 C  2.745749 -0.816127 1.356049
 C  2.353773 -1.290322 -0.035873
 C  4.957784 0.846901 -0.657332
 H  3.214145 1.206832 -1.847851
 O  1.409405 1.881545 -0.340882
 H  3.248873 2.392996 0.441402
 O  3.354767 1.253101 2.503585
 H  3.241229 0.718870 3.308977
 H  1.442252 0.804720 1.817232
 O  2.091593 -1.571016 2.372150
 H  3.815127 -1.007700 1.477838
 O  0.960894 -1.036347 -0.189286
 H  2.544888 -2.362134 -0.145300
 C  0.353385 -1.747051 -1.258225
 O  -0.312348 -2.900181 -0.783997
 C  -1.388741 -2.620455 0.135215
 C  -2.469599 -1.802459 -0.579238
 C  -1.859327 -0.526273 -1.148812
 C  -0.610155 -0.802213 -1.987152
 H  1.119235 -2.106267 -1.949619
 C  -1.900415 -3.954231 0.639330
 H  -1.006199 -2.040431 0.985117
 O  -0.872240 -4.556113 1.430041
 H  -1.225267 -5.396761 1.763667
 H  -2.164836 -4.587485 -0.220271
 H  -2.808379 -3.781691 1.230891
 O  -3.493087 -1.492949 0.369194
 H  -4.036420 -0.781849 -0.017038
 H  -2.877648 -2.399998 -1.409007
 O  -2.871057 0.100800 -1.943866
 H  -2.583714 1.018141 -2.083206
 H  -1.582913 0.119702 -0.307473
 O  0.037350 0.401621 -2.381161
 H  0.435812 0.810918 -1.581283
 H  -0.923286 -1.304925 -2.907832
 O  5.616220 0.192762 -1.742034
 H  6.569475 0.233819 -1.562643
 H  5.231544 0.392875 0.305126
 H  5.227366 1.911997 -0.617730
 C  0.793602 2.996204 0.352215
 H  0.980390 3.903982 -0.233722
```

```
 C  -0.679680 2.733458 0.503832
 C  -1.576484 3.086231 -0.513968
 C  -1.175710 2.082839 1.640306
 C  -2.928865 2.769326 -0.413745
 H  -1.209327 3.614842 -1.390019
 C  -2.525495 1.751924 1.736889
 H  -0.499392 1.825256 2.451121
 C  -3.420828 2.060857 0.698484
 H  -3.608336 3.067267 -1.207011
 H  -2.890262 1.224018 2.614260
 C  -4.813858 1.593412 0.793529
 H  -5.153278 1.347490 1.799451
 C  -5.649576 1.395572 -0.236830
 H  -5.358840 1.579271 -1.267843
 H  -6.659957 1.031485 -0.072334
 H  1.134804 -1.507295 2.199129
 H  1.259112 3.121479 1.334989
Sum of electronic and thermal Free
Energies= -1645.326026
SCF Energies= -1645.778453
S3.out
 O  -0.978415 -2.149280 1.612109
 C  -2.071627 -1.315395 1.160428
 C  -2.684574 -1.899644 -0.125590
 C  -1.603823 -2.071555 -1.192043
 C  -0.414193 -2.855000 -0.624500
 C  0.083633 -2.243684 0.685524
 C  -3.053267 -1.267394 2.318291
 H  -1.695586 -0.306285 0.976228
 O  -3.827953 -1.127719 -0.524836
 H  -3.080424 -2.896297 0.108130
 O  -2.161624 -2.767551 -2.306341
 H  -1.415937 -2.953009 -2.904424
 H  -1.228057 -1.088730 -1.503446
 O  0.623436 -2.969945 -1.594124
 H  -0.739513 -3.875821 -0.405027
 O  0.641185 -0.967980 0.405311
 H  0.835895 -2.888872 1.147118
 C  1.594888 -0.543561 1.368497
 O  2.866286 -1.106188 1.110180
 C  3.432764 -0.733585 -0.165372
 C  3.608450 0.784189 -0.229048
 C  2.273644 1.482475 0.032176
 C  1.664969 0.987443 1.347314
 H  1.306213 -0.897815 2.361758
 C  4.738427 -1.503027 -0.275652
 H  2.763434 -1.056106 -0.970564
 O  4.510119 -2.911846 -0.308221
 H  3.991668 -3.121476 0.487451
 H  5.395210 -1.224672 0.562151
 H  5.239241 -1.238265 -1.209892
 O  4.114218 1.110163 -1.523033
 H  4.108267 2.081138 -1.581868
 H  4.317616 1.095007 0.553537
 O  2.534362 2.884195 0.066219
 H  1.681891 3.341877 0.195164
 H  1.586135 1.242442 -0.793117
 O  0.398490 1.575236 1.620989
 H  -0.181966 1.397188 0.860725
 H  2.321516 1.290197 2.168514
 O  -2.484332 -0.620317 3.456868
 H  -1.653874 -1.088578 3.649219
 H  -3.377219 -2.290622 2.561774
 H  -3.931463 -0.687743 2.026538
 C  -3.696566 -0.150063 -1.570440
 H  -4.727278 0.183214 -1.731813
 C  -2.821883 1.041943 -1.246979
 C  -3.012449 1.783319 -0.071578
 C  -1.818515 1.442975 -2.135671
 C  -2.215801 2.888623 0.210283
 H  -3.791657 1.489290 0.626596
 C  -1.024598 2.556347 -1.862563
 H  -1.655040 0.875243 -3.048469
 C  -1.199000 3.291698 -0.678886
 H  -2.388653 3.454296 1.120900
 H  -0.247750 2.850712 -2.563579
 C  -0.304986 4.429129 -0.402899
 H  0.190618 4.853064 -1.276102
 C  -0.025786 4.937141 0.807524
 H  -0.450825 4.531287 1.721835
 H  0.651743 5.779561 0.915481
 H  0.946513 -2.068891 -1.773188
 H  -3.355151 -0.625713 -2.495498
Sum of electronic and thermal Free
Energies= -1645.335788
SCF Energies= -1645.790897
S30.out
 O  1.051710 -2.047588 1.549050
 C  -0.247480 -1.420487 1.475940
 C  -0.901732 -1.685348 0.105186
 C  0.052002 -1.363587 -1.051033
 C  1.402732 -2.038767 -0.828285
 C  1.953448 -1.641154 0.539880
 C  -1.008020 -2.012100 2.659854
 H  -0.144883 -0.336691 1.615483
 O  -2.060262 -0.862801 -0.028053
 H  -1.171049 -2.749042 0.046397
 O  -0.499736 -1.722351 -2.320190
 H  -0.674891 -2.680459 -2.304091
 H  0.200788 -0.280781 -1.096453
 O  2.342440 -1.687403 -1.842253
 H  1.256946 -3.128487 -0.808477
 O  2.150273 -0.237345 0.574474
 H  2.893670 -2.160091 0.741011
 C  3.299631 0.168245 1.302871
 O  4.478140 -0.152682 0.597736
 C  4.531120 0.481877 -0.700360
 C  4.669374 1.998790 -0.508555
 C  3.425628 2.479882 0.239248
 C  3.208068 1.679123 1.533125
 H  3.351982 -0.368851 2.254604
 C  5.622446 -0.218451 -1.487719
 H  3.588431 0.300562 -1.226246
 O  5.314296 -1.604998 -1.656014
 H  4.356453 -1.674812 -1.844625
 H  6.580161 -0.162456 -0.958684
 H  5.735400 0.286056 -2.458068
 O  4.707851 2.683745 -1.762517
 H  5.607619 2.597506 -2.117457
 H  5.564577 2.221675 0.087786
 O  3.565062 3.866465 0.542369
 H  2.805141 4.092160 1.107231
 H  2.556811 2.321548 -0.419318
 O  1.984403 2.048488 2.164703
 H  1.264904 1.706178 1.603832
 H  4.005838 1.947336 2.231991
```

```
 O  -2.217486 -1.281387 2.863657
 H  -2.702866 -1.727346 3.576049
 H  -0.357406 -1.945071 3.543029
 H  -1.210548 -3.074745 2.467008
 C  -3.275637 -1.583104 -0.280522
 H  -3.433377 -2.320183 0.519905
 C  -4.411521 -0.593953 -0.315246
 C  -5.258160 -0.500472 -1.427056
 C  -4.639123 0.257109 0.774510
 C  -6.309046 0.413393 -1.452521
 H  -5.089463 -1.148146 -2.283854
 C  -5.684205 1.176443 0.747159
 H  -3.988375 0.199375 1.642061
 C  -6.543632 1.273392 -0.363787
 H  -6.945285 0.462640 -2.331289
 H  -5.844815 1.831721 1.600043
 C  -7.633950 2.263175 -0.335678
 H  -7.668061 2.872751 0.567452
 C  -8.558180 2.477687 -1.282170
 H  -8.596692 1.910907 -2.209404
 H  -9.319722 3.241604 -1.151617
 H  1.884361 -1.797749 -2.694531
 H  -3.201747 -2.124412 -1.232504
Sum of electronic and thermal Free
Energies= -1645.320924
SCF Energies= -1645.771895
S32.out
 O  -1.253210 0.190574 -1.206223
 C  0.037702 0.633493 -0.747180
 C  1.100917 -0.421236 -1.087151
 C  0.706791 -1.780894 -0.514759
 C  -0.714855 -2.156009 -0.947204
 C  -1.693929 -1.019570 -0.630166
 C  0.318117 1.968144 -1.419418
 H  0.006960 0.777799 0.340509
 O  2.348057 -0.018624 -0.520880
 H  1.179596 -0.505528 -2.178639
 O  1.652904 -2.748660 -0.969124
 H  1.345764 -3.608774 -0.633854
 H  0.734611 -1.711973 0.582522
 O  -1.136915 -3.384911 -0.356659
 H  -0.723242 -2.316839 -2.028750
 O  -1.769161 -0.961265 0.786448
 H  -2.667913 -1.220222 -1.079195
 C  -2.880405 -0.391753 1.475441
 O  -3.041592 0.991703 1.254241
 C  -3.825490 1.447528 0.126724
 C  -5.208674 0.795272 0.135939
 C  -5.073240 -0.721187 0.134258
 C  -4.210310 -1.170844 1.315857
 H  -2.563615 -0.475038 2.516193
 C  -3.882471 2.962545 0.274793
 H  -3.311740 1.209272 -0.810064
 O  -4.562481 3.373636 1.461287
 H  -4.116143 2.926139 2.200593
 H  -4.430365 3.385831 -0.570488
 H  -2.856211 3.351590 0.252255
 O  -5.902387 1.256121 -1.023493
 H  -6.754438 0.787857 -1.039751
 H  -5.738335 1.097386 1.050191
 O  -6.385521 -1.275016 0.240699
 H  -6.275938 -2.241342 0.267684
 H  -4.618652 -1.031713 -0.816957
 O  -4.014925 -2.581001 1.334263
 H  -3.477153 -2.827726 0.561294
 H  -4.787083 -0.946167 2.219077
 O  -0.611627 2.983613 -1.036873
 H  -0.512682 3.124156 -0.080019
 H  0.223699 1.857535 -2.504258
 H  1.348943 2.265651 -1.188993
 C  3.432188 0.069316 -1.460726
 H  3.315985 0.961677 -2.090555
 C  4.721051 0.117752 -0.684378
 C  5.053590 -0.939512 0.172715
 C  5.602378 1.200289 -0.790389
 C  6.239237 -0.912108 0.900884
 H  4.373583 -1.782803 0.264894
 C  6.792740 1.226501 -0.067255
 H  5.353012 2.031322 -1.445630
 C  7.135402 0.169786 0.796182
 H  6.483532 -1.740548 1.561520
 H  7.455053 2.080518 -0.172972
 C  8.376569 0.144176 1.588916
 H  8.496674 -0.742083 2.212199
 C  9.340391 1.075276 1.617150
 H  9.300177 1.988223 1.027821
 H  10.216664 0.946755 2.246454
 H  -1.209492 -3.220167 0.601358
 H  3.417411 -0.811925 -2.115343
Sum of electronic and thermal Free
Energies= -1645.319869
SCF Energies= -1645.771189
S33.out
 O  -0.989936 -0.722980 0.954667
 C  -2.124594 -1.616911 0.911150
 C  -2.345122 -2.304474 -0.465361
 C  -1.112863 -2.167408 -1.358639
 C  0.137633 -2.374300 -0.496718
 C  0.264776 -1.187272 0.477302
 C  -2.027810 -2.617954 2.064886
 H  -2.970414 -0.961295 1.113463
 O  -3.585291 -1.935968 -1.084646
 H  -2.470456 -3.378906 -0.285907
 O  -1.198488 -3.135977 -2.398507
 H  -0.319802 -3.148020 -2.818927
 H  -1.051451 -1.159496 -1.785802
 O  1.307726 -2.508867 -1.296577
 H  0.048669 -3.309444 0.062458
 O  0.844508 -0.136899 -0.278681
 H  0.912855 -1.428633 1.324483
 C  1.459883 0.911234 0.465109
 O  2.453522 0.433224 1.344126
 C  3.539321 -0.277220 0.705738
 C  4.256472 0.658974 -0.271669
 C  3.249591 1.210331 -1.277662
 C  2.070911 1.874540 -0.559898
 H  0.716724 1.408660 1.094587
 C  4.438350 -0.779743 1.815530
 H  3.141031 -1.136510 0.152908
 O  3.712849 -1.762220 2.558972
 H  4.289062 -2.059303 3.281967
 H  4.733293 0.066474 2.452729
 H  5.345041 -1.207163 1.368975
 O  5.280948 -0.087177 -0.927758
 H  5.656914 0.499384 -1.606438
 H  4.688333 1.501678 0.289063
```

O 3.934683 2.148045 -2.106678
H 3.268098 2.514573 -2.713429
H 2.871907 0.373329 -1.884212
O 1.117901 2.367857 -1.497394
H 0.664798 1.595286 -1.879391
H 2.439110 2.746289 -0.011682
O -1.854821 -1.942711 3.308315
H -1.121757 -1.317312 3.168452
H -1.211817 -3.335961 1.893731
H -2.963078 -3.183122 2.128387
C -3.644154 -0.731683 -1.876035
H -4.659507 -0.750831 -2.283744
C -3.418360 0.538677 -1.087792
C -4.320339 0.912946 -0.082407
C -2.285297 1.334384 -1.294129
C -4.073060 2.025437 0.716953
H -5.209943 0.311584 0.088168
C -2.034970 2.450118 -0.499781
H -1.584385 1.070656 -2.081879
C -2.913266 2.804353 0.539115
H -4.776875 2.291605 1.501918
H -1.139900 3.033493 -0.683357
C -2.664631 3.939092 1.444231
H -3.497550 4.191337 2.100612
C -1.533547 4.651136 1.546946
H -0.651486 4.446795 0.944392
H -1.454419 5.469316 2.257474
H 1.552287 -1.606673 -1.576730
H -2.947646 -0.793951 -2.720197

Sum of electronic and thermal Free Energies= -1645.315404
SCF Energies= -1645.767968

S34.out

O 0.417304 1.762713 0.457843
C -1.011661 1.769136 0.633735
C -1.731490 0.747896 -0.289481
C -0.740224 -0.236572 -0.894485
C 0.240752 -0.681492 0.194406
C 1.105519 0.527803 0.614500
C -1.415028 1.598845 2.095025
H -1.294992 2.777076 0.319167
O -2.414259 1.385475 -1.371338
H -2.448807 0.163587 0.301941
O -1.459917 -1.350621 -1.412705
H -0.790671 -2.039601 -1.576443
H -0.177698 0.265598 -1.695639
O 1.039007 -1.777028 -0.241574
H -0.325368 -1.049892 1.054568
O 2.195797 0.569545 -0.282415
H 1.471679 0.425450 1.641436
C 3.367838 1.202774 0.207320
O 3.946854 0.493553 1.286932
C 4.340350 -0.856848 0.975828
C 5.356612 -0.848936 -0.172297
C 4.810425 -0.098674 -1.382401
C 4.356175 1.297943 -0.963076
H 3.122972 2.191486 0.606584
C 4.917639 -1.436750 2.267744
H 3.463622 -1.445716 0.683653
O 5.156619 -2.838110 2.160135
H 5.645946 -2.962550 1.323853
H 4.193094 -1.292184 3.075253
H 5.834811 -0.888393 2.532753
O 5.647445 -2.214233 -0.498495
H 6.376526 -2.205374 -1.141734
H 6.268992 -0.338889 0.168943
O 5.853418 -0.030972 -2.354150
H 5.502786 0.488618 -3.097847
H 3.949097 -0.651729 -1.783856
O 3.788136 1.925703 -2.107776
H 3.752377 2.881043 -1.934519
H 5.231024 1.854837 -0.604278
O -0.748777 2.600439 2.862093
H -1.005139 2.467495 3.789130
H -1.160399 0.592241 2.456146
H -2.509139 1.704236 2.154753
C -3.676185 1.960501 -1.009641
H -4.000664 2.495717 -1.908684
C -4.709523 0.929159 -0.609240
C -4.831525 -0.270266 -1.328422
C -5.566287 1.151160 0.472180
C -5.790648 -1.214465 -0.982656
H -4.150476 -0.467994 -2.150698
C -6.535929 0.207875 0.815243
H -5.474841 2.066892 1.051616
C -6.670270 -0.992310 0.096520
H -5.854805 -2.135510 -1.554399
H -7.194913 0.398449 1.658928
C -7.706580 -1.955743 0.504254
H -8.276410 -1.660489 1.385526
C -8.009959 -3.119929 -0.086838
H -7.495299 -3.485821 -0.971983
H -8.800897 -3.751810 0.307683
H 1.729456 -1.400171 -0.818980
H -3.554882 2.705026 -0.210585

Sum of electronic and thermal Free Energies= -1645.314140
SCF Energies= -1645.761742

S4.out

O -1.906783 2.396085 -0.540711
C -2.620223 1.194767 -0.905866
C -3.110651 0.392920 0.320578
C -2.003523 0.233687 1.363187
C -1.317067 1.575534 1.641734
C -0.819340 2.181501 0.334715
C -3.767670 1.663510 -1.790646
H -1.962285 0.548805 -1.496127
O -3.643454 -0.814343 -0.255608
H -3.932774 0.937931 0.802839
O -2.569420 -0.274856 2.572486
H -1.834801 -0.318486 3.210029
H -1.236386 -0.448606 0.985764
O -0.265973 1.411057 2.591250
H -2.031647 2.270928 2.089976
O 0.117420 1.262963 -0.207214
H -0.352184 3.157281 0.493146
C 1.022656 1.798804 -1.155511
O 2.093863 2.474367 -0.524893
C 2.873633 1.649689 0.369555
C 3.496442 0.483139 -0.400921
C 2.415770 -0.295871 -1.143910
C 1.545063 0.628536 -1.998004
H 0.521129 2.542899 -1.779997
C 3.903671 2.576349 0.994607
H 2.224874 1.255364 1.159749
O 3.283620 3.592352 1.782700

```
 H  2.662677 4.053845 1.193417
 H  4.527580 3.013099 0.200645
 H  4.548752 2.001905 1.664059
 O  4.164557 -0.356638 0.542625
 H  4.340405 -1.199107 0.087125
 H  4.209555 0.879563 -1.140258
 O  3.081552 -1.268448 -1.950788
 H  2.398789 -1.870616 -2.290198
 H  1.781300 -0.794036 -0.398074
 O  0.485951 -0.085901 -2.629773
 H  -0.027482 -0.519794 -1.924955
 H  2.156331 1.047565 -2.802280
 O  -4.686806 2.505125 -1.093445
 H  -4.162672 3.237323 -0.725610
 H  -4.331156 0.795550 -2.140379
 H  -3.347409 2.180788 -2.664579
 C  -3.468674 -2.086538 0.389927
 H  -4.171614 -2.740195 -0.137902
 C  -2.058456 -2.625939 0.262488
 C  -1.418853 -2.633478 -0.984088
 C  -1.343901 -3.067240 1.383159
 C  -0.090344 -3.037317 -1.098457
 H  -1.958416 -2.296935 -1.865501
 C  -0.010672 -3.457744 1.274250
 H  -1.825685 -3.067769 2.357066
 C  0.651249 -3.424439 0.033949
 H  0.390468 -3.029248 -2.073537
 H  0.523605 -3.785652 2.161417
 C  2.080490 -3.746371 -0.115829
 H  2.391052 -4.016492 -1.124557
 C  3.009595 -3.679293 0.848044
 H  2.774368 -3.372909 1.864613
 H  4.047475 -3.924661 0.640244
 H  0.395450 0.823382 2.183486
 H  -3.770693 -2.041063 1.439577
Sum of electronic and thermal Free
Energies= -1645.331925
SCF Energies= -1645.787313
S5.out
 O  -1.986011 -0.477919 2.161969
 C  -2.345169 0.427242 1.086606
 C  -3.097931 -0.346333 -0.016388
 C  -2.210703 -1.486750 -0.517053
 C  -1.815737 -2.367377 0.677320
 C  -1.143237 -1.533417 1.780161
 C  -3.182087 1.510999 1.742432
 H  -1.432221 0.875621 0.687613
 O  -3.622028 0.518934 -1.031602
 H  -3.991392 -0.791344 0.438671
 O  -2.929873 -2.252859 -1.481733
 H  -2.357924 -3.013614 -1.688539
 H  -1.294290 -1.082644 -0.964059
 O  -1.047473 -3.490803 0.272863
 H  -2.731764 -2.776527 1.116160
 O  0.105717 -0.963486 1.362938
 H  -0.980524 -2.144886 2.673593
 C  1.266649 -1.759132 1.498664
 O  1.559890 -2.455964 0.297678
 C  1.880257 -1.597231 -0.821533
 C  3.179425 -0.862911 -0.491898
 C  2.916600 0.018706 0.729960
 C  2.426446 -0.832095 1.907432
 H  1.111767 -2.534052 2.253995
 C  1.929041 -2.470911 -2.054213
 H  1.078054 -0.864356 -0.952181
 O  0.583532 -2.877403 -2.334325
 H  0.617847 -3.550049 -3.033792
 H  2.577809 -3.337653 -1.870175
 H  2.346668 -1.892091 -2.886882
 O  3.583182 -0.084506 -1.616173
 H  4.261801 0.530785 -1.286176
 H  3.955611 -1.602709 -0.243592
 O  4.135452 0.694507 1.048377
 H  3.894570 1.509636 1.518504
 H  2.142739 0.751681 0.471696
 O  2.054183 -0.032014 3.023524
 H  1.195888 0.369035 2.792254
 H  3.255682 -1.464527 2.238272
 O  -2.403830 2.292653 2.649475
 H  -2.016381 1.667654 3.286071
 H  -4.039710 1.046117 2.251511
 H  -3.562553 2.191993 0.980374
 C  -2.791447 0.877046 -2.154963
 H  -3.471744 1.441912 -2.800170
 C  -1.588308 1.712498 -1.787483
 C  -0.290910 1.246931 -2.032473
 C  -1.745212 2.934082 -1.120206
 C  0.821640 1.951458 -1.581216
 H  -0.150952 0.306310 -2.560544
 C  -0.636499 3.629876 -0.645986
 H  -2.744229 3.321770 -0.939669
 C  0.669357 3.142139 -0.846366
 H  1.809221 1.547469 -1.773249
 H  -0.778477 4.559132 -0.099549
 C  1.804600 3.876498 -0.263059
 H  1.530490 4.788207 0.267864
 C  3.098990 3.527755 -0.304999
 H  3.452318 2.635059 -0.810879
 H  3.855342 4.144147 0.173020
 H  -0.187101 -3.173174 -0.073948
 H  -2.483057 -0.022436 -2.698550
Sum of electronic and thermal Free
Energies= -1645.334544
SCF Energies= -1645.790379
S6.out
 O  -0.634623 2.251555 -1.191556
 C  -0.074856 2.150464 0.142050
 C  1.061769 1.114080 0.181205
 C  0.539398 -0.222498 -0.338665
 C  -0.087466 -0.027663 -1.725297
 C  -1.176894 1.055541 -1.690629
 C  0.361975 3.562058 0.498855
 H  -0.861509 1.837248 0.838173
 O  1.495013 0.956870 1.535724
 H  1.890258 1.444669 -0.457763
 O  1.612157 -1.157677 -0.416020
 H  1.228521 -1.959765 -0.812374
 H  -0.224947 -0.587799 0.359710
 O  -0.523118 -1.254689 -2.293397
 H  0.691993 0.349110 -2.396201
 O  -2.292015 0.716999 -0.854652
 H  -1.537066 1.268423 -2.702666
 C  -3.267433 -0.160340 -1.374665
 O  -2.984581 -1.516927 -1.057073
 C  -2.950514 -1.816420 0.357400
 C  -4.327868 -1.540540 0.963717
```

```
 C  -4.689828 -0.078021 0.710013
 C  -4.621992 0.249571 -0.784073
 H  -3.285412 -0.114201 -2.466950
 C  -2.495507 -3.255226 0.478797
 H  -2.214964 -1.170040 0.849051
 O  -1.137746 -3.315297 0.028126
 H  -0.881172 -4.250798 -0.005667
 H  -3.145912 -3.896092 -0.132033
 H  -2.580546 -3.569826 1.526168
 O  -4.257643 -1.817865 2.361013
 H  -5.094158 -1.505279 2.746878
 H  -5.076637 -2.182463 0.475458
 O  -6.003961 0.141153 1.220890
 H  -6.211929 1.076459 1.051965
 H  -3.964697 0.552698 1.246097
 O  -4.894598 1.625263 -1.026919
 H  -4.116759 2.116182 -0.703591
 H  -5.400325 -0.318748 -1.301245
 O  -0.748645 4.458891 0.513905
 H  -1.173910 4.376234 -0.356928
 H  1.135120 3.895786 -0.209006
 H  0.784940 3.568371 1.505789
 C  2.794956 1.503069 1.834453
 H  2.846061 1.492331 2.927556
 C  3.921193 0.691980 1.240531
 C  4.760529 1.226543 0.254705
 C  4.123208 -0.633810 1.644909
 C  5.780663 0.464013 -0.310088
 H  4.610660 2.251992 -0.074494
 C  5.138214 -1.399726 1.079895
 H  3.471994 -1.068140 2.399241
 C  5.990484 -0.867437 0.092626
 H  6.411325 0.907518 -1.075005
 H  5.281661 -2.427554 1.404713
 C  7.049402 -1.724196 -0.467295
 H  7.043700 -2.749228 -0.096564
 C  7.990666 -1.374971 -1.355266
 H  8.071151 -0.372244 -1.768121
 H  8.723661 -2.099251 -1.699698
 H  -1.244416 -1.616995 -1.734433
 H  2.860797 2.546365 1.502546
Sum of electronic and thermal Free
Energies= -1645.327860
SCF Energies= -1645.778151
S7.out
 O  -0.702606 2.299341 -1.206847
 C  -0.132308 2.222410 0.123274
 C  1.042200 1.230289 0.163313
 C  0.582459 -0.126207 -0.363947
 C  -0.061637 0.045939 -1.745518
 C  -1.196516 1.080418 -1.700865
 C  0.260798 3.647985 0.474256
 H  -0.903395 1.884559 0.825249
 O  1.470509 1.096284 1.522112
 H  1.859050 1.596906 -0.470651
 O  1.700136 -1.006693 -0.454167
 H  1.352529 -1.826454 -0.847556
 H  -0.158814 -0.533576 0.335681
 O  -0.448897 -1.197240 -2.313769
 H  0.695792 0.457934 -2.421031
 O  -2.287578 0.693385 -0.854509
 H  -1.575563 1.276636 -2.709410
 C  -3.231461 -0.222495 -1.366748
 O  -2.891434 -1.565840 -1.052733
 C  -2.827684 -1.861392 0.361385
 C  -4.205679 -1.636482 0.985759
 C  -4.632683 -0.191519 0.732172
 C  -4.595569 0.134869 -0.763615
 H  -3.261365 -0.176006 -2.458743
 C  -2.321311 -3.283229 0.478164
 H  -2.109751 -1.188254 0.842742
 O  -0.970544 -3.300887 0.003388
 H  -0.687021 -4.228437 -0.037217
 H  -2.961187 -3.947224 -0.118981
 H  -2.376810 -3.597420 1.527733
 O  -4.106416 -1.901874 2.383678
 H  -4.940146 -1.595244 2.780547
 H  -4.934529 -2.311222 0.511570
 O  -5.948894 -0.031640 1.260497
 H  -6.191542 0.899845 1.120357
 H  -3.929940 0.471264 1.258947
 O  -4.922877 1.497925 -1.009807
 H  -4.154362 2.018324 -0.711056
 H  -5.355752 -0.466160 -1.270814
 O  -0.878596 4.507798 0.508395
 H  -1.314188 4.413789 -0.356167
 H  1.010170 4.008005 -0.246145
 H  0.701036 3.667347 1.473688
 C  2.775805 1.636928 1.813277
 H  2.819982 1.664596 2.906014
 C  3.886240 0.782867 1.253290
 C  4.647433 1.205659 0.155691
 C  4.129403 -0.489607 1.785799
 C  5.628132 0.385022 -0.396388
 H  4.467641 2.189778 -0.270431
 C  5.107356 -1.312848 1.235908
 H  3.540834 -0.837316 2.631331
 C  5.876690 -0.894895 0.132483
 H  6.199301 0.743445 -1.247665
 H  5.283760 -2.297961 1.661309
 C  6.895106 -1.810527 -0.409360
 H  6.970234 -2.762873 0.115510
 C  7.709803 -1.593366 -1.451266
 H  7.699459 -0.672104 -2.028704
 H  8.425473 -2.349431 -1.762049
 H  -1.147187 -1.592299 -1.748260
 H  2.854412 2.666157 1.441934
Sum of electronic and thermal Free
Energies= -1645.327430
SCF Energies= -1645.778234
S8.out
 O  -0.308281 0.803438 -1.750029
 C  0.263201 1.540731 -0.643823
 C  1.509007 0.795357 -0.173547
 C  1.083727 -0.598037 0.314486
 C  0.255925 -1.337039 -0.745380
 C  -0.837334 -0.442798 -1.348339
 C  0.435267 2.963433 -1.134791
 H  -0.453914 1.567355 0.180596
 O  2.104393 1.482708 0.932533
 H  2.221642 0.686222 -0.999444
 O  2.211503 -1.415896 0.615153
 H  2.776111 -0.904272 1.221216
 H  0.460377 -0.457341 1.211480
 O  -0.295966 -2.553450 -0.253954
 H  0.928922 -1.612945 -1.562977
```

```
 O  -1.855026 -0.264665 -0.375458
 H  -1.253573 -0.901732 -2.249966
 C  -3.042370 0.319213 -0.894637
 O  -3.986178 -0.675669 -1.239999
 C  -4.418966 -1.484663 -0.126402
 C  -5.077700 -0.587147 0.925877
 C  -4.118384 0.515967 1.361307
 C  -3.628678 1.291210 0.141795
 H  -2.820112 0.851977 -1.822920
 C  -5.350561 -2.556290 -0.678635
 H  -3.551564 -1.989080 0.320548
 O  -6.554298 -2.031577 -1.242206
 H  -7.149368 -1.813448 -0.506352
 H  -5.565552 -3.279102 0.117494
 H  -4.831474 -3.081983 -1.485958
 O  -5.457351 -1.409927 2.027644
 H  -5.752616 -0.804805 2.729879
 H  -5.961310 -0.110375 0.476055
 O  -4.831215 1.356547 2.272086
 H  -4.193320 1.999697 2.624659
 H  -3.254519 0.060047 1.864629
 O  -2.696449 2.264955 0.595084
 H  -2.293315 2.726781 -0.169310
 H  -4.493704 1.773345 -0.335064
 O  -0.852522 3.532883 -1.431232
 H  -1.231101 2.988079 -2.143639
 H  1.085460 2.999050 -2.018892
 H  0.877689 3.574978 -0.345475
 C  3.369754 2.114222 0.647319
 H  3.535781 2.791974 1.489809
 C  4.482417 1.099677 0.545545
 C  5.095745 0.805375 -0.678922
 C  4.864666 0.368608 1.679385
 C  6.063321 -0.191973 -0.773090
 H  4.809402 1.363246 -1.566945
 C  5.825082 -0.635270 1.585666
 H  4.399185 0.584912 2.638252
 C  6.441673 -0.940053 0.356933
 H  6.521891 -0.393918 -1.736577
 H  6.107246 -1.194450 2.474409
 C  7.443480 -2.018669 0.312457
 H  7.652064 -2.482293 1.276595
 C  8.094657 -2.473622 -0.767011
 H  7.940538 -2.069416 -1.764597
 H  8.815395 -3.281975 -0.680143
 H  -0.977592 -2.308323 0.396871
 H  3.298855 2.713640 -0.268356
Sum of electronic and thermal Free
Energies= -1645.328574
SCF Energies= -1645.781563
S9.out
 O  -2.036774 -2.807242 -0.094958
 C  -0.727242 -2.566784 -0.661778
 C  0.326383 -2.274439 0.421146
 C  -0.180103 -1.177610 1.357941
 C  -1.555242 -1.573150 1.913336
 C  -2.524563 -1.787592 0.737852
 C  -0.397673 -3.810629 -1.471385
 H  -0.783166 -1.702759 -1.334366
 O  1.493655 -1.837321 -0.273615
 H  0.531649 -3.189098 0.994060
 O  0.756332 -0.938341 2.407207
 H  0.673823 0.010506 2.613815
 H  -0.278674 -0.271409 0.758251
 O  -2.056923 -0.672055 2.888780
 H  -1.465045 -2.540860 2.418538
 O  -2.688701 -0.612439 -0.079979
 H  -3.506414 -2.112329 1.097763
 C  -3.497771 0.432523 0.413900
 O  -2.755808 1.349674 1.216185
 C  -1.687142 2.040303 0.526178
 C  -2.306382 2.893819 -0.579954
 C  -3.088208 1.985393 -1.542798
 C  -4.127784 1.154273 -0.786729
 H  -4.274816 0.036495 1.073732
 C  -0.911714 2.830840 1.569092
 H  -1.013594 1.310713 0.066004
 O  -0.198023 1.993012 2.490375
 H  -0.839410 1.631515 3.123724
 H  -1.592508 3.502508 2.107080
 H  -0.162509 3.435315 1.054215
 O  -1.244838 3.560976 -1.265799
 H  -1.636797 4.303995 -1.752633
 H  -2.998477 3.621638 -0.134891
 O  -3.785101 2.750623 -2.526174
 H  -3.117645 3.114996 -3.131016
 H  -2.370277 1.306513 -2.025924
 O  -4.803466 0.225880 -1.624186
 H  -4.152686 -0.464850 -1.845084
 H  -4.892276 1.833064 -0.395998
 O  -1.310990 -4.001789 -2.550906
 H  -2.196756 -4.058286 -2.153936
 H  -0.385221 -4.683219 -0.801431
 H  0.596893 -3.696211 -1.909097
 C  2.750873 -2.216487 0.317039
 H  3.071954 -3.183943 -0.091439
 C  3.759940 -1.138957 0.013653
 C  3.536290 0.172783 0.466986
 C  4.917302 -1.405204 -0.720599
 C  4.444964 1.186109 0.191368
 H  2.640532 0.390492 1.042947
 C  5.834879 -0.388773 -0.993252
 H  5.102941 -2.412456 -1.085473
 C  5.617694 0.925895 -0.548642
 H  4.245611 2.188380 0.559056
 H  6.730794 -0.614808 -1.566565
 C  6.614213 1.960805 -0.871380
 H  7.483412 1.595966 -1.418941
 C  6.556855 3.265366 -0.569189
 H  5.725411 3.713167 -0.030444
 H  7.359714 3.937082 -0.860315
 H  -2.215254 0.185109 2.436869
 H  2.630457 -2.325947 1.399332
Sum of electronic and thermal Free
Energies= -1645.324983
SCF Energies= -1645.77889
```

Conformations for **O6** (Energies in Hartree)

S0.out

```
 O  -0.733303 1.933969 1.370714
 C  0.372960 1.865275 0.444699
 C  0.325317 3.106240 -0.443765
 C  -0.984751 3.040027 -1.234453
 C  -2.199303 2.881263 -0.307575
 C  -1.983813 1.775856 0.733091
 C  1.627115 1.654356 1.260586
 H  0.255077 0.986420 -0.194278
 O  1.453373 3.086672 -1.316369
 H  0.329413 4.011713 0.180713
 O  -1.091533 4.233924 -2.009471
 H  -1.912585 4.155869 -2.525226
 H  -0.931293 2.163441 -1.897840
 O  -3.398774 2.686303 -1.051478
 H  -2.328570 3.818598 0.241519
 O  -2.058034 0.518899 0.076687
 H  -2.737648 1.833914 1.524066
 C  -2.108201 -0.583395 0.970621
 O  -3.443146 -0.995294 1.191761
 C  -4.125601 -1.439635 -0.000857
 C  -3.395520 -2.649778 -0.586998
 C  -1.933759 -2.297799 -0.856154
 C  -1.276285 -1.747677 0.406542
 H  -1.720168 -0.287809 1.948321
 C  -5.551665 -1.747212 0.425678
 H  -4.137352 -0.626291 -0.736894
 O  -6.218180 -0.580351 0.906890
 H  -5.667488 -0.230773 1.628288
 H  -5.536813 -2.540374 1.188234
 H  -6.117934 -2.107135 -0.436598
 O  -4.061433 -3.023551 -1.792031
 H  -3.502472 -3.699530 -2.212929
 H  -3.425710 -3.472859 0.143523
 O  -1.291870 -3.491558 -1.309108
 H  -0.383141 -3.249134 -1.554651
 H  -1.898090 -1.526905 -1.638705
 O  0.055427 -1.375729 0.074778
 H  0.480568 -0.918124 0.833080
 H  -1.281629 -2.535302 1.173037
 O  1.490678 0.367260 1.881168
 H  1.746056 2.430249 2.029462
 H  2.498323 1.678658 0.596356
 H  -3.334958 1.804003 -1.459521
 C  2.703896 -0.126086 2.473699
 C  3.745390 -0.501278 1.444949
 H  2.390643 -1.004209 3.046378
 C  3.473592 -1.499324 0.499618
 C  4.984463 0.150384 1.393655
 C  4.419730 -1.836146 -0.464359
 H  2.513909 -2.008380 0.514994
 C  5.935125 -0.189854 0.434221
 H  5.204938 0.934680 2.113768
 C  5.671663 -1.193180 -0.516351
 H  4.193233 -2.613607 -1.190101
 H  6.884304 0.337446 0.421056
 C  6.635262 -1.595880 -1.555138
 H  6.268846 -2.360273 -2.240548
 C  7.879713 -1.130227 -1.730842
```

```
 H  8.324706 -0.372919 -1.089850
 H  8.502655 -1.505578 -2.538008
 H  1.304459 3.785112 -1.976763
 H  3.101132 0.619183 3.175598
Sum of electronic and thermal Free Energies= -1645.331161
SCF Energies= -1645.782144
S1.out
 O  2.046012 0.235225 -0.932713
 C  2.885556 0.217640 0.238572
 C  3.715389 -1.075902 0.257218
 C  2.828233 -2.313268 0.110413
 C  1.915182 -2.177821 -1.103762
 C  1.146696 -0.856604 -1.012283
 C  3.789995 1.443424 0.178945
 H  2.259904 0.264694 1.137906
 O  4.433230 -1.117401 1.490235
 H  4.413024 -1.057507 -0.594691
 O  3.705657 -3.436440 -0.005608
 H  3.152279 -4.234419 0.030946
 H  2.208443 -2.408187 1.011694
 O  1.044065 -3.306537 -1.129756
 H  2.533366 -2.139756 -2.010501
 O  0.308147 -0.928212 0.124642
 H  0.552121 -0.684409 -1.914269
 C  -0.793843 -0.042978 0.062396
 O  -1.761354 -0.499072 -0.864584
 C  -2.296227 -1.798607 -0.536455
 C  -3.037862 -1.698229 0.798640
 C  -2.067807 -1.222959 1.882457
 C  -1.403319 0.083620 1.462286
 H  -0.466308 0.925799 -0.307349
 C  -3.166662 -2.224134 -1.698578
 H  -1.473278 -2.516549 -0.439596
 O  -2.301926 -2.447931 -2.817918
 H  -2.856277 -2.750580 -3.555341
 H  -3.903724 -1.437101 -1.914661
 H  -3.706592 -3.138784 -1.424004
 O  -3.567435 -2.982270 1.122877
 H  -3.893850 -2.919018 2.037323
 H  -3.845040 -0.955253 0.700544
 O  -2.827063 -1.061617 3.082625
 H  -2.195932 -0.839087 3.787367
 H  -1.296926 -1.993870 2.021785
 O  -0.424150 0.425634 2.441444
 H  -0.109205 1.323092 2.233003
 H  -2.180628 0.855036 1.402725
 O  3.134327 2.682735 0.434451
 H  4.301834 1.467609 -0.793258
 H  4.546871 1.341493 0.961408
 H  0.461155 -3.218504 -1.904124
 C  2.463703 3.294634 -0.676810
 C  0.957473 3.264565 -0.537004
 H  2.765330 2.824218 -1.618815
 C  0.350843 3.474667 0.708966
 C  0.137756 3.064938 -1.654683
 C  -1.037194 3.451553 0.836874
 H  0.971151 3.641856 1.584807
 C  -1.250702 3.030862 -1.527822
 H  0.591118 2.913622 -2.631307
 C  -1.862873 3.190894 -0.272404
 H  -1.489315 3.594739 1.815440
 H  -1.865897 2.856982 -2.405960
 C  -3.312125 3.017358 -0.069951
```

```
 H  -3.733927 3.541266 0.787780
 C  -4.105432 2.225878 -0.805311
 H  -3.724847 1.637337 -1.636548
 H  -5.165464 2.133349 -0.585037
 H  4.888931 -1.976562 1.512251
 H  2.804942 4.338370 -0.705294
Sum of electronic and thermal Free Energies= -1645.331366
SCF Energies= -1645.783016
S10.out
 O  -2.148907 0.074257 -1.156850
 C  -3.033598 1.033543 -0.540915
 C  -3.930728 0.369486 0.524259
 C  -4.170281 -1.097797 0.158707
 C  -2.848058 -1.884992 0.103657
 C  -1.712092 -0.903886 -0.215442
 C  -2.250849 2.211905 0.016507
 H  -3.684468 1.383964 -1.347465
 O  -5.154409 1.098953 0.555140
 H  -3.449272 0.410654 1.513464
 O  -5.082874 -1.623849 1.121912
 H  -5.430275 -2.458719 0.767105
 H  -4.615869 -1.125737 -0.844584
 O  -2.995830 -2.899938 -0.886274
 H  -2.653165 -2.325456 1.091051
 O  -0.634757 -1.610399 -0.766336
 H  -1.395490 -0.408117 0.709335
 C  0.559208 -0.835664 -0.918972
 O  0.948352 -0.222355 0.283764
 C  1.253252 -1.120810 1.369572
 C  2.405667 -2.040298 0.964958
 C  2.044332 -2.778981 -0.322411
 C  1.645864 -1.788504 -1.422370
 H  0.380564 -0.019034 -1.620545
 C  1.572949 -0.222532 2.556628
 H  0.369879 -1.728331 1.602474
 O  0.494305 0.671653 2.835362
 H  0.409264 1.248157 2.055537
 H  2.500713 0.331157 2.357501
 H  1.719873 -0.837845 3.447192
 O  2.630156 -2.950460 2.041892
 H  3.312271 -3.574019 1.739113
 H  3.302501 -1.430544 0.777710
 O  3.184332 -3.545686 -0.711137
 H  2.936960 -4.019535 -1.523921
 H  1.192527 -3.443253 -0.114059
 O  1.259399 -2.458035 -2.618898
 H  0.411967 -2.901266 -2.434201
 H  2.519954 -1.181226 -1.677413
 O  -1.757200 2.971736 -1.083736
 H  -1.427155 1.847922 0.646580
 H  -2.909438 2.832209 0.643380
 H  -2.147692 -3.373089 -0.937286
 C  -0.788161 3.958022 -0.700505
 C  0.579018 3.357622 -0.461854
 H  -1.132209 4.504562 0.188414
 C  1.250353 2.715493 -1.514866
 C  1.199083 3.412801 0.789658
 C  2.499498 2.138368 -1.321611
 H  0.782332 2.671871 -2.495065
 C  2.457082 2.838002 0.985899
 H  0.697404 3.909407 1.616712
 C  3.121033 2.171931 -0.057295
 H  2.996236 1.653359 -2.156669
```

```
 H  2.919135 2.880325 1.968942
 C  4.401338 1.501908 0.222455
 H  4.865136 1.777493 1.169478
 C  5.003643 0.579261 -0.542277
 H  4.587189 0.234489 -1.485737
 H  5.945696 0.132456 -0.236822
 H  -5.742938 0.610051 1.156947
 H  -0.753478 4.661839 -1.538573
Sum of electronic and thermal Free Energies= -1645.326379
SCF Energies= -1645.77901
S11.out
 O  -0.196571 -0.813130 -0.471356
 C  -0.273060 -0.434174 0.923476
 C  -0.368112 1.089465 1.074192
 C  0.776504 1.758505 0.323520
 C  0.768015 1.295706 -1.133745
 C  0.862304 -0.237894 -1.194175
 C  -1.462583 -1.164023 1.539171
 H  0.632159 -0.782571 1.437309
 O  -0.316316 1.371819 2.473291
 H  -1.319576 1.433879 0.646821
 O  0.619292 3.175327 0.412630
 H  1.247694 3.552486 -0.229111
 H  1.720856 1.459297 0.796384
 O  1.742862 1.966001 -1.919952
 H  -0.199278 1.558556 -1.575432
 O  2.079953 -0.755633 -0.636479
 H  0.763351 -0.587530 -2.227076
 C  3.248105 -0.699491 -1.426987
 O  3.978563 0.502038 -1.213337
 C  4.443388 0.694758 0.140810
 C  5.414493 -0.429771 0.504463
 C  4.700491 -1.769810 0.342367
 C  4.113730 -1.913059 -1.065373
 H  2.995082 -0.701091 -2.490743
 C  5.050756 2.087303 0.196110
 H  3.589744 0.653123 0.827853
 O  4.087134 3.102003 -0.099682
 H  3.414294 3.084714 0.602110
 H  5.835571 2.177174 -0.561200
 H  5.501027 2.240304 1.184105
 O  5.830951 -0.231055 1.854894
 H  6.319513 -1.032028 2.112262
 H  6.277295 -0.400490 -0.178365
 O  5.649530 -2.801993 0.608601
 H  5.174531 -3.645463 0.510960
 H  3.879846 -1.810829 1.074500
 O  3.382927 -3.127156 -1.201166
 H  2.565461 -3.010999 -0.682581
 H  4.937502 -1.962800 -1.783367
 O  -2.735789 -0.609978 1.224390
 H  -1.373937 -1.098133 2.626543
 H  -1.417051 -2.223589 1.248726
 H  2.631931 1.750738 -1.562219
 C  -3.192777 -0.861627 -0.112219
 C  -4.667649 -0.558857 -0.188210
 H  -3.004943 -1.917286 -0.362949
 C  -5.188653 0.213944 -1.229460
 C  -5.553842 -1.074912 0.771075
 C  -6.559954 0.456138 -1.318184
 H  -4.518535 0.630132 -1.977788
 C  -6.918966 -0.827464 0.689806
 H  -5.162456 -1.671531 1.590343
```

```
 C  -7.453566 -0.056072 -0.362357
 H  -6.946013 1.058357 -2.137201
 H  -7.576629 -1.241981 1.448266
 C  -8.890297 0.234208 -0.503067
 H  -9.147514 0.825559 -1.382043
 C  -9.879710 -0.144447 0.317997
 H  -9.711256 -0.732920 1.216650
 H  -10.909803 0.129659 0.107513
 H  -0.351354 2.339149 2.563597
 H  -2.639493 -0.250387 -0.833794
Sum of electronic and thermal Free Energies= -1645.328888
SCF Energies= -1645.780711
S12.out
 O  0.447643 1.270264 -1.020806
 C  0.142736 1.355973 0.388545
 C  0.439835 2.773360 0.879605
 C  1.906350 3.098267 0.593801
 C  2.233751 2.887466 -0.882893
 C  1.826162 1.480041 -1.345258
 C  -1.302697 0.925556 0.549917
 H  0.779899 0.662111 0.945494
 O  0.169338 2.815583 2.278799
 H  -0.194245 3.490284 0.336664
 O  2.124692 4.455511 0.978147
 H  3.062688 4.645839 0.805118
 H  2.533055 2.425953 1.197387
 O  3.626987 3.124902 -1.051322
 H  1.641566 3.600268 -1.470440
 O  2.662668 0.526894 -0.736877
 H  1.875207 1.396731 -2.435329
 C  2.916018 -0.697815 -1.444791
 O  4.052576 -1.284240 -0.859234
 C  3.892246 -1.695351 0.519947
 C  2.728092 -2.683121 0.659322
 C  1.467015 -2.065249 0.060805
 C  1.737602 -1.691148 -1.400368
 H  3.179585 -0.463807 -2.481897
 C  5.232095 -2.286077 0.927921
 H  3.685218 -0.813770 1.137996
 O  6.274093 -1.312457 0.875273
 H  6.270977 -0.960367 -0.031155
 H  5.458848 -3.147119 0.281457
 H  5.172097 -2.636683 1.961197
 O  2.551744 -2.954014 2.048502
 H  1.689507 -3.401094 2.119249
 H  2.967332 -3.609150 0.113143
 O  0.384482 -2.987155 0.196642
 H  -0.408952 -2.437918 0.325075
 H  1.238487 -1.163329 0.633477
 O  0.592823 -1.227160 -2.096610
 H  0.274625 -0.420671 -1.636531
 H  2.071462 -2.585895 -1.936830
 O  -1.419368 -0.466542 0.212116
 H  -1.947523 1.535472 -0.092310
 H  -1.612290 1.071559 1.588800
 H  3.783133 3.317919 -1.990575
 C  -2.343691 -0.752799 -0.840110
 C  -3.791994 -0.598818 -0.429953
 H  -2.134046 -1.790646 -1.122352
 C  -4.191175 -0.765387 0.899699
 C  -4.770570 -0.316612 -1.394080
 C  -5.535059 -0.655950 1.253976
 H  -3.443868 -0.974260 1.659321
```

```
 C  -6.112916 -0.216296 -1.043536
 H  -4.474305 -0.172206 -2.430637
 C  -6.525207 -0.383962 0.293004
 H  -5.826918 -0.784559 2.293660
 H  -6.844819 0.004141 -1.815087
 C  -7.930087 -0.284651 0.723186
 H  -8.087176 -0.428288 1.792452
 C  -8.999384 -0.046425 -0.049098
 H  -8.930756 0.107243 -1.123361
 H  -9.995418 0.004804 0.381968
 H  0.488040 3.677760 2.596945
 H  -2.127566 -0.129018 -1.717779
Sum of electronic and thermal Free Energies= -1645.326919
SCF Energies= -1645.778411
S13.out
 O  -1.715088 -0.219459 0.453601
 C  -2.476022 -1.279823 -0.153486
 C  -2.681781 -2.409636 0.864516
 C  -1.335756 -2.876354 1.415738
 C  -0.541746 -1.697599 1.983790
 C  -0.443358 -0.583564 0.938493
 C  -3.798875 -0.678601 -0.608836
 H  -1.934414 -1.673031 -1.022801
 O  -3.358885 -3.479110 0.204398
 H  -3.285552 -2.027161 1.702137
 O  -1.602714 -3.853998 2.422290
 H  -0.738145 -4.151778 2.753850
 H  -0.762942 -3.326544 0.591802
 O  0.746833 -2.103876 2.442045
 H  -1.069701 -1.302156 2.856066
 O  0.402177 -1.084879 -0.085846
 H  -0.022622 0.330153 1.365127
 C  0.871136 -0.113730 -1.006248
 O  1.682842 0.858553 -0.377296
 C  2.849993 0.338147 0.296160
 C  3.735535 -0.387870 -0.725155
 C  2.922354 -1.457828 -1.455022
 C  1.666630 -0.851087 -2.080241
 H  0.029889 0.435800 -1.432745
 C  3.484332 1.563920 0.955971
 H  2.542902 -0.372043 1.076148
 O  4.574837 1.239589 1.813959
 H  4.225023 0.671968 2.521112
 H  2.694758 2.101611 1.499023
 H  3.879972 2.233398 0.185197
 O  4.839824 -0.990653 -0.053070
 H  5.233807 -1.602129 -0.700703
 H  4.089079 0.347205 -1.465421
 O  3.777297 -2.030958 -2.452524
 H  3.445420 -2.923930 -2.640459
 H  2.626298 -2.226535 -0.730452
 O  0.824890 -1.839589 -2.668388
 H  1.304813 -2.198555 -3.433907
 H  1.969564 -0.105253 -2.827237
 O  -3.643484 0.130228 -1.779338
 H  -4.233522 -0.103728 0.217691
 H  -4.484506 -1.496810 -0.855244
 H  1.264150 -2.328996 1.647466
 C  -3.971280 1.525029 -1.630060
 C  -2.851467 2.308437 -0.989152
 H  -4.903927 1.635240 -1.062105
 C  -1.658915 2.513292 -1.694012
 C  -2.928958 2.754627 0.336411
```

```
 C  -0.562044 3.107692 -1.077315
 H  -1.582844 2.180903 -2.726535
 C  -1.831740 3.344876 0.959079
 H  -3.851789 2.614255 0.894002
 C  -0.615977 3.511945 0.269632
 H  0.363444 3.236143 -1.632646
 H  -1.918755 3.666569 1.992822
 C  0.599569 4.064439 0.889924
 H  1.436250 4.198021 0.204532
 C  0.778945 4.383027 2.179907
 H  0.001550 4.265872 2.931067
 H  1.730579 4.777051 2.525599
 H  -3.389783 -4.216368 0.838034
 H  -4.150687 1.878018 -2.650619
Sum of electronic and thermal Free Energies= -1645.327066
SCF Energies= -1645.778769
S14.out
 O  1.422476 -1.707358 1.136794
 C  1.541526 -2.060812 -0.254961
 C  2.952245 -2.593908 -0.506290
 C  3.940941 -1.482512 -0.154436
 C  3.720312 -0.968694 1.273554
 C  2.242926 -0.624599 1.520478
 C  0.414505 -3.024287 -0.561917
 H  1.391939 -1.168865 -0.874373
 O  3.059925 -2.961359 -1.880938
 H  3.136604 -3.460957 0.145439
 O  5.261481 -2.002025 -0.311572
 H  5.869567 -1.272953 -0.099248
 H  3.777538 -0.650539 -0.856202
 O  4.565826 0.143290 1.555056
 H  4.001740 -1.760750 1.973606
 O  1.955627 0.549131 0.780832
 H  2.053626 -0.461511 2.584791
 C  1.140183 1.562853 1.367038
 O  1.544565 2.792756 0.812237
 C  1.357838 2.900774 -0.620243
 C  -0.117972 2.707251 -0.981029
 C  -0.629998 1.391973 -0.398626
 C  -0.359869 1.364751 1.105157
 H  1.340594 1.621695 2.441833
 C  1.891576 4.273104 -0.997067
 H  1.955086 2.131336 -1.122921
 O  3.287076 4.389022 -0.721744
 H  3.395124 4.187244 0.223495
 H  1.315223 5.043265 -0.462880
 H  1.762019 4.428056 -2.071067
 O  -0.226530 2.713678 -2.403022
 H  -1.135764 2.425860 -2.598950
 H  -0.705129 3.530909 -0.545642
 O  -2.035579 1.306165 -0.667661
 H  -2.246849 0.376186 -0.854573
 H  -0.110325 0.559561 -0.883802
 O  -0.794021 0.162943 1.723494
 H  -1.707069 0.003509 1.424695
 H  -0.866083 2.229310 1.560088
 O  -0.786914 -2.266542 -0.455213
 H  0.414746 -3.861320 0.152275
 H  0.536342 -3.429549 -1.575422
 H  4.185583 0.898030 1.067709
 C  -1.977516 -3.011364 -0.727028
 C  -3.132096 -2.084020 -0.457619
 H  -2.021002 -3.895037 -0.072740
```

```
 C  -3.858282 -1.495244 -1.496727
 C  -3.434441 -1.719256 0.865796
 C  -4.863173 -0.564621 -1.220447
 H  -3.634071 -1.759477 -2.526933
 C  -4.425359 -0.784667 1.141546
 H  -2.875725 -2.170932 1.681898
 C  -5.161064 -0.184041 0.098570
 H  -5.417392 -0.115690 -2.040862
 H  -4.632119 -0.522952 2.174701
 C  -6.217857 0.814913 0.329084
 H  -6.711001 1.168052 -0.576446
 C  -6.614530 1.316933 1.506601
 H  -6.173574 1.021779 2.455520
 H  -7.409644 2.055877 1.553134
 H  3.999649 -3.154383 -2.042258
 H  -1.980445 -3.360523 -1.769565
Sum of electronic and thermal Free Energies= -1645.330234
SCF Energies= -1645.779799
S15.out
 O  0.087913 -0.000035 -1.458532
 C  -0.815636 -0.476480 -0.443440
 C  -1.378390 0.702516 0.367532
 C  -0.230035 1.518743 0.957593
 C  0.739081 1.946263 -0.149984
 C  1.190632 0.729913 -0.962785
 C  -1.839739 -1.384255 -1.126534
 H  -0.270190 -1.120107 0.260879
 O  -2.205921 0.153528 1.393627
 H  -1.959576 1.367017 -0.277470
 O  -0.785752 2.658397 1.612141
 H  -0.031739 3.209158 1.886543
 H  0.310607 0.889285 1.681180
 O  1.849772 2.668740 0.378526
 H  0.221166 2.632399 -0.826183
 O  1.993415 -0.052411 -0.091604
 H  1.769539 1.029107 -1.840339
 C  2.798930 -1.031714 -0.727206
 O  3.898968 -0.452342 -1.401021
 C  4.790342 0.297428 -0.554965
 C  5.350317 -0.617005 0.542367
 C  4.219930 -1.269740 1.331159
 C  3.257320 -1.986726 0.378776
 H  2.223436 -1.555657 -1.494589
 C  5.881362 0.850459 -1.472959
 H  4.253710 1.136608 -0.095702
 O  6.719567 1.784714 -0.797495
 H  6.970967 1.355314 0.043677
 H  5.408116 1.379782 -2.305871
 H  6.461350 0.012509 -1.889454
 O  6.177826 0.189718 1.392330
 H  6.646887 -0.412221 1.994414
 H  5.950313 -1.406888 0.068469
 O  4.802459 -2.184383 2.258525
 H  4.063121 -2.612041 2.724216
 H  3.670524 -0.481179 1.867042
 O  2.150299 -2.548172 1.079687
 H  1.631076 -1.799196 1.424268
 H  3.782317 -2.823551 -0.090401
 O  -2.393802 -0.915365 -2.355933
 H  -2.620938 -1.629091 -0.397779
 H  -1.331881 -2.312205 -1.404014
 H  2.357676 2.040391 0.923120
 C  -3.304171 0.193976 -2.309714
```

```
 C  -4.455597 0.016069 -1.346034
 H  -3.682934 0.262256 -3.335744
 C  -4.805094 1.023083 -0.436217
 C  -5.196494 -1.171982 -1.343931
 C  -5.870509 0.855905 0.444689
 H  -4.234728 1.948473 -0.415916
 C  -6.257028 -1.345463 -0.458443
 H  -4.930192 -1.967921 -2.034472
 C  -6.619674 -0.335598 0.452882
 H  -6.113944 1.656763 1.136638
 H  -6.819459 -2.276020 -0.470542
 C  -7.752762 -0.571094 1.363754
 H  -8.214457 -1.553866 1.267600
 C  -8.256261 0.281535 2.267000
 H  -7.856637 1.280594 2.423393
 H  -9.101000 -0.002565 2.888469
 H  -2.822158 0.851241 1.668962
 H  -2.768083 1.127497 -2.103629
Sum of electronic and thermal Free Energies= -1645.326032
SCF Energies= -1645.777509
S16.out
 O  1.834925 -1.334975 1.106132
 C  1.814790 -1.762363 -0.270737
 C  3.214235 -2.230883 -0.677963
 C  4.184560 -1.066654 -0.490486
 C  4.118696 -0.531458 0.941706
 C  2.673364 -0.224215 1.357594
 C  0.746670 -2.830539 -0.387608
 H  1.526546 -0.921607 -0.913956
 O  3.169152 -2.646818 -2.042471
 H  3.522981 -3.063327 -0.027799
 O  5.496477 -1.534567 -0.805674
 H  6.094227 -0.775513 -0.692524
 H  3.892255 -0.264315 -1.184563
 O  4.953439 0.611299 1.110246
 H  4.505063 -1.300521 1.617288
 O  2.251226 0.918571 0.628487
 H  2.617104 -0.039411 2.430192
 C  1.524068 1.946321 1.306978
 O  1.335500 2.980218 0.370125
 C  0.524487 2.621701 -0.777301
 C  -0.868500 2.168307 -0.327893
 C  -0.739647 1.057516 0.710735
 C  0.150991 1.526326 1.854758
 H  2.146652 2.357429 2.108421
 C  0.492119 3.859881 -1.657663
 H  1.008862 1.803854 -1.322998
 O  1.789369 4.197056 -2.148612
 H  2.352419 4.321846 -1.365881
 H  0.052085 4.693512 -1.090351
 H  -0.138626 3.664029 -2.528246
 O  -1.571463 1.714609 -1.484530
 H  -2.399401 1.314083 -1.164313
 H  -1.394475 3.018516 0.132918
 O  -2.026908 0.717514 1.246087
 H  -2.261773 -0.162403 0.907575
 H  -0.297919 0.175787 0.242058
 O  0.284700 0.534515 2.862811
 H  -0.591500 0.113209 2.929288
 H  -0.284517 2.441090 2.285680
 O  -0.510291 -2.179218 -0.233800
 H  0.889652 -3.600104 0.385733
 H  0.814086 -3.312054 -1.372327
```

```
 H  4.511458 1.337817 0.633053
 C  -1.636171 -3.047183 -0.398867
 C  -2.868546 -2.182310 -0.379410
 H  -1.663687 -3.794211 0.407087
 C  -3.122109 -1.304528 -1.442690
 C  -3.738220 -2.171282 0.720386
 C  -4.217372 -0.444400 -1.406402
 H  -2.448909 -1.287595 -2.295453
 C  -4.832037 -1.308260 0.760139
 H  -3.549219 -2.838379 1.557424
 C  -5.091507 -0.422980 -0.302052
 H  -4.399717 0.228182 -2.241324
 H  -5.481080 -1.319487 1.630335
 C  -6.221387 0.521479 -0.308666
 H  -6.282817 1.148204 -1.198200
 C  -7.147362 0.677978 0.646953
 H  -7.156262 0.092594 1.563245
 H  -7.940471 1.412271 0.536461
 H  4.090865 -2.800581 -2.312434
 H  -1.549618 -3.583290 -1.355866
Sum of electronic and thermal Free Energies= -1645.329082
SCF Energies= -1645.780123
S18.out
 O  -1.771446 -0.945381 -0.832332
 C  -3.106058 -1.341121 -0.455177
 C  -3.148912 -2.405385 0.666819
 C  -1.776536 -2.587390 1.304610
 C  -1.161506 -1.207961 1.541942
 C  -0.838424 -0.573528 0.175859
 C  -3.967495 -0.126811 -0.120833
 H  -3.501531 -1.800989 -1.364583
 O  -3.641680 -3.624712 0.105977
 H  -3.826349 -2.065554 1.464260
 O  -1.942286 -3.299909 2.526693
 H  -1.102148 -3.195808 3.008949
 H  -1.133409 -3.153154 0.614068
 O  -0.009533 -1.277504 2.373882
 H  -1.878479 -0.578853 2.078112
 O  0.408161 -1.101825 -0.240205
 H  -0.768202 0.516273 0.246648
 C  1.210332 -0.233821 -1.032173
 O  2.010668 0.615391 -0.239377
 C  2.987303 -0.048137 0.591620
 C  3.926448 -0.893718 -0.274657
 C  3.108467 -1.877438 -1.105944
 C  2.063546 -1.129066 -1.935188
 H  0.573897 0.427192 -1.623869
 C  3.711230 1.042032 1.367070
 H  2.475705 -0.699789 1.308538
 O  2.863103 1.671125 2.324345
 H  2.237066 2.223957 1.822115
 H  4.129310 1.774142 0.661037
 H  4.537023 0.588624 1.920994
 O  4.822819 -1.578740 0.599961
 H  5.339760 -2.186498 0.043811
 H  4.480645 -0.232014 -0.958019
 O  4.011460 -2.598586 -1.944164
 H  3.469754 -3.222013 -2.458314
 H  2.595119 -2.567150 -0.419850
 O  1.252319 -2.021680 -2.692491
 H  0.625845 -2.421727 -2.061185
 H  2.580882 -0.488402 -2.655496
 O  -4.069170 0.698898 -1.278845
```

```
 H  -3.529892 0.421224 0.722456
 H  -4.968996 -0.464445 0.182467
 H  0.695016 -1.674513 1.829897
 C  -4.031263 2.107465 -1.000127
 C  -2.629143 2.581818 -0.695620
 H  -4.716217 2.355188 -0.178368
 C  -1.659509 2.571917 -1.706823
 C  -2.248547 2.979797 0.592598
 C  -0.353753 2.972795 -1.441094
 H  -1.932812 2.246677 -2.707408
 C  -0.940379 3.378172 0.863778
 H  -2.985906 2.976682 1.391530
 C  0.030147 3.394233 -0.153542
 H  0.385125 2.967202 -2.238729
 H  -0.673928 3.670518 1.875194
 C  1.420851 3.825073 0.063955
 H  2.089316 3.642714 -0.776536
 C  1.925759 4.405058 1.164062
 H  1.323214 4.636422 2.038922
 H  2.975160 4.680933 1.211850
 H  -3.699930 -4.263681 0.837356
 H  -4.405697 2.586310 -1.910215
Sum of electronic and thermal Free Energies= -1645.324457
SCF Energies= -1645.777671
S19.out
 O  0.747379 0.516679 0.340017
 C  0.547613 1.086530 -0.975506
 C  0.059015 2.534546 -0.854935
 C  -1.195433 2.587214 0.011937
 C  -0.929452 1.922143 1.362516
 C  -0.397526 0.494529 1.154581
 C  1.875261 0.982056 -1.696245
 H  -0.203393 0.500065 -1.517504
 O  -0.203192 3.014673 -2.173247
 H  0.841787 3.138461 -0.371159
 O  -1.553543 3.959514 0.175856
 H  -2.307239 3.971202 0.791556
 H  -2.001238 2.047073 -0.505525
 O  -2.061258 1.988171 2.220811
 H  -0.134690 2.478881 1.869903
 O  -1.353168 -0.362320 0.517218
 H  -0.095353 0.052980 2.109648
 C  -2.331270 -0.991002 1.318251
 O  -3.527097 -0.223928 1.375980
 C  -4.178753 -0.022716 0.097177
 C  -4.548663 -1.385108 -0.490626
 C  -3.292838 -2.249377 -0.639729
 C  -2.578284 -2.380360 0.709931
 H  -1.987459 -1.074302 2.352709
 C  -5.355269 0.900484 0.339741
 H  -3.489217 0.483074 -0.589212
 O  -6.296840 0.255119 1.197776
 H  -7.060479 0.848606 1.280350
 H  -5.800721 1.150748 -0.631711
 H  -4.977871 1.829067 0.792595
 O  -5.164785 -1.165489 -1.756522
 H  -5.200025 -2.037671 -2.188057
 H  -5.243232 -1.892104 0.195849
 O  -3.615898 -3.517301 -1.212664
 H  -4.193321 -3.984013 -0.582057
 H  -2.620129 -1.769519 -1.359116
 O  -1.356706 -3.099844 0.617864
 H  -0.732268 -2.511589 0.154561
```

```
 H  -3.220737 -2.939505 1.398325
 O  2.118864 -0.395187 -1.976747
 H  2.665622 1.402289 -1.059990
 H  1.837009 1.559529 -2.629317
 H  -2.748332 1.376010 1.877602
 C  3.447100 -0.648570 -2.427179
 C  4.487474 -0.573092 -1.326575
 H  3.712262 0.032334 -3.249432
 C  5.816030 -0.257933 -1.627380
 C  4.149805 -0.859768 0.004395
 C  6.786861 -0.245761 -0.626670
 H  6.094651 -0.020031 -2.651453
 C  5.115866 -0.838787 1.005062
 H  3.116084 -1.080149 0.252944
 C  6.459647 -0.535917 0.709877
 H  7.815187 0.001128 -0.880104
 H  4.821224 -1.058583 2.027260
 C  7.523201 -0.502715 1.727772
 H  8.506966 -0.230831 1.344726
 C  7.402900 -0.768140 3.036061
 H  6.459460 -1.049648 3.497429
 H  8.264706 -0.711791 3.695314
 H  -0.588230 3.901887 -2.071159
 H  3.419241 -1.663829 -2.840436
Sum of electronic and thermal Free Energies= -1645.327264
SCF Energies= -1645.776378
S2.out
 O  0.444319 0.702335 0.506194
 C  0.494546 1.988939 -0.146694
 C  0.169545 3.087104 0.871887
 C  -1.197951 2.815324 1.497307
 C  -1.260073 1.403871 2.088560
 C  -0.819087 0.373954 1.044745
 C  1.881991 2.117390 -0.738921
 H  -0.245377 2.018269 -0.955645
 O  0.178484 4.339461 0.187207
 H  0.930155 3.073896 1.667416
 O  -1.417150 3.805440 2.502361
 H  -2.297988 3.629502 2.875763
 H  -1.958043 2.901602 0.707048
 O  -2.557426 1.108128 2.602450
 H  -0.571600 1.344662 2.936276
 O  -1.829172 0.362901 0.048222
 H  -0.707990 -0.620344 1.484746
 C  -1.751808 -0.721040 -0.862937
 O  -1.992933 -1.958539 -0.224966
 C  -3.276154 -2.045983 0.432034
 C  -4.391402 -1.869740 -0.603210
 C  -4.199192 -0.552649 -1.354239
 C  -2.792902 -0.474269 -1.953812
 H  -0.743331 -0.789941 -1.280316
 C  -3.320808 -3.391385 1.126720
 H  -3.355731 -1.254608 1.187576
 O  -2.340844 -3.380315 2.167841
 H  -2.355386 -4.256952 2.584713
 H  -3.115843 -4.185525 0.394321
 H  -4.330049 -3.545859 1.529692
 O  -5.643798 -1.883688 0.079716
 H  -6.308912 -1.615162 -0.578254
 H  -4.337204 -2.695883 -1.329190
 O  -5.202757 -0.494486 -2.374542
 H  -5.332628 0.440934 -2.601244
 H  -4.334052 0.275660 -0.647154
```

```
 O  -2.531761 0.795157 -2.547134
 H  -3.095349 0.860409 -3.336228
 H  -2.682114 -1.278633 -2.693069
 O  1.980120 1.187302 -1.817980
 H  2.629960 1.903740 0.036090
 H  2.040664 3.140379 -1.103976
 H  -3.151858 1.038493 1.833344
 C  3.316644 0.985285 -2.268561
 C  4.149574 0.121515 -1.340386
 H  3.816773 1.950084 -2.439882
 C  3.551792 -0.815421 -0.491461
 C  5.548429 0.218978 -1.352289
 C  4.334667 -1.636265 0.319006
 H  2.469783 -0.888859 -0.454259
 C  6.330992 -0.606554 -0.551144
 H  6.028735 0.951799 -1.996904
 C  5.738568 -1.556755 0.303419
 H  3.852021 -2.355645 0.976699
 H  7.411630 -0.502695 -0.583369
 C  6.513636 -2.456200 1.174417
 H  5.907092 -3.108473 1.803073
 C  7.847626 -2.552001 1.263307
 H  8.525958 -1.943707 0.669836
 H  8.307454 -3.259890 1.947398
 H  -0.124652 5.005969 0.827462
 H  3.219439 0.492629 -3.243406
Sum of electronic and thermal Free Energies= -1645.326868
SCF Energies= -1645.775402
S20.out
 O  0.575460 1.944895 -1.044565
 C  0.207493 2.543934 0.218569
 C  1.337569 3.482705 0.680668
 C  2.638873 2.690751 0.792350
 C  2.929959 1.927951 -0.500542
 C  1.712553 1.111679 -0.956200
 C  -1.135426 3.237652 0.019643
 H  0.077272 1.759371 0.973866
 O  1.051447 4.025281 1.971318
 H  1.470453 4.284486 -0.057693
 O  3.696047 3.604606 1.086294
 H  4.515553 3.081087 1.098722
 H  2.528398 1.961427 1.609032
 O  4.087372 1.133673 -0.264727
 H  3.120038 2.665113 -1.293550
 O  1.477322 0.036389 -0.059405
 H  1.881992 0.727115 -1.965557
 C  1.069773 -1.153147 -0.709769
 O  2.155138 -1.737001 -1.405254
 C  3.261748 -2.064817 -0.534072
 C  2.823542 -3.206768 0.378115
 C  1.646386 -2.698203 1.215867
 C  0.528604 -2.140952 0.325247
 H  0.309376 -0.933305 -1.465153
 C  4.445438 -2.318639 -1.445500
 H  3.502784 -1.196481 0.084459
 O  4.763266 -1.121477 -2.175668
 H  3.981605 -0.921771 -2.720401
 H  4.235049 -3.147963 -2.134057
 H  5.325128 -2.569975 -0.849521
 O  3.921810 -3.574950 1.209465
 H  3.559140 -4.165534 1.892765
 H  2.492604 -4.060434 -0.232443
 O  1.172470 -3.791885 2.007419
```

```
 H  0.629590 -3.420388 2.722927
 H  2.013721 -1.893448 1.866626
 O  -0.475458 -1.480623 1.096865
 H  -1.033180 -2.165687 1.501317
 H  0.095131 -2.976141 -0.238652
 O  -2.256482 2.377596 0.215558
 H  -1.162112 3.694531 -0.981363
 H  -1.253255 4.027377 0.765982
 H  4.283295 0.581458 -1.049464
 C  -2.347273 1.296063 -0.727637
 C  -3.678646 0.616133 -0.543007
 H  -1.531942 0.581827 -0.571765
 C  -3.759087 -0.704497 -0.080601
 C  -4.867595 1.302040 -0.820967
 C  -4.992202 -1.330465 0.085098
 H  -2.844996 -1.242744 0.157675
 C  -6.101521 0.680006 -0.650854
 H  -4.823230 2.329187 -1.174414
 C  -6.191120 -0.651069 -0.200195
 H  -5.019616 -2.354072 0.447156
 H  -7.014626 1.226120 -0.875810
 C  -7.522974 -1.262436 -0.051975
 H  -8.354729 -0.587249 -0.253499
 C  -7.801479 -2.528796 0.287381
 H  -7.032204 -3.268339 0.496078
 H  -8.830570 -2.868802 0.364283
 H  0.557117 4.849993 1.842666
 H  -2.252631 1.696460 -1.748328
Sum of electronic and thermal Free Energies= -1645.326297
SCF Energies= -1645.778115
S21.out
 O  -0.405444 -2.614068 -1.173901
 C  0.472200 -2.396709 -0.046691
 C  -0.199057 -2.889366 1.243942
 C  -1.564093 -2.228364 1.411139
 C  -2.410006 -2.417502 0.150284
 C  -1.631326 -1.927137 -1.080051
 C  1.773355 -3.143108 -0.305788
 H  0.672205 -1.325001 0.052736
 O  0.665826 -2.569366 2.333777
 H  -0.348845 -3.977655 1.175081
 O  -2.193130 -2.820943 2.548491
 H  -3.063855 -2.394903 2.631375
 H  -1.408685 -1.155196 1.585206
 O  -3.698319 -1.829376 0.277989
 H  -2.580372 -3.489420 0.005349
 O  -1.326898 -0.527837 -1.005957
 H  -2.184181 -2.133755 -2.001986
 C  -2.273286 0.412990 -1.462193
 O  -3.151437 0.822506 -0.419918
 C  -2.521312 1.498068 0.698855
 C  -1.777968 2.734246 0.195230
 C  -0.757551 2.323511 -0.867642
 C  -1.470364 1.600376 -2.016700
 H  -2.916234 -0.024538 -2.230870
 C  -3.642599 1.800608 1.680305
 H  -1.803351 0.823949 1.179478
 O  -4.606550 2.711452 1.154514
 H  -4.948013 2.312908 0.335893
 H  -3.218664 2.264943 2.574080
 H  -4.112228 0.850447 1.974180
 O  -1.129843 3.337516 1.311394
 H  -0.495781 3.974035 0.935399
```

```
 H  -2.505099 3.427891 -0.253600
 O  0.008317 3.443637 -1.310440
 H  -0.593127 4.050033 -1.778827
 H  -0.030926 1.648571 -0.406672
 O  -0.582941 1.160838 -3.036251
 H  -0.102960 0.397787 -2.667996
 H  -2.173108 2.292406 -2.492489
 O  2.420664 -2.868056 -1.551949
 H  1.580949 -4.220733 -0.321266
 H  2.443219 -2.925610 0.534318
 H  -3.600421 -0.853787 0.231364
 C  2.423670 -1.517568 -2.021608
 C  3.027024 -0.493473 -1.085132
 H  1.404497 -1.213419 -2.291537
 C  2.551869 0.822264 -1.103332
 C  4.068553 -0.816772 -0.204232
 C  3.087297 1.785884 -0.251526
 H  1.757910 1.098106 -1.790123
 C  4.601516 0.142984 0.651560
 H  4.457343 -1.830970 -0.187115
 C  4.116065 1.465701 0.652283
 H  2.690272 2.798011 -0.277127
 H  5.404703 -0.139915 1.325708
 C  4.630147 2.516743 1.546269
 H  4.182121 3.498582 1.391889
 C  5.560726 2.387019 2.502138
 H  6.051252 1.442622 2.725561
 H  5.861099 3.241199 3.102761
 H  0.185976 -2.806833 3.145800
 H  3.003191 -1.562556 -2.951226
Sum of electronic and thermal Free Energies= -1645.329869
SCF Energies= -1645.78468
S22.out
 O  1.496922 -1.330625 -1.028102
 C  1.554391 -2.597152 -0.345862
 C  2.980208 -2.880446 0.178983
 C  3.999931 -2.072274 -0.627426
 C  3.742006 -0.558756 -0.520542
 C  2.230628 -0.332430 -0.330068
 C  0.515684 -2.676087 0.767487
 H  1.322652 -3.336060 -1.117181
 O  3.215743 -4.280333 0.049076
 H  3.064823 -2.584966 1.236333
 O  5.294375 -2.436719 -0.148987
 H  5.941951 -2.134061 -0.806998
 H  3.890964 -2.351062 -1.683733
 O  4.242503 0.033764 -1.716740
 H  4.267739 -0.165989 0.360329
 O  1.888637 0.925033 -0.850261
 H  1.984569 -0.373211 0.737663
 C  0.503056 1.259218 -0.777533
 O  0.000193 1.180846 0.535347
 C  0.615423 2.068487 1.492847
 C  0.421967 3.517123 1.044933
 C  0.992890 3.694749 -0.360885
 C  0.372595 2.681965 -1.330255
 H  -0.084069 0.543287 -1.354856
 C  -0.047949 1.735411 2.819852
 H  1.687936 1.848762 1.557494
 O  0.153460 0.363499 3.164965
 H  -0.192056 -0.155510 2.419021
 H  -1.120049 1.973642 2.759167
 H  0.397400 2.337713 3.614828
```

```
 O  1.088945 4.353050 1.989029
 H  1.038082 5.259549 1.640774
 H  -0.654736 3.743888 1.016304
 O  0.717092 5.032565 -0.774216
 H  1.061031 5.117363 -1.680365
 H  2.079074 3.525592 -0.317425
 O  0.927973 2.800431 -2.636578
 H  1.848325 2.485850 -2.581543
 H  -0.694558 2.901146 -1.429430
 O  -0.749816 -2.331340 0.221312
 H  0.772992 -1.994359 1.591608
 H  0.514137 -3.699352 1.173557
 H  4.013509 0.978458 -1.684564
 C  -1.805228 -2.400559 1.187610
 C  -3.034485 -1.761603 0.596867
 H  -1.502091 -1.866200 2.100873
 C  -3.036251 -0.390727 0.306193
 C  -4.182271 -2.510948 0.310671
 C  -4.160325 0.210669 -0.253180
 H  -2.152849 0.204949 0.518924
 C  -5.309560 -1.909391 -0.244098
 H  -4.192558 -3.576754 0.525462
 C  -5.321143 -0.533538 -0.539299
 H  -4.146304 1.275999 -0.471605
 H  -6.184470 -2.518113 -0.452266
 C  -6.480663 0.157540 -1.128581
 H  -6.332708 1.224501 -1.296187
 C  -7.659685 -0.380678 -1.470206
 H  -7.889240 -1.435255 -1.337736
 H  -8.445227 0.233225 -1.902031
 H  4.147311 -4.420806 0.294488
 H  -1.997102 -3.447047 1.465275
Sum of electronic and thermal Free Energies= -1645.318956
SCF Energies= -1645.76914
S23.out
 O  0.047418 0.024375 -0.555046
 C  -0.031019 0.020913 0.893427
 C  -0.359825 1.424088 1.404354
 C  0.675665 2.415990 0.886531
 C  0.756641 2.352585 -0.640023
 C  1.007720 0.916371 -1.112294
 C  -1.053921 -1.033747 1.300527
 H  0.941403 -0.285475 1.298899
 O  -0.355054 1.361885 2.830040
 H  -1.350738 1.720208 1.032898
 O  0.288850 3.718565 1.322244
 H  0.940019 4.337126 0.948038
 H  1.656692 2.150050 1.307955
 O  1.748894 3.238717 -1.146468
 H  -0.199213 2.683936 -1.056165
 O  2.319220 0.570126 -0.729524
 H  0.886702 0.830973 -2.195746
 C  3.054908 -0.332955 -1.566606
 O  4.414617 0.004602 -1.461756
 C  4.976078 -0.142884 -0.136735
 C  4.831509 -1.591742 0.345357
 C  3.370736 -2.027202 0.256724
 C  2.840973 -1.798911 -1.160393
 H  2.768053 -0.174979 -2.611134
 C  6.424110 0.294496 -0.228116
 H  4.445471 0.518658 0.558573
 O  6.450940 1.693552 -0.518971
 H  7.384646 1.952675 -0.577759
```

```
 H  6.925287 -0.286602 -1.015885
 H  6.917196 0.075392 0.727444
 O  5.306843 -1.651158 1.690496
 H  5.125345 -2.552908 2.006049
 H  5.429552 -2.247958 -0.305361
 O  3.304362 -3.408085 0.613640
 H  2.376786 -3.673641 0.486242
 H  2.784613 -1.426221 0.966378
 O  1.497862 -2.241728 -1.309551
 H  0.898706 -1.567373 -0.922660
 H  3.436842 -2.405577 -1.850587
 O  -2.414107 -0.652928 1.132257
 H  -0.931139 -1.227589 2.369178
 H  -0.835873 -1.962568 0.752183
 H  2.610459 2.849609 -0.906896
 C  -2.867836 -0.613098 -0.230667
 C  -4.373441 -0.559137 -0.233237
 H  -2.510578 -1.513361 -0.753613
 C  -5.057301 0.461191 -0.906703
 C  -5.120622 -1.540763 0.429855
 C  -6.449331 0.499650 -0.927205
 H  -4.491392 1.233783 -1.421690
 C  -6.512256 -1.501418 0.416014
 H  -4.606149 -2.337014 0.961169
 C  -7.207300 -0.481182 -0.261435
 H  -6.947804 1.301986 -1.463154
 H  -7.076623 -2.272416 0.935348
 C  -8.680058 -0.488561 -0.240682
 H  -9.120669 -1.342907 0.273369
 C  -9.502844 0.427068 -0.770807
 H  -9.145418 1.311909 -1.291961
 H  -10.580748 0.314847 -0.693635
 H  -0.492871 2.270678 3.147039
 H  -2.452826 0.256877 -0.750725
Sum of electronic and thermal Free Energies= -1645.326078
SCF Energies= -1645.774538
S24.out
 O  -0.034246 2.048567 -1.051112
 C  0.726497 1.434893 0.015093
 C  1.320573 0.092161 -0.436165
 C  0.239583 -0.808835 -1.023795
 C  -0.525887 -0.055898 -2.113179
 C  -1.084251 1.261773 -1.556099
 C  1.787843 2.438735 0.432284
 H  0.069736 1.261162 0.877157
 O  1.931021 -0.515236 0.705537
 H  2.070529 0.286064 -1.210222
 O  0.865607 -1.973441 -1.564422
 H  0.169957 -2.434927 -2.065587
 H  -0.455679 -1.092634 -0.221132
 O  -1.505617 -0.874050 -2.742718
 H  0.184213 0.218268 -2.900812
 O  -2.022914 1.061940 -0.491097
 H  -1.558076 1.845390 -2.352764
 C  -3.370970 0.851558 -0.831826
 O  -3.659331 -0.535858 -1.013982
 C  -3.470044 -1.354923 0.166380
 C  -4.386806 -0.861567 1.288191
 C  -4.118684 0.615141 1.563252
 C  -4.264754 1.425331 0.278834
 H  -3.601143 1.316814 -1.795489
 C  -3.712207 -2.792096 -0.249248
 H  -2.430259 -1.273863 0.503471
```

```
 O  -5.070313 -2.943591 -0.664072
 H  -5.201626 -3.882417 -0.873122
 H  -3.477057 -3.441537 0.603775
 H  -3.017208 -3.035328 -1.066093
 O  -4.114454 -1.657646 2.440130
 H  -4.647973 -1.286731 3.163791
 H  -5.433631 -0.975968 0.976153
 O  -5.056392 1.040350 2.552534
 H  -4.865503 1.976237 2.734325
 H  -3.091888 0.723440 1.940843
 O  -3.934541 2.775920 0.582283
 H  -4.276726 3.333943 -0.135605
 H  -5.303278 1.343196 -0.066317
 O  2.699311 2.677788 -0.643485
 H  2.300421 2.039949 1.312961
 H  1.303406 3.382525 0.715850
 H  -2.270787 -0.966899 -2.133779
 C  4.079405 2.758812 -0.243012
 C  4.632660 1.407761 0.145031
 H  4.195461 3.477838 0.578741
 C  4.915237 1.087240 1.475353
 C  4.783761 0.408145 -0.830280
 C  5.324478 -0.199509 1.827672
 H  4.804628 1.847249 2.244808
 C  5.184862 -0.876959 -0.483582
 H  4.569197 0.641319 -1.870269
 C  5.459923 -1.209799 0.860694
 H  5.534325 -0.429996 2.869241
 H  5.287474 -1.627728 -1.261297
 C  5.879403 -2.554567 1.289167
 H  6.061572 -2.650759 2.359515
 C  6.051631 -3.634457 0.514418
 H  5.889101 -3.622929 -0.560605
 H  6.365348 -4.581260 0.945092
 H  2.725951 -0.979619 0.395764
 H  4.600964 3.153600 -1.120281
Sum of electronic and thermal Free Energies= -1645.324952
SCF Energies= -1645.775899
S25.out
 O  -2.102158 -0.292760 -1.112727
 C  -3.418482 0.244109 -0.862806
 C  -4.169407 -0.569213 0.208605
 C  -3.749490 -2.035943 0.130354
 C  -2.247993 -2.199266 0.417497
 C  -1.500889 -0.909753 0.023244
 C  -3.345045 1.735783 -0.572564
 H  -3.962665 0.116268 -1.804486
 O  -5.561918 -0.415191 -0.057318
 H  -3.936753 -0.190803 1.213122
 O  -4.564334 -2.753856 1.058147
 H  -4.493940 -3.697559 0.839196
 H  -3.935607 -2.389612 -0.892656
 O  -1.797977 -3.334311 -0.319186
 H  -2.105816 -2.353308 1.496090
 O  -0.195451 -1.251764 -0.351443
 H  -1.490264 -0.205057 0.863352
 C  0.757730 -0.189571 -0.297849
 O  1.522699 -0.262245 0.883060
 C  2.321593 -1.451262 1.019134
 C  3.280360 -1.575938 -0.171839
 C  2.502699 -1.561402 -1.482220
 C  1.634643 -0.302835 -1.547750
 H  0.243596 0.771278 -0.271770
```

```
 C  3.054661 -1.315151 2.354077
 H  1.673950 -2.336669 1.055419
 O  3.704195 -2.527480 2.728885
 H  4.209051 -2.811833 1.942130
 H  2.325448 -1.080199 3.135471
 H  3.766975 -0.477834 2.291316
 O  4.009862 -2.800463 -0.010552
 H  4.707379 -2.809370 -0.687766
 H  3.970068 -0.719611 -0.160696
 O  3.441917 -1.592393 -2.556335
 H  2.922399 -1.505601 -3.374467
 H  1.853883 -2.449439 -1.517237
 O  0.848057 -0.264248 -2.734634
 H  0.125635 -0.906252 -2.606686
 H  2.289852 0.571665 -1.579050
 O  -2.839315 1.958185 0.743531
 H  -4.346534 2.180953 -0.670241
 H  -2.692298 2.189696 -1.327647
 H  -0.831978 -3.374423 -0.210395
 C  -2.274730 3.271319 0.937206
 C  -0.800176 3.275260 0.615973
 H  -2.435795 3.509027 1.992937
 C  0.124660 2.886253 1.597985
 C  -0.323300 3.583377 -0.664389
 C  1.480136 2.786577 1.308167
 H  -0.228646 2.660014 2.601216
 C  1.035463 3.471292 -0.961550
 H  -1.017711 3.911095 -1.433556
 C  1.959549 3.051131 0.011019
 H  2.171162 2.491225 2.091162
 H  1.386766 3.697068 -1.965371
 C  3.370810 2.871284 -0.367334
 H  3.655815 3.327607 -1.315287
 C  4.292090 2.174618 0.314103
 H  4.070263 1.666651 1.249234
 H  5.310168 2.087471 -0.055183
 H  -6.017847 -1.030839 0.543074
 H  -2.820472 4.006590 0.332982
Sum of electronic and thermal Free Energies= -1645.322936
SCF Energies= -1645.774107
S26.out
 O  -0.203387 -0.861208 -0.555067
 C  -0.239934 -0.556149 0.858644
 C  -0.360123 0.958342 1.083296
 C  0.772426 1.670763 0.350344
 C  0.706849 1.305313 -1.134932
 C  0.822362 -0.225118 -1.274578
 C  -1.386313 -1.349451 1.453298
 H  0.686557 -0.902460 1.333197
 O  -0.286149 1.192026 2.488753
 H  -1.322382 1.309130 0.684813
 O  0.654244 3.077511 0.567741
 H  1.562554 3.426033 0.530420
 H  1.717835 1.323777 0.775398
 O  1.639274 2.009133 -1.941241
 H  -0.282823 1.575206 -1.518800
 O  2.067852 -0.744657 -0.770191
 H  0.708557 -0.526315 -2.321143
 C  3.229835 -0.576635 -1.550314
 O  3.900283 0.649069 -1.260594
 C  4.359123 0.772703 0.108164
 C  5.400023 -0.321036 0.401937
 C  4.758232 -1.682310 0.149565
```

```
 C  4.168566 -1.751620 -1.264797
 H  2.978375 -0.526378 -2.613599
 C  4.880329 2.191140 0.275617
 H  3.514578 0.628178 0.789239
 O  3.842042 3.177451 0.203520
 H  3.598687 3.289489 -0.729439
 H  5.660017 2.392203 -0.470316
 H  5.319901 2.283524 1.271725
 O  5.805408 -0.275536 1.771197
 H  6.526384 0.370077 1.845782
 H  6.263270 -0.200236 -0.265952
 O  5.741876 -2.700273 0.318098
 H  5.323329 -3.524834 0.013289
 H  3.943311 -1.815677 0.878327
 O  3.522369 -2.999827 -1.488917
 H  2.707051 -2.987099 -0.954475
 H  4.992585 -1.698165 -1.982143
 O  -2.611637 -0.911801 0.879888
 H  -1.387593 -1.203046 2.542896
 H  -1.230586 -2.420009 1.253123
 H  2.537490 1.724708 -1.666788
 C  -3.745256 -1.550400 1.474344
 C  -4.994897 -1.049853 0.797578
 H  -3.767436 -1.321595 2.552238
 C  -5.941463 -1.937699 0.279622
 C  -5.235113 0.329162 0.684055
 C  -7.101256 -1.462758 -0.333770
 H  -5.771224 -3.008917 0.353482
 C  -6.384549 0.804395 0.063994
 H  -4.508953 1.031656 1.084216
 C  -7.343917 -0.084814 -0.462400
 H  -7.825821 -2.169846 -0.730574
 H  -6.543918 1.876572 -0.003980
 C  -8.575045 0.362517 -1.135322
 H  -9.260506 -0.440965 -1.405356
 C  -8.916153 1.620493 -1.447474
 H  -8.283723 2.476554 -1.225073
 H  -9.857011 1.832142 -1.947995
 H  -0.155492 2.151674 2.588344
 H  -3.662767 -2.642398 1.372409
Sum of electronic and thermal Free Energies= -1645.325570
SCF Energies= -1645.778781
S27.out
 O  -0.066563 -0.900622 1.613456
 C  -0.418381 -1.260265 0.261516
 C  0.304573 -2.543987 -0.195656
 C  1.803875 -2.405032 0.026049
 C  2.073066 -2.001984 1.479215
 C  1.309325 -0.716912 1.835357
 C  -1.934471 -1.417626 0.298875
 H  -0.149715 -0.448260 -0.424742
 O  0.076412 -2.779707 -1.584288
 H  -0.061912 -3.388575 0.409268
 O  2.438744 -3.648112 -0.272377
 H  3.372796 -3.526973 -0.025223
 H  2.180961 -1.622115 -0.645069
 O  3.462309 -1.935340 1.768827
 H  1.671806 -2.784889 2.131392
 O  1.714539 0.417998 1.056604
 H  1.426131 -0.484759 2.898939
 C  2.890314 1.100200 1.439265
 O  4.040840 0.590088 0.777291
 C  4.015914 0.704985 -0.664719
```

```
 C  3.938712 2.182382 -1.054723
 C  2.695236 2.798312 -0.417289
 C  2.696994 2.583029 1.098655
 H  3.084925 0.964096 2.506785
 C  5.255421 -0.000473 -1.173109
 H  3.130057 0.192369 -1.055916
 O  5.106007 -1.396683 -0.895424
 H  5.954948 -1.826566 -1.088234
 H  6.140183 0.412326 -0.669805
 H  5.351690 0.181646 -2.250719
 O  3.877382 2.256802 -2.478027
 H  3.663444 3.180246 -2.696237
 H  4.828975 2.706120 -0.674703
 O  2.690341 4.189041 -0.737345
 H  1.887115 4.562220 -0.335034
 H  1.809038 2.306478 -0.845567
 O  1.515689 3.101688 1.699959
 H  0.794081 2.496282 1.448298
 H  3.535231 3.138416 1.529072
 O  -2.383119 -1.706454 -1.027224
 H  -2.390958 -0.492400 0.671431
 H  -2.203238 -2.237727 0.980029
 H  3.859415 -1.222161 1.223769
 C  -3.763127 -2.091416 -1.093496
 C  -4.706993 -0.961733 -0.747821
 H  -3.941551 -2.956030 -0.439534
 C  -5.812761 -1.175419 0.084793
 C  -4.496706 0.320851 -1.268577
 C  -6.696683 -0.140703 0.379951
 H  -5.981676 -2.163251 0.506917
 C  -5.373800 1.359220 -0.966146
 H  -3.635723 0.504625 -1.905415
 C  -6.493765 1.151674 -0.138861
 H  -7.545313 -0.340434 1.027447
 H  -5.194498 2.350089 -1.376719
 C  -7.388468 2.286459 0.145575
 H  -7.098280 3.222109 -0.332522
 C  -8.489328 2.278213 0.909897
 H  -8.846812 1.388202 1.422140
 H  -9.076119 3.182111 1.047682
 H  -0.889190 -2.687346 -1.712451
 H  -3.910143 -2.414092 -2.129401
Sum of electronic and thermal Free Energies= -1645.328409
SCF Energies= -1645.778565
S28.out
 O  1.456033 -1.356340 -1.045292
 C  1.512588 -2.591358 -0.308373
 C  2.954025 -2.879637 0.171122
 C  3.956101 -2.128190 -0.712429
 C  3.727669 -0.604435 -0.678547
 C  2.236142 -0.347657 -0.413248
 C  0.517072 -2.583541 0.846545
 H  1.233953 -3.361481 -1.032542
 O  3.160255 -4.288192 0.092861
 H  3.086956 -2.541827 1.210587
 O  5.260924 -2.493872 -0.264263
 H  5.890098 -2.221028 -0.952466
 H  3.801608 -2.458860 -1.747909
 O  4.158824 -0.085184 -1.934562
 H  4.311051 -0.171196 0.145525
 O  1.875715 0.901562 -0.940971
 H  2.052501 -0.362779 0.666463
 C  0.495033 1.228229 -0.784787
```

```
 O  0.068133 1.125153 0.555328
 C  0.710233 2.018766 1.486985
 C  0.475893 3.468989 1.057143
 C  0.947063 3.668892 -0.381892
 C  0.288564 2.654329 -1.312658
 H  -0.117805 0.507753 -1.330213
 C  0.124462 1.705543 2.849270
 H  1.789702 1.822147 1.503444
 O  0.548220 0.390954 3.226942
 H  -0.014146 0.102112 3.963692
 H  -0.970056 1.768309 2.790955
 H  0.477962 2.453444 3.570226
 O  1.198157 4.314608 1.950201
 H  1.130778 5.215400 1.589031
 H  -0.602345 3.686077 1.103270
 O  0.609785 5.007130 -0.750084
 H  0.950671 5.145521 -1.650169
 H  2.036322 3.526892 -0.414925
 O  0.843937 2.841695 -2.610727
 H  0.280628 2.367762 -3.245099
 H  -0.793687 2.839157 -1.319044
 O  -0.771305 -2.282167 0.324745
 H  0.804422 -1.834054 1.596236
 H  0.531632 -3.568463 1.338902
 H  3.884529 0.847798 -1.962491
 C  -1.718136 -1.971429 1.358377
 C  -2.989550 -1.493484 0.708327
 H  -1.298838 -1.190130 2.008532
 C  -4.096934 -2.341039 0.571557
 C  -3.070185 -0.195607 0.186981
 C  -5.259853 -1.906022 -0.058584
 H  -4.045421 -3.353680 0.964402
 C  -4.231213 0.240292 -0.447284
 H  -2.221621 0.475407 0.286561
 C  -5.351392 -0.601778 -0.580828
 H  -6.099693 -2.588912 -0.146932
 H  -4.279081 1.252685 -0.841733
 C  -6.555253 -0.081112 -1.251166
 H  -6.449912 0.928513 -1.648467
 C  -7.731179 -0.704583 -1.408894
 H  -7.923843 -1.707893 -1.036643
 H  -8.552705 -0.214981 -1.924564
 H  4.095366 -4.435945 0.319515
 H  -1.905371 -2.861526 1.976737
Sum of electronic and thermal Free Energies= -1645.315369
SCF Energies= -1645.763689
S29.out
 O  -2.076240 0.976552 -1.019352
 C  -2.064100 2.337299 -0.530329
 C  -2.937622 2.492412 0.733521
 C  -4.057208 1.454673 0.721869
 C  -3.480356 0.031832 0.744340
 C  -2.103266 0.033341 0.048716
 C  -0.652803 2.866029 -0.283566
 H  -2.528866 2.925234 -1.326961
 O  -3.455110 3.820258 0.717438
 H  -2.330591 2.342001 1.640204
 O  -4.898190 1.719742 1.844364
 H  -5.718692 1.215452 1.715764
 H  -4.620898 1.572221 -0.213316
 O  -4.424214 -0.814941 0.093493
 H  -3.332923 -0.277142 1.788392
 O  -1.893121 -1.254923 -0.460952
```

```
 H  -1.321407 0.285688 0.774852
 C  -0.647566 -1.496369 -1.112914
 O  0.456238 -1.103990 -0.336095
 C  0.601667 -1.787025 0.927626
 C  0.755795 -3.288496 0.682744
 C  -0.439052 -3.801822 -0.117877
 C  -0.608998 -2.999622 -1.412508
 H  -0.590265 -0.906332 -2.029685
 C  1.809043 -1.153661 1.602746
 H  -0.288622 -1.613702 1.544454
 O  1.620192 0.245245 1.816985
 H  1.629928 0.668473 0.941237
 H  2.706806 -1.339502 0.997625
 H  1.950985 -1.612128 2.584365
 O  0.841954 -3.929247 1.954997
 H  0.818145 -4.886674 1.785187
 H  1.670574 -3.464167 0.096145
 O  -0.207042 -5.182318 -0.396950
 H  -0.977447 -5.496318 -0.900648
 H  -1.344133 -3.683816 0.495869
 O  -1.751917 -3.426661 -2.147733
 H  -2.533830 -3.162628 -1.630058
 H  0.256964 -3.186050 -2.054370
 O  0.043674 3.167247 -1.495058
 H  -0.083745 2.165601 0.339916
 H  -0.738211 3.810323 0.264690
 H  -4.013459 -1.693974 0.022548
 C  0.848662 2.109456 -2.012388
 C  2.136613 1.881990 -1.244879
 H  1.081530 2.403603 -3.042840
 C  2.863635 0.699007 -1.454858
 C  2.642750 2.824863 -0.344873
 C  4.054749 0.461223 -0.779464
 H  2.480081 -0.047821 -2.145115
 C  3.832797 2.581238 0.342289
 H  2.096807 3.747107 -0.173679
 C  4.559981 1.395233 0.147022
 H  4.591588 -0.463966 -0.966337
 H  4.202614 3.320715 1.048587
 C  5.796790 1.177850 0.915484
 H  6.099336 2.021510 1.536015
 C  6.554395 0.072306 0.931852
 H  6.316124 -0.816044 0.351732
 H  7.452347 0.023315 1.541609
 H  -4.053150 3.886818 1.482211
 H  0.277176 1.175940 -2.064818
Sum of electronic and thermal Free Energies= -1645.323188
SCF Energies= -1645.774064
S3.out
 O  -0.228431 1.113516 -0.427430
 C  0.048054 1.412462 0.959714
 C  0.365775 2.902533 1.093811
 C  1.569736 3.222952 0.209179
 C  1.314707 2.794055 -1.238918
 C  0.865285 1.329721 -1.312565
 C  -1.163204 0.958563 1.745225
 H  0.920157 0.839071 1.291891
 O  0.650288 3.170417 2.465298
 H  -0.497418 3.492247 0.750812
 O  1.807676 4.627581 0.288473
 H  2.555328 4.812915 -0.306056
 H  2.436989 2.667383 0.597146
 O  2.454586 3.028215 -2.058552
```

```
 H  0.507579 3.410266 -1.645490
 O  1.972726 0.516944 -0.989965
 H  0.485288 1.087174 -2.308642
 C  2.077659 -0.764509 -1.634111
 O  3.408719 -1.189678 -1.487401
 C  3.823181 -1.450871 -0.127253
 C  2.925892 -2.518968 0.512311
 C  1.464982 -2.094567 0.405778
 C  1.116652 -1.821376 -1.058117
 H  1.904185 -0.637493 -2.707874
 C  5.280417 -1.882974 -0.191289
 H  3.744682 -0.527392 0.461226
 O  6.132858 -0.857397 -0.700138
 H  6.121785 -0.131217 -0.054036
 H  5.374416 -2.732688 -0.875409
 H  5.595657 -2.208956 0.807970
 O  3.317989 -2.659548 1.877332
 H  2.631064 -3.205541 2.298062
 H  3.057339 -3.469733 -0.027390
 O  0.658936 -3.137331 0.956068
 H  -0.232723 -2.763736 1.061742
 H  1.332578 -1.179848 0.993622
 O  -0.252338 -1.499174 -1.252484
 H  -0.453800 -0.695815 -0.725429
 H  1.292169 -2.736623 -1.633558
 O  -1.172608 -0.469771 1.728231
 H  -2.072626 1.366007 1.284623
 H  -1.100568 1.326578 2.777373
 H  3.118774 2.364062 -1.797623
 C  -2.396880 -1.040612 2.211988
 C  -3.545724 -0.834799 1.251714
 H  -2.639723 -0.629940 3.201979
 C  -3.444154 -1.306054 -0.067646
 C  -4.703477 -0.151493 1.631053
 C  -4.472729 -1.100359 -0.978529
 H  -2.545566 -1.832213 -0.377554
 C  -5.741193 0.049899 0.719517
 H  -4.794646 0.229170 2.645489
 C  -5.646998 -0.414907 -0.603015
 H  -4.365371 -1.478611 -1.990948
 H  -6.634690 0.584514 1.033051
 C  -6.765646 -0.163668 -1.527231
 H  -7.615918 0.349925 -1.078268
 C  -6.834494 -0.489262 -2.825621
 H  -6.029750 -0.996958 -3.351854
 H  -7.717461 -0.249018 -3.411437
 H  0.968033 4.088695 2.506144
 H  -2.176048 -2.107022 2.329028
Sum of electronic and thermal Free Energies= -1645.331188
SCF Energies= -1645.783198
S30.out
 O  -0.122632 0.169349 -0.335202
 C  -0.428642 -1.221065 -0.578095
 C  -0.704906 -1.939495 0.746415
 C  0.449076 -1.742027 1.725779
 C  0.754034 -0.256664 1.888553
 C  0.990714 0.379800 0.513665
 C  -1.607393 -1.285666 -1.544693
 H  0.429345 -1.693584 -1.072997
 O  -0.893538 -3.322842 0.449793
 H  -1.613854 -1.514509 1.194842
 O  0.053040 -2.333612 2.964847
 H  0.803309 -2.235263 3.575113
```

```
 H  1.340291 -2.248796 1.330279
 O  1.891430 -0.137006 2.740563
 H  -0.120347 0.235027 2.333772
 O  2.168047 -0.192101 -0.023851
 H  1.100168 1.465224 0.593399
 C  2.760695 0.550524 -1.078711
 O  3.399280 1.714156 -0.597711
 C  4.434327 1.448337 0.375086
 C  5.525860 0.561351 -0.249316
 C  4.920107 -0.726244 -0.825228
 C  3.749413 -0.398925 -1.765238
 H  1.994213 0.894468 -1.778501
 C  4.948867 2.786910 0.864891
 H  3.996591 0.922523 1.234673
 O  5.561904 3.488941 -0.219082
 H  5.978652 4.282029 0.154694
 H  5.663526 2.600720 1.676560
 H  4.104386 3.358063 1.276393
 O  6.558106 0.279689 0.694236
 H  6.162082 -0.251373 1.407616
 H  6.008255 1.115729 -1.061125
 O  5.902994 -1.533448 -1.469672
 H  6.271161 -1.011228 -2.204382
 H  4.541793 -1.335305 0.005323
 O  3.088852 -1.568470 -2.238057
 H  2.690819 -1.998025 -1.460165
 H  4.140689 0.112037 -2.651121
 O  -2.878537 -1.015179 -0.962743
 H  -1.673280 -2.305274 -1.933208
 H  -1.412689 -0.604011 -2.385446
 H  1.968183 0.795372 3.004490
 C  -3.114822 0.365154 -0.647770
 C  -4.586663 0.556122 -0.388818
 H  -2.789582 0.987580 -1.495853
 C  -5.038630 1.181218 0.776124
 C  -5.535602 0.123066 -1.329015
 C  -6.402843 1.380954 0.992506
 H  -4.319958 1.515259 1.520434
 C  -6.894737 0.314744 -1.112986
 H  -5.197990 -0.374351 -2.234198
 C  -7.358612 0.955270 0.054645
 H  -6.735018 1.871136 1.904544
 H  -7.602592 -0.036340 -1.857971
 C  -8.785063 1.195610 0.331199
 H  -8.986290 1.655830 1.298754
 C  -9.824216 0.919743 -0.469334
 H  -9.711048 0.468750 -1.452170
 H  -10.840045 1.145795 -0.157116
 H  -0.999996 -3.774690 1.304415
 H  -2.528128 0.669099 0.226028
Sum of electronic and thermal Free Energies= -1645.326171
SCF Energies= -1645.774049
S31.out
 O  -0.457107 0.858876 0.214259
 C  -0.146538 1.959264 -0.667500
 C  -0.456994 3.289541 0.042552
 C  -1.908146 3.310180 0.531670
 C  -2.201636 2.070044 1.368581
 C  -1.816234 0.811122 0.592738
 C  1.313240 1.820891 -1.038426
 H  -0.757764 1.884018 -1.573845
 O  -0.306665 4.402203 -0.843559
 H  0.203499 3.395837 0.913157
```

```
 O  -2.163780 4.449019 1.352803
 H  -1.976650 5.230626 0.804944
 H  -2.571075 3.316289 -0.344435
 O  -3.578559 1.943182 1.716333
 H  -1.578754 2.103844 2.272817
 O  -2.671053 0.744904 -0.532769
 H  -1.918023 -0.060003 1.239646
 C  -3.027345 -0.500544 -1.124197
 O  -1.928912 -1.298844 -1.501600
 C  -1.351394 -2.220009 -0.547358
 C  -2.432148 -3.123977 0.046509
 C  -3.498351 -2.260109 0.712621
 C  -4.086684 -1.271072 -0.296989
 H  -3.487355 -0.188247 -2.063141
 C  -0.282961 -2.976509 -1.319706
 H  -0.860070 -1.671709 0.264201
 O  0.881262 -2.187141 -1.556635
 H  0.621085 -1.265454 -1.744018
 H  -0.722169 -3.335120 -2.262651
 H  0.037378 -3.845285 -0.738938
 O  -1.802732 -3.985880 0.993100
 H  -2.517903 -4.460354 1.450628
 H  -2.901680 -3.707512 -0.760201
 O  -4.515814 -3.135122 1.203335
 H  -5.182468 -2.570788 1.631370
 H  -3.038947 -1.723775 1.554718
 O  -5.021881 -0.384924 0.305973
 H  -4.523731 0.326246 0.757490
 H  -4.655608 -1.871221 -1.015126
 O  1.468558 0.631402 -1.813818
 H  1.923203 1.777048 -0.126950
 H  1.627909 2.694301 -1.626094
 H  -3.869274 2.793018 2.088916
 C  2.819651 0.380219 -2.205448
 C  3.745800 0.035144 -1.056037
 H  3.214892 1.243074 -2.760819
 C  3.279876 -0.641501 0.076990
 C  5.106554 0.363464 -1.129044
 C  4.157502 -0.987397 1.102620
 H  2.228004 -0.896038 0.150253
 C  5.985737 0.007592 -0.110583
 H  5.480454 0.905966 -1.994458
 C  5.528557 -0.681122 1.029221
 H  3.778108 -1.510578 1.977407
 H  7.033671 0.279306 -0.198378
 C  6.410243 -1.088973 2.135868
 H  5.894169 -1.552763 2.976691
 C  7.742892 -0.960761 2.201126
 H  8.333651 -0.518918 1.402295
 H  8.290933 -1.303642 3.074378
 H  0.622818 4.681018 -0.819203
 H  2.755431 -0.463522 -2.901268
Sum of electronic and thermal Free Energies= -1645.324767
SCF Energies= -1645.775262
S32.out
 O  -0.387132 -2.606778 -1.183954
 C  0.488223 -2.394183 -0.055037
 C  -0.176922 -2.919393 1.224819
 C  -1.547000 -2.269606 1.403458
 C  -2.392163 -2.440856 0.138704
 C  -1.614103 -1.921921 -1.079036
 C  1.803529 -3.105669 -0.338494
 H  0.669336 -1.321185 0.063879
```

```
 O  0.685917 -2.615303 2.320873
 H  -0.318505 -4.007183 1.133367
 O  -2.172655 -2.885252 2.530631
 H  -3.041711 -2.458713 2.627280
 H  -1.396822 -1.198759 1.595741
 O  -3.682517 -1.857570 0.273631
 H  -2.557518 -3.511185 -0.023619
 O  -1.316447 -0.526761 -0.967534
 H  -2.164924 -2.110415 -2.006208
 C  -2.220557 0.413435 -1.486964
 O  -3.196267 0.794716 -0.516712
 C  -2.662660 1.460023 0.659357
 C  -1.861408 2.713244 0.270278
 C  -0.777111 2.333224 -0.728407
 C  -1.424034 1.646475 -1.933358
 H  -2.791671 -0.011714 -2.318439
 C  -3.867141 1.750610 1.541019
 H  -1.993547 0.775759 1.193313
 O  -4.776712 2.673406 0.943112
 H  -5.026635 2.295654 0.082529
 H  -3.529013 2.198361 2.479510
 H  -4.362983 0.797923 1.776808
 O  -1.227974 3.257865 1.428571
 H  -1.880808 3.810942 1.887315
 H  -2.532602 3.449132 -0.188660
 O  -0.073255 3.507850 -1.128898
 H  0.533320 3.230529 -1.837679
 H  -0.087520 1.631810 -0.240463
 O  -0.389418 1.299397 -2.847361
 H  -0.797677 1.128220 -3.712272
 H  -2.129976 2.345891 -2.398242
 O  2.408040 -2.803724 -1.599256
 H  1.642431 -4.188374 -0.355933
 H  2.486441 -2.871800 0.487013
 H  -3.599716 -0.886916 0.154918
 C  2.397064 -1.437837 -2.029547
 C  3.033450 -0.447298 -1.079603
 H  1.372414 -1.118273 -2.257452
 C  4.140896 -0.780620 -0.287465
 C  2.515250 0.848861 -0.993320
 C  4.704254 0.155359 0.575223
 H  4.555248 -1.783551 -0.343006
 C  3.077838 1.788331 -0.132271
 H  1.665160 1.121043 -1.609491
 C  4.183602 1.461571 0.672767
 H  5.555779 -0.134639 1.183930
 H  2.642608 2.783736 -0.075695
 C  4.739991 2.487555 1.570229
 H  4.191079 3.429435 1.574255
 C  5.824714 2.381367 2.350431
 H  6.431288 1.480196 2.400129
 H  6.143248 3.212231 2.973918
 H  0.206919 -2.869879 3.128168
 H  2.949452 -1.457070 -2.976432
Sum of electronic and thermal Free Energies= -1645.327776
SCF Energies= -1645.780865
S33.out
 O  2.088088 -0.813364 0.781943
 C  2.846325 -1.172415 -0.390453
 C  4.276842 -0.628733 -0.280650
 C  4.257886 0.873110 -0.010219
 C  3.389748 1.190481 1.209667
 C  1.999298 0.572373 1.036676
```

```
 C  2.833360 -2.692076 -0.488999
 H  2.363302 -0.749234 -1.279568
 O  4.947348 -0.922079 -1.506600
 H  4.781300 -1.123622 0.563659
 O  5.607454 1.291807 0.196702
 H  5.570371 2.245145 0.387188
 H  3.835277 1.379605 -0.890003
 O  3.321849 2.592841 1.452652
 H  3.848853 0.745152 2.096898
 O  1.389759 1.282613 -0.031090
 H  1.403964 0.669148 1.946485
 C  0.006582 1.053052 -0.242637
 O  -0.695814 1.388810 0.946012
 C  -1.905616 2.166880 0.805427
 C  -2.672376 1.650838 -0.419291
 C  -1.888453 1.915679 -1.701431
 C  -0.368865 1.927821 -1.440534
 H  -0.162174 -0.005869 -0.467138
 C  -2.670446 1.985643 2.106915
 H  -1.659244 3.228924 0.685031
 O  -3.145443 0.651332 2.290498
 H  -2.395248 0.055058 2.119453
 H  -3.548506 2.636733 2.100829
 H  -2.022130 2.291676 2.940545
 O  -3.964344 2.246523 -0.530980
 H  -4.570674 1.692185 -0.010468
 H  -2.764127 0.568314 -0.304541
 O  -2.255384 0.900631 -2.636652
 H  -1.886638 1.149745 -3.500862
 H  -2.157879 2.910372 -2.080495
 O  0.019186 3.281784 -1.207616
 H  0.917963 3.254432 -0.832843
 H  0.146478 1.521681 -2.322063
 O  1.532506 -3.217709 -0.733317
 H  3.270064 -3.126784 0.420110
 H  3.454086 -2.985379 -1.340006
 H  2.790172 2.974261 0.730546
 C  0.744771 -3.493575 0.428398
 C  -0.651001 -2.924577 0.309940
 H  1.225486 -3.100498 1.328944
 C  -1.455020 -2.835585 1.453847
 C  -1.192907 -2.531185 -0.919977
 C  -2.764399 -2.368258 1.368105
 H  -1.052984 -3.137498 2.418374
 C  -2.500123 -2.056335 -1.005488
 H  -0.584911 -2.595251 -1.816039
 C  -3.311297 -1.954848 0.138801
 H  -3.369426 -2.299571 2.268933
 H  -2.891089 -1.758642 -1.972688
 C  -4.677462 -1.404953 0.109051
 H  -5.265615 -1.591160 1.007372
 C  -5.230050 -0.687229 -0.880462
 H  -4.691041 -0.422668 -1.786316
 H  -6.251113 -0.324328 -0.800001
 H  5.820810 -0.497950 -1.451599
 H  0.682266 -4.586139 0.547742
Sum of electronic and thermal Free Energies= -1645.324595
SCF Energies= -1645.778476
S34.out
 O  -0.355925 -1.671889 -1.128033
 C  -0.113062 -2.458099 0.059254
 C  -1.185645 -3.549771 0.168036
 C  -2.576587 -2.921538 0.152814
```

```
 C  -2.764700 -2.011023 -1.064582
 C  -1.604841 -1.010674 -1.144283
 C  1.290957 -3.039680 -0.054391
 H  -0.162075 -1.812354 0.944769
 O  -0.967008 -4.263636 1.385412
 H  -1.097486 -4.224440 -0.697666
 O  -3.527749 -3.987502 0.150818
 H  -4.406575 -3.570478 0.141165
 H  -2.689382 -2.318181 1.065869
 O  -4.029509 -1.357908 -1.028385
 H  -2.751788 -2.624263 -1.970392
 O  -1.771980 -0.167245 -0.024636
 H  -1.626309 -0.432692 -2.071957
 C  -1.118019 1.083894 -0.019075
 O  -1.677841 1.975870 -0.960364
 C  -3.121948 2.090560 -0.900736
 C  -3.656166 2.143110 0.549992
 C  -2.544679 2.516183 1.552649
 C  -1.270983 1.637297 1.415023
 H  -0.068957 0.970575 -0.306189
 C  -3.471124 3.316481 -1.733989
 H  -3.564870 1.219656 -1.396083
 O  -3.037853 4.550887 -1.139016
 H  -3.764284 4.880926 -0.583872
 H  -4.551554 3.333082 -1.912978
 H  -2.961827 3.236023 -2.698754
 O  -4.227913 0.862644 0.857325
 H  -4.671490 0.929092 1.719337
 H  -4.437453 2.910549 0.618427
 O  -2.223631 3.903548 1.451141
 H  -2.165569 4.133289 0.499525
 H  -2.931630 2.362828 2.565512
 O  -1.202660 0.590892 2.380627
 H  -1.795132 -0.112311 2.060428
 H  -0.422778 2.296033 1.616122
 O  2.328594 -2.115475 0.257114
 H  1.428770 -3.457945 -1.062949
 H  1.390370 -3.848676 0.673664
 H  -4.010730 -0.707259 -0.292987
 C  2.563546 -1.110175 -0.740085
 C  3.894687 -0.459603 -0.466389
 H  1.763779 -0.361451 -0.731947
 C  4.003238 0.930628 -0.333474
 C  5.055339 -1.235403 -0.353821
 C  5.237672 1.534987 -0.108715
 H  3.109158 1.545563 -0.404741
 C  6.289540 -0.634418 -0.122143
 H  4.987172 -2.316079 -0.445992
 C  6.409414 0.763350 -0.000865
 H  5.286009 2.615017 -0.005339
 H  7.180733 -1.252023 -0.039173
 C  7.742005 1.345359 0.232480
 H  8.540168 0.613024 0.355066
 C  8.058442 2.646070 0.299757
 H  7.325410 3.440126 0.178832
 H  9.083492 2.959148 0.477674
 H  -1.732725 -4.852499 1.499184
 H  2.562845 -1.580988 -1.735317
Sum of electronic and thermal Free Energies= -1645.324068
SCF Energies= -1645.774518
S35.out
 O  -1.658936 -0.957353 -0.925561
 C  -1.454668 -2.123124 -0.103661
```

```
 C  -2.759155 -2.923327 -0.058788
 C  -3.855851 -2.031567 0.525170
 C  -3.969862 -0.713261 -0.249006
 C  -2.595966 -0.043407 -0.384295
 C  -0.269973 -2.881500 -0.664728
 H  -1.196131 -1.813609 0.915397
 O  -2.555588 -4.077507 0.754885
 H  -3.041127 -3.212952 -1.082346
 O  -5.079882 -2.766030 0.473421
 H  -5.754937 -2.206509 0.894264
 H  -3.593832 -1.808752 1.569434
 O  -4.923399 0.163990 0.343620
 H  -4.332404 -0.934951 -1.257186
 O  -2.233693 0.378859 0.915906
 H  -2.649629 0.791088 -1.086124
 C  -1.164269 1.300782 1.149149
 O  -0.021035 1.097066 0.354865
 C  0.045155 1.708608 -0.959544
 C  -0.191155 3.217899 -0.846377
 C  -1.556422 3.454114 -0.209043
 C  -1.617864 2.777405 1.154566
 H  -0.854635 1.042582 2.163424
 C  1.397263 1.325640 -1.542747
 H  -0.721651 1.286394 -1.616008
 O  1.405928 0.004244 -2.070855
 H  1.121973 -0.615694 -1.364314
 H  2.173491 1.463404 -0.774886
 H  1.623240 1.992540 -2.379903
 O  -0.224234 3.833688 -2.136943
 H  0.683127 4.086393 -2.370668
 H  0.585767 3.673385 -0.218608
 O  -1.803059 4.843184 0.008781
 H  -1.684780 5.279129 -0.853042
 H  -2.328939 3.032439 -0.869124
 O  -2.919780 2.836805 1.727101
 H  -3.155690 3.779045 1.772328
 H  -0.895427 3.303344 1.796448
 O  0.898440 -2.124393 -0.342700
 H  -0.361756 -3.008773 -1.751987
 H  -0.215673 -3.871524 -0.196143
 H  -4.487046 0.557232 1.121760
 C  2.126123 -2.806974 -0.596565
 C  3.279941 -1.922821 -0.185022
 H  2.203712 -3.068717 -1.661487
 C  3.114010 -0.879036 0.737105
 C  4.555317 -2.152485 -0.712249
 C  4.192327 -0.085134 1.116661
 H  2.129365 -0.668693 1.139716
 C  5.636498 -1.363534 -0.324200
 H  4.703565 -2.950088 -1.436415
 C  5.480963 -0.313405 0.598721
 H  4.024454 0.723830 1.821610
 H  6.619235 -1.556848 -0.747673
 C  6.656669 0.491028 0.971774
 H  7.570609 0.231724 0.437019
 C  6.711204 1.472258 1.883459
 H  5.848735 1.786878 2.466185
 H  7.641948 1.998256 2.077325
 H  -3.434068 -4.471661 0.893965
 H  2.138684 -3.748253 -0.025402
Sum of electronic and thermal Free Energies= -1645.323832
SCF Energies= -1645.775106
S36.out
```

```
 O  2.121017 -0.270003 0.904957
 C  2.943746 -0.490355 -0.258249
 C  3.765832 0.768204 -0.569222
 C  2.863643 1.992133 -0.676627
 C  1.994517 2.129418 0.568150
 C  1.224580 0.818494 0.809935
 C  3.862836 -1.667796 0.046664
 H  2.309895 -0.729144 -1.120580
 O  4.458724 0.540478 -1.796500
 H  4.480009 0.938218 0.251461
 O  3.716075 3.126507 -0.851556
 H  3.134495 3.898459 -0.956710
 H  2.209798 1.871841 -1.552424
 O  1.148416 3.252469 0.370358
 H  2.647864 2.278560 1.439411
 O  0.292177 0.633001 -0.243800
 H  0.703300 0.854014 1.767770
 C  -1.021655 0.225795 0.132635
 O  -1.559514 1.082998 1.112363
 C  -1.995237 2.338252 0.555628
 C  -3.276102 2.117749 -0.273624
 C  -3.293414 0.687170 -0.864021
 C  -1.859905 0.229975 -1.176089
 H  -0.998841 -0.764051 0.589941
 C  -2.131885 3.298696 1.719752
 H  -1.214726 2.716898 -0.110171
 O  -0.868396 3.486105 2.382800
 H  -0.638282 2.627434 2.779936
 H  -2.881491 2.930947 2.432386
 H  -2.447129 4.278045 1.351396
 O  -3.362222 3.106315 -1.301561
 H  -2.624447 2.903434 -1.907689
 H  -4.169590 2.235645 0.347662
 O  -3.929158 -0.181648 0.068557
 H  -3.932670 -1.079593 -0.317803
 H  -3.855930 0.730346 -1.806549
 O  -1.349090 1.149465 -2.149900
 H  -0.405393 1.278842 -1.937117
 H  -1.860628 -0.785326 -1.588616
 O  3.247642 -2.950151 -0.006259
 H  4.334036 -1.504108 1.026782
 H  4.648028 -1.691592 -0.713031
 H  0.558738 3.364810 1.150188
 C  2.377962 -3.278809 1.076859
 C  0.908589 -3.233516 0.709168
 H  2.571251 -2.633606 1.941592
 C  -0.056122 -3.325009 1.720341
 C  0.479805 -3.181972 -0.622747
 C  -1.412011 -3.379389 1.406264
 H  0.257946 -3.362845 2.761000
 C  -0.875850 -3.231221 -0.938409
 H  1.216806 -3.113825 -1.415769
 C  -1.851217 -3.331116 0.070344
 H  -2.146684 -3.450511 2.204706
 H  -1.176097 -3.205583 -1.981706
 C  -3.295619 -3.368984 -0.205465
 H  -3.916818 -3.624648 0.652955
 C  -3.905751 -3.095644 -1.371024
 H  -3.360984 -2.810967 -2.267828
 H  -4.986727 -3.158600 -1.459344
 H  4.907327 1.375070 -2.015938
 H  2.631143 -4.304912 1.376847
Sum of electronic and thermal Free Energies= -1645.330278
```

```
SCF Energies= -1645.78723
S37.out
 O  1.903256 0.304982 -0.535429
 C  2.890489 -0.082259 0.439541
 C  3.832569 -1.126423 -0.173416
 C  3.024818 -2.305616 -0.710774
 C  1.943955 -1.830362 -1.684459
 C  1.094288 -0.737744 -1.029950
 C  3.626365 1.181130 0.863923
 H  2.394597 -0.519713 1.314796
 O  4.738156 -1.552529 0.844773
 H  4.379011 -0.667337 -1.011644
 O  3.937653 -3.196140 -1.353308
 H  3.403752 -3.929560 -1.705036
 H  2.541073 -2.808406 0.139957
 O  1.148147 -2.915989 -2.151698
 H  2.427657 -1.398851 -2.565418
 O  0.347392 -1.374864 -0.000368
 H  0.415505 -0.266799 -1.745553
 C  -0.614483 -0.547314 0.639891
 O  -1.667483 -0.215320 -0.241367
 C  -2.751693 -1.150147 -0.243532
 C  -3.476342 -1.054209 1.108656
 C  -2.484868 -0.872213 2.281861
 C  -1.069406 -1.314996 1.899290
 H  -0.155980 0.402039 0.915277
 C  -3.663248 -0.799117 -1.414819
 H  -2.377299 -2.171043 -0.377513
 O  -4.698196 -1.772306 -1.566769
 H  -4.984882 -2.019140 -0.666038
 H  -3.081135 -0.787421 -2.342116
 H  -4.077690 0.209002 -1.264250
 O  -4.262676 -2.246434 1.225335
 H  -4.905929 -2.105286 1.940568
 H  -4.128767 -0.171284 1.102075
 O  -2.488835 0.516466 2.624844
 H  -1.817029 0.658527 3.313476
 H  -2.831426 -1.485928 3.124265
 O  -1.105029 -2.725636 1.702332
 H  -0.316981 -2.950189 1.175787
 H  -0.370739 -1.061225 2.709831
 O  2.849675 1.979341 1.761855
 H  3.912408 1.749030 -0.029525
 H  4.540972 0.885272 1.389402
 H  0.607294 -3.208624 -1.395940
 C  2.462538 3.285293 1.292949
 C  1.175920 3.261296 0.502849
 H  3.273821 3.731260 0.703962
 C  -0.039866 3.023732 1.156853
 C  1.167632 3.404925 -0.890827
 C  -1.224185 2.905101 0.434882
 H  -0.054757 2.908007 2.238315
 C  -0.013700 3.278123 -1.617834
 H  2.101522 3.599832 -1.412362
 C  -1.231757 3.004875 -0.968280
 H  -2.151462 2.687229 0.956694
 H  0.012631 3.389952 -2.697866
 C  -2.500258 2.788407 -1.683858
 H  -3.380816 2.746014 -1.042969
 C  -2.663856 2.608190 -3.001903
 H  -1.834170 2.610890 -3.704840
 H  -3.652622 2.443059 -3.420834
 H  5.250038 -2.288587 0.467862
```

```
 H  2.335448 3.882683 2.201768
Sum of electronic and thermal Free Energies= -1645.323062
SCF Energies= -1645.773932
S38.out
 O  0.237937 1.713499 0.828723
 C  -0.362502 2.952111 0.412341
 C  0.701828 4.021789 0.074245
 C  2.079619 3.370979 -0.048912
 C  1.964516 2.094898 -0.886101
 C  1.078501 1.072573 -0.125084
 C  -1.348244 2.748420 -0.734543
 H  -0.918190 3.282950 1.293083
 O  0.679245 5.018579 1.098148
 H  0.468840 4.482451 -0.897570
 O  2.959779 4.311503 -0.658581
 H  3.781296 3.824455 -0.848573
 H  2.435353 3.107867 0.958005
 O  3.245745 1.563233 -1.210183
 H  1.495229 2.343139 -1.842751
 O  1.935450 0.238479 0.618210
 H  0.480683 0.468459 -0.815709
 C  1.452017 -1.083822 0.848373
 O  1.363060 -1.832852 -0.342954
 C  2.615520 -2.007927 -1.043072
 C  3.612871 -2.726487 -0.129916
 C  3.788752 -1.944666 1.167658
 C  2.428756 -1.725420 1.838184
 H  0.436893 -1.042822 1.252235
 C  2.306841 -2.765409 -2.327797
 H  3.019741 -1.026542 -1.318989
 O  1.814550 -4.088643 -2.108901
 H  2.574550 -4.648877 -1.881633
 H  3.205510 -2.772631 -2.956380
 H  1.520215 -2.226265 -2.864712
 O  4.843454 -2.844548 -0.843095
 H  5.487041 -3.225618 -0.221545
 H  3.212542 -3.720233 0.119447
 O  4.661471 -2.693457 2.013148
 H  4.729068 -2.196283 2.846773
 H  4.235842 -0.967135 0.931250
 O  2.548347 -0.969024 3.039120
 H  2.780590 -0.060249 2.776021
 H  2.020375 -2.698164 2.126685
 O  -2.264785 1.733576 -0.352269
 H  -0.829905 2.465758 -1.663234
 H  -1.867416 3.700650 -0.925082
 H  3.541822 1.059953 -0.429015
 C  -3.216535 1.442190 -1.382156
 C  -4.187660 0.417008 -0.859116
 H  -2.701315 1.069992 -2.279562
 C  -4.346391 -0.823095 -1.482294
 C  -4.954554 0.698029 0.283411
 C  -5.255832 -1.756945 -0.983217
 H  -3.756474 -1.062005 -2.363668
 C  -5.854463 -0.232927 0.786747
 H  -4.836688 1.657640 0.780122
 C  -6.025046 -1.484942 0.160586
 H  -5.367943 -2.716004 -1.483242
 H  -6.434756 0.016239 1.670298
 C  -6.964885 -2.508490 0.648037
 H  -7.012768 -3.408198 0.034420
 C  -7.737741 -2.443427 1.741062
 H  -7.746657 -1.585691 2.409380
```

```
 H  -8.397329 -3.265994 2.003438
 H  1.342155 5.686325 0.851622
 H  -3.744509 2.367430 -1.662649
Sum of electronic and thermal Free Energies= -1645.314895
SCF Energies= -1645.762722
S39.out
 O  -0.169628 0.808434 -0.818267
 C  1.076400 1.328444 -0.321446
 C  0.878765 2.538208 0.634799
 C  -0.574431 2.614934 1.106420
 C  -1.066110 1.203831 1.441296
 C  -1.126973 0.372986 0.140502
 C  1.948427 0.241588 0.298500
 H  1.580700 1.690135 -1.221420
 O  1.318630 3.766376 0.055870
 H  1.504289 2.405570 1.524067
 O  -0.642319 3.461147 2.249348
 H  -1.515372 3.290350 2.647044
 H  -1.194604 3.019635 0.290836
 O  -2.322204 1.230591 2.112576
 H  -0.365919 0.741488 2.142984
 O  -2.395192 0.614814 -0.430519
 H  -1.003700 -0.696632 0.341627
 C  -2.868539 -0.391067 -1.315247
 O  -3.021628 -1.639722 -0.671607
 C  -3.931827 -1.622729 0.451405
 C  -5.326424 -1.218849 -0.027617
 C  -5.262634 0.124596 -0.754081
 C  -4.219157 0.083915 -1.869994
 H  -2.141236 -0.559724 -2.115052
 C  -3.869111 -3.019495 1.046195
 H  -3.577629 -0.901375 1.196194
 O  -2.558137 -3.317223 1.528932
 H  -1.958955 -3.211312 0.770221
 H  -4.190790 -3.752290 0.291396
 H  -4.546857 -3.082506 1.900836
 O  -6.174169 -1.142490 1.117228
 H  -7.024896 -0.788760 0.805718
 H  -5.697098 -1.976522 -0.734934
 O  -6.568286 0.383106 -1.272215
 H  -6.534650 1.255071 -1.700955
 H  -4.980493 0.900612 -0.028238
 O  -4.144702 1.385937 -2.440696
 H  -3.673914 1.309732 -3.287669
 H  -4.538229 -0.654551 -2.616541
 O  2.097262 -0.803598 -0.656888
 H  1.507717 -0.156728 1.224324
 H  2.919180 0.687058 0.556702
 H  -2.999474 1.365533 1.423277
 C  2.971066 -1.843971 -0.218620
 C  4.427365 -1.428048 -0.165530
 H  2.837228 -2.652249 -0.947046
 C  4.942240 -0.510738 -1.093938
 C  5.293234 -1.970342 0.788208
 C  6.283966 -0.146768 -1.070346
 H  4.274817 -0.072047 -1.830326
 C  6.641978 -1.615170 0.806278
 H  4.911471 -2.674117 1.524249
 C  7.166233 -0.694350 -0.117702
 H  6.648813 0.570299 -1.800051
 H  7.300258 -2.048127 1.555840
 C  8.594297 -0.343420 -0.042181
 H  9.146576 -0.863854 0.740536
```

```
 C  9.258307 0.527777 -0.814710
 H  8.783354 1.090362 -1.614900
 H  10.319151 0.706871 -0.662827
 H  0.780482 3.917674 -0.740753
 H  2.650325 -2.226542 0.761628
Sum of electronic and thermal Free Energies= -1645.314507
SCF Energies= -1645.762578
S40.out
 O  -0.422187 0.991674 -1.587855
 C  0.980094 1.323729 -1.572091
 C  1.453896 1.961131 -0.232703
 C  0.339905 1.927886 0.809307
 C  -0.263221 0.521640 0.833127
 C  -0.975055 0.247313 -0.509735
 C  1.839071 0.148374 -2.012065
 H  1.072435 2.092262 -2.345244
 O  1.973138 3.277891 -0.425773
 H  2.294182 1.384882 0.166319
 O  0.889498 2.260841 2.080458
 H  0.217233 1.988537 2.731283
 H  -0.443081 2.650885 0.527715
 O  -1.137154 0.346476 1.945453
 H  0.542611 -0.202339 0.966607
 O  -2.307015 0.704077 -0.369071
 H  -0.979346 -0.820701 -0.745979
 C  -3.258270 0.064683 -1.213445
 O  -3.429803 -1.296483 -0.885888
 C  -3.882656 -1.538687 0.465934
 C  -5.237567 -0.862239 0.667067
 C  -5.133188 0.636599 0.356173
 C  -4.565459 0.853231 -1.052591
 H  -2.910002 0.080708 -2.249565
 C  -3.920370 -3.049988 0.621719
 H  -3.154563 -1.125904 1.172704
 O  -2.618145 -3.620377 0.487648
 H  -2.292444 -3.353377 -0.388773
 H  -4.619380 -3.476026 -0.113311
 H  -4.277555 -3.300669 1.623451
 O  -5.647785 -1.069431 2.016694
 H  -6.411169 -0.480620 2.154089
 H  -5.964312 -1.310186 -0.030690
 O  -6.395568 1.278468 0.539818
 H  -7.008554 0.911339 -0.122340
 H  -4.463249 1.098181 1.090090
 O  -4.376844 2.225973 -1.368258
 H  -3.636212 2.536662 -0.817649
 H  -5.279044 0.461814 -1.785415
 O  1.701002 -0.914622 -1.072650
 H  2.882262 0.488602 -2.074818
 H  1.526245 -0.193145 -3.008940
 H  -1.974310 0.789414 1.712962
 C  2.725721 -1.910067 -1.181657
 C  4.054285 -1.426194 -0.645392
 H  2.825752 -2.241591 -2.224514
 C  5.228295 -1.533717 -1.394234
 C  4.122385 -0.843485 0.631177
 C  6.445164 -1.087273 -0.875675
 H  5.192781 -1.968164 -2.390363
 C  5.330797 -0.390963 1.145986
 H  3.214863 -0.744911 1.221215
 C  6.523043 -0.507026 0.401419
 H  7.349133 -1.180758 -1.472716
 H  5.350217 0.053180 2.136837
```

```
 C  7.831929 -0.051148 0.898419
 H  8.658008 -0.206385 0.204295
 C  8.096400 0.515876 2.083784
 H  7.331497 0.706254 2.832730
 H  9.109330 0.811430 2.342906
 H  1.243616 3.833394 -0.752716
 H  2.358768 -2.756716 -0.591930
Sum of electronic and thermal Free Energies= -1645.317030
SCF Energies= -1645.767883
S41.out
 O  0.209607 1.990526 -1.578078
 C  -0.914572 1.990553 -0.675180
 C  -0.752496 3.116280 0.350634
 C  0.562352 2.922143 1.106282
 C  1.733423 2.805046 0.126418
 C  1.440910 1.740116 -0.935812
 C  -2.172750 2.134611 -1.518036
 H  -0.943473 1.040403 -0.130854
 O  -1.868692 3.065432 1.238215
 H  -0.717026 4.082497 -0.175274
 O  0.726849 4.039030 1.979967
 H  1.555960 3.890679 2.466349
 H  0.490820 1.991750 1.689367
 O  2.964105 2.552407 0.798061
 H  1.855662 3.763257 -0.386727
 O  1.420782 0.475454 -0.287753
 H  2.206097 1.753959 -1.715571
 C  1.994647 -0.607292 -1.002543
 O  3.391664 -0.622739 -0.811184
 C  3.762833 -1.201486 0.455626
 C  3.492888 -2.720271 0.433730
 C  2.306341 -3.054771 -0.499067
 C  1.298030 -1.900273 -0.503776
 H  1.840525 -0.482362 -2.076105
 C  5.210252 -0.826540 0.698098
 H  3.152220 -0.749068 1.246534
 O  5.357525 0.579594 0.903306
 H  4.912882 1.017460 0.156597
 H  5.822916 -1.172891 -0.147568
 H  5.562360 -1.324236 1.606385
 O  3.263106 -3.190967 1.762182
 H  2.424628 -2.780884 2.045217
 H  4.370844 -3.259158 0.063311
 O  2.812821 -3.287601 -1.812894
 H  2.062321 -3.554683 -2.370864
 H  1.817360 -3.953424 -0.101626
 O  0.811152 -1.784611 0.837769
 H  0.517520 -0.862075 0.952389
 H  0.465271 -2.118198 -1.184938
 O  -2.273508 1.175152 -2.572503
 H  -2.179298 3.109113 -2.015958
 H  -3.041999 2.078461 -0.851515
 H  2.927929 1.637872 1.132456
 C  -2.114273 -0.198004 -2.184972
 C  -3.088798 -0.654979 -1.123829
 H  -1.082618 -0.390287 -1.862770
 C  -2.651574 -1.337640 0.014758
 C  -4.460688 -0.392159 -1.264828
 C  -3.565148 -1.761958 0.980661
 H  -1.592191 -1.537865 0.154618
 C  -5.370583 -0.806050 -0.299662
 H  -4.809514 0.149816 -2.140224
 C  -4.940243 -1.505237 0.846945
```

```
 H  -3.207297 -2.294074 1.858996
 H  -6.425082 -0.585851 -0.437558
 C  -5.858206 -1.970233 1.900314
 H  -5.372123 -2.490237 2.725920
 C  -7.189813 -1.822371 1.939220
 H  -7.752079 -1.317793 1.157171
 H  -7.766338 -2.211224 2.773984
 H  -1.679514 3.694058 1.955875
 H  -2.275249 -0.755331 -3.114195
Sum of electronic and thermal Free Energies= -1645.324711
SCF Energies= -1645.777717
S42.out
 O  -0.262052 -0.844814 -0.977375
 C  -0.515914 -1.929665 -0.061482
 C  -1.131753 -1.376683 1.228737
 C  -0.218987 -0.315755 1.838588
 C  0.083612 0.768277 0.806997
 C  0.636267 0.127239 -0.476016
 C  -1.368158 -2.950204 -0.808488
 H  0.432690 -2.423725 0.189165
 O  -1.319839 -2.471460 2.125586
 H  -2.090072 -0.894596 1.002196
 O  -0.900220 0.215421 2.977514
 H  -0.288136 0.834315 3.409995
 H  0.724235 -0.788352 2.146126
 O  0.981538 1.695638 1.404641
 H  -0.860316 1.260941 0.532550
 O  1.902017 -0.453348 -0.205576
 H  0.725239 0.880755 -1.263009
 C  2.817625 -0.327154 -1.278943
 O  3.215679 1.020213 -1.438235
 C  3.845103 1.544558 -0.246875
 C  5.190058 0.841439 -0.059735
 C  4.919415 -0.665144 0.126326
 C  4.042603 -1.216236 -1.007605
 H  2.336925 -0.612712 -2.220664
 C  3.862618 3.050317 -0.405739
 H  3.216591 1.319079 0.619865
 O  2.514978 3.553756 -0.436857
 H  2.100009 3.171968 -1.230142
 H  4.405148 3.342652 -1.314811
 H  4.351384 3.505363 0.457883
 O  5.928925 1.381025 1.033688
 H  5.407717 1.229542 1.842014
 H  5.812927 0.993910 -0.948782
 O  6.123686 -1.414899 0.261325
 H  6.625528 -1.310213 -0.566114
 H  4.384891 -0.798592 1.074887
 O  3.663899 -2.546788 -0.670759
 H  3.251157 -2.940073 -1.458229
 H  4.642381 -1.202212 -1.929527
 O  -2.587518 -2.423967 -1.323712
 H  -1.544888 -3.816167 -0.159534
 H  -0.797116 -3.288729 -1.678876
 H  1.272175 2.355526 0.741294
 C  -3.719529 -2.458969 -0.451642
 C  -4.430756 -1.122473 -0.420772
 H  -3.414769 -2.739607 0.564544
 C  -5.745573 -1.049487 0.054247
 C  -3.798020 0.062988 -0.821682
 C  -6.404783 0.174973 0.136318
 H  -6.257956 -1.958066 0.362804
 C  -4.458680 1.286328 -0.743505
```

```
 H  -2.780111 0.022202 -1.193681
 C  -5.778697 1.370347 -0.263249
 H  -7.425934 0.209306 0.508754
 H  -3.936403 2.184943 -1.059115
 C  -6.526992 2.634904 -0.165916
 H  -7.522551 2.538549 0.268005
 C  -6.119219 3.852072 -0.552224
 H  -5.145628 4.035049 -1.000676
 H  -6.764127 4.717784 -0.429434
 H  -1.619837 -2.086190 2.966998
 H  -4.411326 -3.238897 -0.800444
Sum of electronic and thermal Free Energies= -1645.323561
SCF Energies= -1645.777195
S44.out
 O  -1.693062 0.606997 0.222428
 C  -2.597158 0.068524 -0.762448
 C  -3.903307 -0.324868 -0.066576
 C  -3.594567 -1.332055 1.042302
 C  -2.533711 -0.790124 2.006670
 C  -1.307371 -0.300057 1.230709
 C  -2.762550 1.124549 -1.841811
 H  -2.157552 -0.826478 -1.219359
 O  -4.775640 -0.893921 -1.042421
 H  -4.356320 0.571177 0.384448
 O  -4.816757 -1.607042 1.727605
 H  -4.605275 -2.260878 2.415893
 H  -3.211311 -2.248969 0.570633
 O  -2.194757 -1.748191 3.005203
 H  -2.953157 0.069793 2.536706
 O  -0.668271 -1.454212 0.692590
 H  -0.613287 0.249402 1.872831
 C  0.526199 -1.186110 -0.018640
 O  1.585220 -1.041661 0.925156
 C  2.829907 -1.696380 0.604792
 C  3.115894 -1.464200 -0.879881
 C  2.073247 -2.175450 -1.748455
 C  0.727573 -2.326707 -1.010168
 H  0.415186 -0.250418 -0.570831
 C  3.918987 -1.129439 1.510704
 H  2.743978 -2.770008 0.811432
 O  4.392781 0.161292 1.121028
 H  4.888901 0.039174 0.293267
 H  4.747616 -1.846771 1.546218
 H  3.515136 -1.024029 2.521650
 O  4.449420 -1.889490 -1.160409
 H  4.625808 -1.667900 -2.090691
 H  3.017347 -0.384584 -1.060243
 O  1.941388 -1.397746 -2.939929
 H  1.365768 -1.886471 -3.552668
 H  2.437582 -3.185858 -1.975357
 O  0.724475 -3.594144 -0.354779
 H  -0.036149 -3.595696 0.252682
 H  -0.088247 -2.267451 -1.745027
 O  -1.594891 1.159407 -2.672673
 H  -2.954574 2.097152 -1.375009
 H  -3.624663 0.865756 -2.466668
 H  -1.713388 -2.465507 2.555252
 C  -0.946434 2.441698 -2.780286
 C  -0.180400 2.792569 -1.528767
 H  -1.683649 3.219422 -3.018672
 C  -0.681346 3.712670 -0.603887
 C  1.002892 2.104124 -1.214749
 C  -0.037608 3.915125 0.616913
```

```
 H  -1.591455 4.262026 -0.831770
 C  1.644181 2.296687 0.003408
 H  1.404896 1.384517 -1.925121
 C  1.124502 3.200207 0.954252
 H  -0.449299 4.625674 1.329767
 H  2.542473 1.729375 0.224059
 C  1.733852 3.423849 2.276036
 H  1.245691 4.194924 2.872462
 C  2.786654 2.783385 2.803809
 H  3.326731 1.997579 2.282657
 H  3.141428 3.036674 3.799387
 H  -5.546016 -1.236870 -0.557765
 H  -0.270052 2.336949 -3.634119
Sum of electronic and thermal Free Energies= -1645.319823
SCF Energies= -1645.772784
S5.out
 O  2.045699 -0.237519 0.929408
 C  2.881224 -0.222263 -0.244834
 C  3.709865 1.072227 -0.271518
 C  2.823408 2.309782 -0.121904
 C  1.917863 2.174776 1.097611
 C  1.147082 0.854911 1.009829
 C  3.787960 -1.446368 -0.184063
 H  2.252469 -0.273314 -1.141774
 O  4.420212 1.110831 -1.508985
 H  4.412656 1.056453 0.576172
 O  3.700707 3.433416 -0.011533
 H  3.145058 4.230396 -0.034018
 H  2.198667 2.403565 -1.019914
 O  1.047574 3.304282 1.130305
 H  2.541490 2.135856 2.000366
 O  0.306193 0.925525 -0.125490
 H  0.554033 0.685274 1.913328
 C  -0.798671 0.044061 -0.057380
 O  -1.760959 0.506706 0.871532
 C  -2.292649 1.805653 0.540588
 C  -3.042783 1.701150 -0.789125
 C  -2.080130 1.219778 -1.877033
 C  -1.413577 -0.085301 -1.454824
 H  -0.473032 -0.924746 0.314159
 C  -3.149751 2.242268 1.715945
 H  -1.466041 2.518691 0.428511
 O  -2.360276 2.428210 2.895032
 H  -1.769268 3.181680 2.726007
 H  -3.880070 1.461003 1.950350
 H  -3.692963 3.157060 1.449286
 O  -3.571152 2.985774 -1.114162
 H  -3.908276 2.919329 -2.024439
 H  -3.851076 0.960406 -0.682897
 O  -2.846000 1.052826 -3.072337
 H  -2.218787 0.825900 -3.779212
 H  -1.309688 1.989676 -2.024577
 O  -0.438450 -0.430736 -2.436941
 H  -0.123567 -1.327962 -2.227369
 H  -2.190916 -0.856240 -1.390171
 O  3.134478 -2.687691 -0.435082
 H  4.301731 -1.467005 0.787223
 H  4.543057 -1.345110 -0.968299
 H  0.496982 3.233106 1.929467
 C  2.463802 -3.295891 0.678028
 C  0.957495 -3.265176 0.538993
 H  2.766343 -2.823322 1.618684
 C  0.138512 -3.066198 1.657302
```

```
 C  0.350106 -3.475185 -0.706605
 C  -1.250065 -3.032988 1.531476
 H  0.592495 -2.915006 2.633662
 C  -1.038068 -3.452898 -0.833489
 H  0.969914 -3.641822 -1.582899
 C  -1.863083 -3.193288 0.276524
 H  -1.864774 -2.859770 2.410084
 H  -1.490822 -3.596258 -1.811753
 C  -3.312723 -3.021198 0.075546
 H  -3.735310 -3.546947 -0.780672
 C  -4.105465 -2.228919 0.810649
 H  -3.723853 -1.638457 1.640072
 H  -5.165881 -2.137461 0.591787
 H  4.878918 1.968268 -1.534478
 H  2.804179 -4.339830 0.709045
Sum of electronic and thermal Free Energies= -1645.331298
SCF Energies= -1645.784597
S6.out
 O  -0.997918 -2.013139 -1.425458
 C  -1.139218 -2.413050 -0.042844
 C  -2.561984 -2.168421 0.487159
 C  -2.994462 -0.741344 0.179269
 C  -2.894288 -0.514337 -1.331280
 C  -1.422071 -0.714200 -1.748079
 C  -0.807879 -3.898240 0.009976
 H  -0.439663 -1.837886 0.574711
 O  -2.537237 -2.394675 1.895936
 H  -3.260693 -2.866416 -0.001173
 O  -4.309988 -0.527051 0.687735
 H  -4.322703 0.406275 0.973702
 H  -2.302807 -0.072377 0.694419
 O  -3.442409 0.719476 -1.767052
 H  -3.466815 -1.292289 -1.847840
 O  -0.518307 0.205133 -1.099913
 H  -1.310859 -0.609458 -2.832589
 C  -0.548580 1.551749 -1.521404
 O  -1.501510 2.325193 -0.788478
 C  -1.256514 2.401149 0.633820
 C  0.078680 3.108401 0.860398
 C  1.188377 2.340687 0.140623
 C  0.849610 2.154455 -1.343264
 H  -0.868187 1.620682 -2.564971
 C  -2.446694 3.114867 1.255926
 H  -1.187134 1.391719 1.050202
 O  -3.673871 2.385550 1.108070
 H  -3.972277 2.494426 0.190534
 H  -2.545762 4.118788 0.824260
 H  -2.268714 3.214178 2.328943
 O  0.324244 3.154065 2.264732
 H  1.254284 3.423196 2.365425
 H  0.025986 4.125193 0.441724
 O  2.386619 3.093019 0.312840
 H  3.128386 2.535110 0.009726
 H  1.288034 1.352808 0.613231
 O  1.823840 1.383041 -2.032868
 H  1.783369 0.481734 -1.663483
 H  0.842809 3.139439 -1.818977
 O  0.550929 -4.217899 -0.270673
 H  -1.402976 -4.413181 -0.751420
 H  -1.094743 -4.287095 0.995678
 H  -2.933661 1.434079 -1.326950
 C  1.461798 -3.923395 0.792202
 C  2.189821 -2.605112 0.634748
```

```
 H  2.201130 -4.734572 0.781094
 C  2.623601 -2.173533 -0.627776
 C  2.540452 -1.849194 1.757551
 C  3.430693 -1.047812 -0.757108
 H  2.344655 -2.742507 -1.509539
 C  3.339522 -0.712737 1.628763
 H  2.200063 -2.159224 2.742582
 C  3.812025 -0.296380 0.373241
 H  3.790471 -0.765149 -1.742294
 H  3.607245 -0.140781 2.513707
 C  4.676180 0.892791 0.296308
 H  5.017842 1.269779 1.260142
 C  5.054391 1.547301 -0.814249
 H  4.734038 1.252748 -1.809593
 H  5.702692 2.416611 -0.749241
 H  -3.368587 -2.015428 2.233489
 H  0.948716 -3.963974 1.761641
Sum of electronic and thermal Free Energies= -1645.337865
SCF Energies= -1645.794716
S7.out
 O  -0.149731 2.015805 -0.730866
 C  0.188102 2.476085 0.597723
 C  1.508718 3.254798 0.565478
 C  2.600704 2.403251 -0.077269
 C  2.142357 1.912107 -1.451878
 C  0.801329 1.170615 -1.326908
 C  -0.978487 3.323699 1.085629
 H  0.296871 1.611057 1.261947
 O  1.840884 3.596878 1.911097
 H  1.374615 4.162469 -0.042751
 O  3.774879 3.207687 -0.188849
 H  4.420987 2.671996 -0.681952
 H  2.795604 1.539441 0.573288
 O  3.152568 1.166768 -2.118743
 H  1.950997 2.788394 -2.080369
 O  0.885520 -0.015108 -0.522825
 H  0.412098 0.908333 -2.316012
 C  1.279015 -1.208141 -1.152773
 O  2.697400 -1.373957 -1.118509
 C  3.269579 -1.487721 0.208780
 C  2.671875 -2.700993 0.920128
 C  1.150194 -2.588238 0.955118
 C  0.604926 -2.400459 -0.457447
 H  1.021866 -1.185319 -2.216462
 C  4.774439 -1.568451 0.002669
 H  3.040846 -0.585793 0.787589
 O  5.170217 -2.727278 -0.729761
 H  4.700981 -2.691597 -1.580807
 H  5.266427 -1.622493 0.976702
 H  5.103138 -0.648533 -0.502410
 O  3.217628 -2.731619 2.237029
 H  2.770527 -3.458494 2.703874
 H  2.946009 -3.609003 0.365135
 O  0.651171 -3.786725 1.549932
 H  -0.312173 -3.684510 1.630175
 H  0.873971 -1.716039 1.564238
 O  -0.802563 -2.232251 -0.352540
 H  -1.178195 -2.188221 -1.248185
 H  0.848927 -3.293923 -1.047162
 O  -2.161861 2.540784 1.233682
 H  -1.140993 4.168370 0.403576
 H  -0.724766 3.724235 2.071426
 H  3.195011 0.271411 -1.716844
```

```
 C  -3.063179 2.595953 0.115482
 C  -3.830070 1.300795 0.023163
 H  -2.497928 2.756555 -0.808886
 C  -3.148949 0.077395 -0.037819
 C  -5.229708 1.292106 -0.030505
 C  -3.855126 -1.117316 -0.149973
 H  -2.063898 0.058932 -0.004371
 C  -5.936706 0.098073 -0.152922
 H  -5.772139 2.232978 0.024544
 C  -5.261669 -1.134679 -0.212924
 H  -3.312297 -2.057965 -0.187620
 H  -7.021590 0.128269 -0.193442
 C  -5.950576 -2.430534 -0.335335
 H  -5.285397 -3.293820 -0.363338
 C  -7.271423 -2.644834 -0.413513
 H  -8.003495 -1.841027 -0.392931
 H  -7.664648 -3.653836 -0.502553
 H  2.708671 4.034737 1.879034
 H  -3.750987 3.444450 0.237960
Sum of electronic and thermal Free Energies= -1645.327690
SCF Energies= -1645.77934
S8.out
 O  -0.684608 0.853999 -0.332958
 C  -0.791518 1.845303 0.712684
 C  -0.379723 3.221189 0.180746
 C  1.010813 3.165328 -0.447808
 C  1.070089 2.061129 -1.498670
 C  0.609660 0.730946 -0.889731
 C  -2.214367 1.809945 1.260691
 H  -0.121387 1.565743 1.535700
 O  -0.407750 4.128448 1.282156
 H  -1.095510 3.532928 -0.592463
 O  1.263600 4.448859 -1.022808
 H  2.168923 4.426204 -1.376105
 H  1.745698 2.949960 0.340326
 O  2.407774 1.993892 -1.987005
 H  0.371722 2.309840 -2.307998
 O  1.558655 0.349684 0.089665
 H  0.528599 -0.044162 -1.657219
 C  1.544406 -1.030468 0.417226
 O  2.131101 -1.804693 -0.609976
 C  3.506658 -1.464707 -0.898773
 C  4.345386 -1.664435 0.364419
 C  3.786495 -0.839729 1.527523
 C  2.303783 -1.165512 1.744102
 H  0.516138 -1.389742 0.513731
 C  3.924513 -2.362359 -2.053587
 H  3.569254 -0.418031 -1.220603
 O  3.883775 -3.749016 -1.714259
 H  2.978042 -3.930305 -1.409715
 H  4.955925 -2.132837 -2.332727
 H  3.276770 -2.149438 -2.915887
 O  5.687020 -1.279468 0.072216
 H  6.149046 -1.263941 0.929195
 H  4.301289 -2.728937 0.641807
 O  4.569274 -1.036366 2.707060
 H  4.486311 -1.973636 2.959743
 H  3.890933 0.223699 1.286160
 O  1.703709 -0.368338 2.758245
 H  1.713440 0.549444 2.433739
 H  2.213256 -2.205114 2.076203
 O  -3.200909 2.446753 0.449826
 H  -2.226118 2.358068 2.206011
```

```
 H  -2.483695 0.765943 1.466746
 H  2.405344 1.437837 -2.784478
 C  -3.531329 1.783246 -0.783996
 C  -4.061335 0.381627 -0.586796
 H  -2.670872 1.774375 -1.460334
 C  -3.492833 -0.711362 -1.246225
 C  -5.139166 0.153328 0.283773
 C  -3.999891 -1.997645 -1.056791
 H  -2.646395 -0.557026 -1.910094
 C  -5.640820 -1.127242 0.480727
 H  -5.580627 0.993510 0.813702
 C  -5.080433 -2.233943 -0.190094
 H  -3.545843 -2.835727 -1.580228
 H  -6.475989 -1.270220 1.160093
 C  -5.570785 -3.612038 -0.020460
 H  -5.034023 -4.358435 -0.606221
 C  -6.579695 -4.023038 0.760310
 H  -7.166052 -3.344967 1.375722
 H  -6.853295 -5.073583 0.804569
 H  -0.080096 4.979861 0.945183
 H  -4.303360 2.421282 -1.227477
Sum of electronic and thermal Free Energies= -1645.330134
SCF Energies= -1645.779531
S9.out
 O  -0.258639 2.292103 -1.313494
 C  -1.450754 1.962103 -0.561457
 C  -1.538644 2.898008 0.652088
 C  -0.269277 2.770768 1.492800
 C  0.972457 3.046934 0.643654
 C  0.958793 2.163402 -0.605809
 C  -2.576098 2.137576 -1.587549
 H  -1.400064 0.921866 -0.224196
 O  -2.686370 2.565306 1.432593
 H  -1.612437 3.934353 0.286494
 O  -0.373066 3.702693 2.570496
 H  0.433475 3.596561 3.103581
 H  -0.214572 1.744423 1.884775
 O  2.171752 2.881123 1.395669
 H  0.952820 4.091933 0.321916
 O  1.167722 0.833377 -0.162319
 H  1.742993 2.457162 -1.309548
 C  1.530161 -0.076339 -1.184391
 O  2.913430 -0.010392 -1.476957
 C  3.771378 -0.340779 -0.362799
 C  3.496552 -1.776911 0.091204
 C  2.019611 -1.935020 0.444079
 C  1.140727 -1.484246 -0.719266
 H  1.017351 0.182432 -2.114972
 C  5.191425 -0.124769 -0.860201
 H  3.573942 0.351291 0.464728
 O  5.416406 1.240666 -1.210565
 H  4.726078 1.472296 -1.855457
 H  5.381840 -0.792440 -1.713832
 H  5.897298 -0.372255 -0.063907
 O  4.327175 -2.046098 1.219684
 H  4.061405 -2.920860 1.551508
 H  3.732754 -2.463731 -0.736038
 O  1.793464 -3.309752 0.759068
 H  0.851371 -3.401554 0.993922
 H  1.800794 -1.303095 1.316737
 O  -0.202098 -1.534287 -0.262685
 H  -0.804420 -1.517269 -1.024877
 H  1.298813 -2.167750 -1.563099
```

```
 O  -3.865799 1.760968 -1.112216
 H  -2.308916 1.565243 -2.485151
 H  -2.631020 3.196792 -1.866141
 H  2.244816 1.930964 1.597743
 C  -4.337161 0.480317 -1.542065
 C  -3.757279 -0.693172 -0.781031
 H  -4.164685 0.354732 -2.619804
 C  -3.384875 -1.866576 -1.451089
 C  -3.633681 -0.649469 0.613432
 C  -2.879703 -2.961648 -0.751071
 H  -3.492855 -1.923522 -2.531689
 C  -3.121116 -1.738467 1.313150
 H  -3.912891 0.253343 1.146364
 C  -2.707115 -2.903705 0.643515
 H  -2.596840 -3.858511 -1.294520
 H  -3.006240 -1.678117 2.392785
 C  -2.042956 -3.971709 1.408404
 H  -2.238356 -3.966061 2.480752
 C  -1.196461 -4.886890 0.912001
 H  -0.928108 -4.920571 -0.141283
 H  -0.741372 -5.635123 1.555158
 H  -2.589187 3.046085 2.272949
 H  -5.421508 0.519291 -1.384683
Sum of electronic and thermal Free Energies= -1645.330452
SCF Energies= -1645.783868
```