Electronic Supplementary Material (ESI) for Environmental Science: Processes & Impacts.

Towards a Comprehensive Understanding of Malathion Degradation: Comparison of Degradation Reactions under Alkaline and Radical Conditions

*Robert W. Lamb[1,2], Harley McAlexander[3], Christa M. Woodley[3], and Manoj K. Shukla[3]**

[1]Oak Ridge Institute for Science and Education, Oak Ridge, TN, USA

[2]Current affiliation: Simetri Inc., 7005 University Blvd, Winter Park, FL 32792, USA

[3]US Army Engineer Research and Development Center, Environmental Laboratory, 3909 Halls Ferry Road, Vicksburg, MS 39180, USA

Supporting Information

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Additional Reaction Pathways

With OH^-, the free energy of activation association to the ß ester position, **TS13**, is more endergonic than association to the α position in **TS9** (8.7 vs 5.3 kcal mol^{-1}) indicating the reaction at the α site will be kinetically favored. However, reaction at the ß site is still quite feasible and could be expected to occur to some degree. Subsequent dissociation of the OMe group, **TS14**, has a slightly lower free energy of activation indicating that the dissociation step will likely occur should OH^- bind. Similarly, initial binding with OH• is endergonic, **TS13** (14.5 kcal mol^{-1}), while the subsequent dissociation of OMe, **TS14**, is slightly lower in energy (12.0 kcal mol^{-1}) indicating facile degradation upon association of OH• to the ß site. Although these energies are still feasible at room temperature, degradation with OH• is notably higher in energy, and therefore slower, than degradation by OH^-. Interestingly, following dissociation of the OMe group as methanol, it is lower in energy for this structure to reorganize to the carboxylic acid form with a proximal OMe• radical, **28**. Although, the carboxylic acid will likely become deprotonated once the OMe• migrates away in bulk solution.

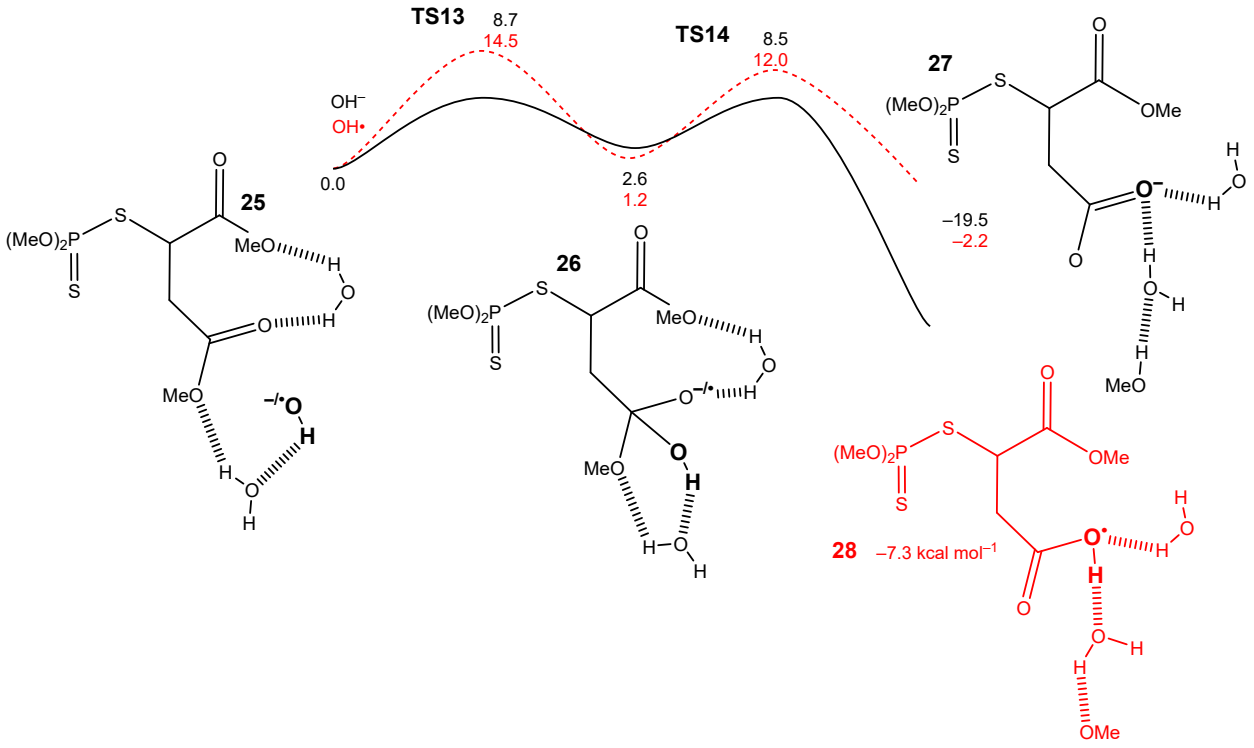

Figure S1. Initial ß-ester degradation at the M06-2X/aug-cc-pVTZ//M06-2X/6-31G(d,p) level of theory in bulk water. Non-bolded numbers indicate relative free energies in kcal mol^{-1}. Bolded numbers denote the compound numbers as local minimum (standard) or transition state (leading "TS") geometries. Atoms corresponding to the hydroxide ion or hydroxyl radical are bolded and enlarged throughout the reaction. The position of the negative charge or radical electron are also noted when localized to a single atom.

Following degradation of the ß position, and exchange of the MeOH byproduct for an additional OH^- or OH•, the α position can then be degraded in a similar way. Degradation by OH^- remains quite facile with the initial association **TS15** being only slightly higher in energy (8.9 kcal mol^{-1}) than association at the α position in **TS13** (8.7 kcal mol^{-1}). Similarly, initial association of the OH• to **29** is slightly higher in energy than the previous association to **25** (15.6 vs 14.5 kcal mol^{-1}) while

the subsequent dissociation of OMe• is lower in energy. Again, the lower energy structure **32** is with the α carboxyl group retaining a proton as a carboxylic acid and a proximal OMe• radical.

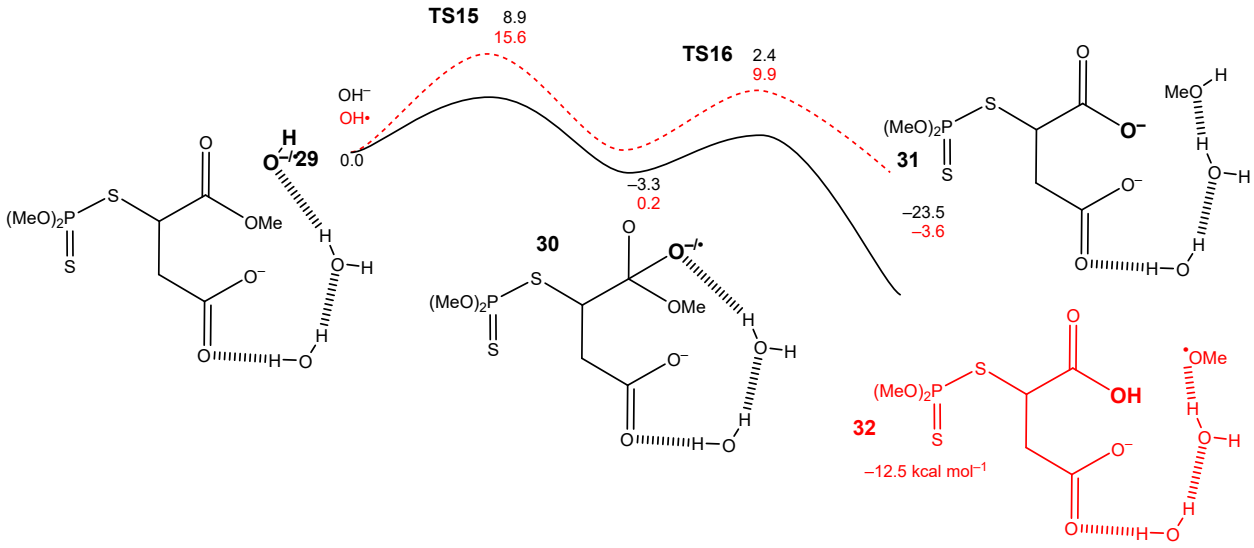

Figure S2. α-ester degradation following ß-ester hydrolysis at the M06-2X/aug-cc-pVTZ//M06-2X/6-31G(d,p) level of theory in bulk water. Non-bolded numbers indicate relative free energies in kcal mol^{-1}. Bolded numbers denote the compound numbers as local minimum (standard) or transition state (leading "TS") geometries. Atoms corresponding to the hydroxide ion or hydroxyl radical are bolded and enlarged throughout the reaction. The position of the negative charge or radical electron are also noted when localized to a single atom.

Energy Tables

Table S1: Relative free energies in kcal mol^{-1}. Free energies for single-point computations were obtained by applying the thermodynamic corrections from M06-2X/6-31G(d,p) to the SCF energies from computations with aug-cc-pVTZ.

	M06-2X/6-31G(d,p)	M06-2X/aug-cc-pVTZ// M06-2X/6-31G(d,p)	MP2/aug-cc-pVTZ// M06-2X/6-31G(d,p)
1	0.0	0.0	0.0
TS1	6.9	4.6	16.0
3	–19.1	–22.9	–10.1
4	0.0	0.0	0.0
TS2	16.6	17.8	31.1
5	3.0	5.4	11.2
TS3	6.7	15.7	32.9
6	–14.9	–13.7	–6.2
7	–2.9	–1.7	3.9
8	0.0	0.0	0.0
TS4	18.4	20.3	34.6
9	7.4	15.6	29.6
TS5	13.7	21.4	50.9
10	–10.6	–8.5	–4.6
11	1.1	2.1	2.7
12	0.0	0.0	0.0
TS6	5.3	5.3	12.2
13	–28.3	–27.8	–13.6
TS7	–1.7	2.5	18.0
14	–8.4	–2.3	0.6
15	–5.0	–0.7	1.4
TS8	–0.1	4.6	20.1
16	–25.2	–21.7	3.3
18	0.0	0.0	0.0
TS9	16.9	17.5	29.7
19	–1.2	2.3	70.7
TS10	9.5	11.5	91.2
20	5.2	–1.6	12.9
21	–10.6	–9.9	–7.4

Table S1 cont.

	M06-2X/6-31G(d,p)	M06-2X/aug-cc-pVTZ// M06-2X/6-31G(d,p)	MP2/aug-cc-pVTZ// M06-2X/6-31G(d,p)
22	0.0	0.0	0.0
TS11	16.7	17.8	29.9
23	–0.7	2.1	5.4
TS12	22.5	30.6	65.0
24	–4.5	–1.3	12.9
25	–33.8	0.0	0.0
TS13	–20.2	14.5	27.3
26	–35.0	1.2	4.9
TS14	–23.4	12.0	28.7
27	–33.0	–2.2	27.6
28	–41.9	–7.3	–4.6
29	0.0	0.0	0.0
TS15	13.0	15.6	25.4
30	–4.8	0.2	10.7
TS16	5.9	9.9	32.2
31	–4.0	–3.6	45.4
32	–14.8	–12.5	–8.6
33	–9.7	0.0	0.0
TS17	7.7	15.6	43.3
37	–16.9	–6.6	2.9
38	–5.3	0.0	0.0
TS21	14.6	19.7	51.9
39	–50.6	–48.4	–39.1
41	0.0	0.0	0.0
TS22	22.2	22.9	87.3
42	–0.9	1.4	48.9
TS23	8.4	9.0	71.0
43	–0.4	–5.6	19.6

Table S1 cont.

	M06-2X/6-31G(d,p)	M06-2X/aug-cc-pVTZ// M06-2X/6-31G(d,p)	MP2/aug-cc-pVTZ// M06-2X/6-31G(d,p)
44	8.8	0.0	0.0
TS24	24.7	16.0	17.0
45	11.2	5.5	25.4
TS25	13.6	7.9	–28.5
46	1.0	–6.9	–34.2
47	–7.4	–13.9	–67.8

Table S2: Absolute electronic and free energies in hartrees. Free energies for single-point computations were obtained by applying the thermodynamic corrections from M06-2X/6-31G(d,p) to the SCF energies from computations with aug-cc-pVTZ.

	M06-2X/6-31G(d,p)	M06-2X/6-31G(d,p)	M06-2X/aug-cc-pVTZ// M06-2X/6-31G(d,p)	MP2/aug-cc-pVTZ// M06-2X/6-31G(d,p)
	E	G	E	E
1	–2131.16994	–2130.92208	–2131.71738	–2124.65520
TS1	–2131.15574	–2130.91103	–2131.70691	–2124.62660
3	–2131.20043	–2130.95246	–2131.75391	–2124.67135
4	–762.65826	–762.50638	–762.98748	–759.09097
TS2	–762.63421	–762.47996	–762.96152	–759.04373
5	–762.65883	–762.50153	–762.98421	–759.07849
TS3	–762.64558	–762.49066	–762.96152	–759.04163
6	–762.67574	–762.52511	–763.00408	–759.09957
7	–762.65834	–762.50594	–762.98683	–759.08525
8	–722.89991	–722.78783	–723.23893	–719.58951
TS4	–722.87343	–722.75855	–723.20937	–719.53712
9	–722.89396	–722.77603	–723.21997	–719.54817
TS5	–722.88440	–722.76597	–723.21115	–719.51479
10	–722.91731	–722.80477	–723.25286	–719.59722
11	–722.89591	–722.78614	–723.23329	–719.58296
12	–683.15674	–683.08032	–683.50138	–680.09213
TS6	–683.15040	–683.07186	–683.49500	–680.07482
13	–683.20242	–683.12544	–683.54623	–680.11430
TS7	–683.16076	–683.08305	–683.49864	–680.06479
14	–683.17641	–683.09366	–683.51142	–680.09746
15	–683.17017	–683.08825	–683.50805	–680.09539
TS8	–683.15542	–683.08043	–683.49263	–680.05865
16	–683.20113	–683.12045	–683.54018	–680.09109
18	–2131.16928	–2130.91900	–2131.71586	–2124.65539
TS9	–2131.14180	–2130.89204	–2131.68751	–2124.60757
19	–2131.17568	–2130.92093	–2131.71661	–2124.54724
TS10	–2131.15593	–2130.90391	–2131.69932	–2124.51177
20	–2131.16082	–2130.91079	–2131.71817	–2124.63458
21	–2131.18148	–2130.93591	–2131.72695	–2124.66239

Table S2 cont.

	M06-2X/6-31G(d,p) E	M06-2X/6-31G(d,p) G	M06-2X/aug-cc-pVTZ// M06-2X/6-31G(d,p) E	MP2/aug-cc-pVTZ// M06-2X/6-31G(d,p) E
22	–2091.42178	–2091.21016	–2091.97325	–2085.15636
TS11	–2091.39520	–2091.18359	–2091.94492	–2085.10864
23	–2091.42618	–2091.21123	–2091.97326	–2085.15112
TS12	–2091.38449	–2091.17429	–2091.92305	–2085.05129
24	–2091.42620	–2091.21738	–2091.97250	–2085.13295
25	–2131.16655	–2130.91700	–2131.71444	–2124.65388
TS13	–2131.14543	–2130.89522	–2131.69202	–2124.61097
26	–2131.17045	–2130.91876	–2131.71469	–2124.64824
TS14	–2131.15136	–2130.90043	–2131.69670	–2124.60948
27	–2131.16545	–2130.91572	–2131.71815	–2124.61002
28	–2131.17559	–2130.92988	–2131.72227	–2124.65737
29	–2091.42582	–2091.21299	–2091.97418	–2085.14957
TS15	–2091.40737	–2091.19222	–2091.95171	–2085.11139
30	–2091.43794	–2091.22069	–2091.97826	–2085.13686
TS16	–2091.42047	–2091.20360	–2091.96237	–2085.10225
31	–2091.42936	–2091.21938	–2091.97706	–2085.07436
32	–2091.45003	–2091.23663	–2091.99470	–2085.16386
33	–2051.66267	–2051.49163	–2052.22280	–2045.64558
TS17	–2051.63613	–2051.46392	–2052.19909	–2045.57766
37	–2051.66960	–2051.50308	–2052.22885	–2045.63644
38	–2131.16692	–2130.91897	–2131.71586	–2124.65725
TS21	–2131.13855	–2130.88718	–2131.68785	–2124.57795
39	–2131.23865	–2130.99110	–2131.79257	–2124.71911
41	–1162.04628	–1161.86773	–1162.41092	–1157.81576
TS22	–1162.01019	–1161.83233	–1162.37380	–1157.67593
42	–1162.05064	–1161.86915	–1162.41156	–1157.74082
TS23	–1162.03070	–1161.85437	–1162.39434	–1157.70036
43	–1162.04762	–1161.86845	–1162.42044	–1157.78509

Table S2 cont.

	M06-2X/6-31G(d,p)	M06-2X/6-31G(d,p)	M06-2X/aug-cc-pVTZ// M06-2X/6-31G(d,p)	MP2/aug-cc-pVTZ// M06-2X/6-31G(d,p)
	E	G	E	E
44	–1122.28883	–1122.15306	–1122.65942	–1118.21667
TS24	–1122.26476	–1122.12773	–1122.63520	–1118.19089
45	–1122.29111	–1122.14927	–1122.65679	–1118.18233
TS25	–1122.28567	–1122.14534	–1122.65132	–1118.26667
46	–1122.29972	–1122.16551	–1122.66879	–1118.26966
47	–1122.31335	–1122.17890	–1122.68023	–1118.32334

XYZ Coordinates

```
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P    -2.154902 -0.574826  0.383624
O    -2.251907 -2.166977  0.335044
O    -3.587038 -0.169901 -0.217599
C    -2.795664 -2.838185 -0.822222
H    -3.850993 -2.588493 -0.928558
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H    -2.668063 -3.901678 -0.631697
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H    -3.179614  1.801946 -0.771870
H    -4.885991  1.267521 -0.826925
H    -4.102527  1.596914  0.748234
S    -1.727638  0.089607  2.148613
S    -0.886558 -0.025991 -1.223201
C     0.536056  0.751997 -0.371904
C     0.474895  2.260862 -0.545913
O    -0.618869  2.774539  0.013945
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C     5.189226 -0.036482  0.626978
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O     2.883690  1.179181  1.039122
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H     5.991176 -0.645592  0.217136
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H     4.942454 -0.353909  1.641012
O     0.269024 -2.876978 -1.282893
H     0.203221 -2.558104 -0.344716
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H     3.566394 -2.241774 -0.432405
O     0.883269 -1.799055  1.140022
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H    -1.800719 -3.881113 -0.768458
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H    -4.825909  0.969462  0.431167
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S    -1.133594  0.385072 -1.291163
C     0.395771  0.728303 -0.343840
C     0.718370  2.220726 -0.321103
O    -0.309725  2.956139  0.073496
C    -0.056562  4.366434  0.172771
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C     2.774929  0.047860  0.016284
O     3.916158  0.076747 -0.651831
C     5.100272  0.039114  0.160023
O     1.814482  2.654155 -0.591239
O     2.694429  0.083842  1.229975
H     0.216215  0.441630  0.697491
H    -0.990613  4.808818  0.509172
H     0.741496  4.551647  0.892755
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H     1.825741  0.201089 -1.925487
H     5.934200  0.059012 -0.537337
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H     5.099175 -0.881513  0.745162
O     0.805624 -2.434665 -0.668974
H     0.568831 -2.272460  0.287280
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O    -3.596936 -0.295315 -0.310336
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H    -5.009732  1.004180 -0.972880
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C     0.519653  0.827862 -0.322312
C     0.558962  2.348326 -0.491987
O    -0.571961  2.914211 -0.084796
C    -0.612720  4.345409 -0.176893
C     1.794959  0.207013 -0.769575
C     2.936021  0.337365  0.121310
O     4.058171 -0.204589 -0.396849
C     5.216866 -0.114387  0.443045
O     1.517087  2.952132 -0.910477
O     2.895069  0.873169  1.211837
H     0.384813  0.626864  0.748092
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H     0.173688  4.782350  0.440018
H    -0.479207  4.657346 -1.213652
H     0.264210 -2.356924 -1.891831
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H     6.026264 -0.572425 -0.120393
H     5.441651  0.930371  0.661218
H     5.045105 -0.652126  1.377517
O     0.451914 -3.018431 -1.214809
H     0.223735 -2.575013 -0.373306
O     2.941833 -2.852215 -0.006690
H     2.234481 -3.033013 -0.655932
H     3.504975 -2.184804 -0.420549
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O     3.612612 -0.909846 -0.057075
C     4.930857 -0.435915  0.241301
C     0.251376  0.205862 -0.425778
C    -1.071055 -0.387334 -0.744925
O    -1.985428  0.557392 -0.983056
C    -3.305761  0.091547 -1.302365
O     2.855802  1.195195  0.170315
O    -1.311668 -1.576933 -0.795807
H     1.275950 -1.637659 -0.564625
H     5.576742 -1.309611  0.201431
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H     4.952266  0.013966  1.235215
H     0.291397  1.273925 -0.231429
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H    -3.271548 -0.555932 -2.179003
H    -3.714703 -0.456715 -0.452779
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H    -3.906360 -2.132298  1.409170
H    -2.416988 -0.302209  1.748729
O    -2.968969 -1.918558  1.483034
H    -2.560471 -2.197454  0.648828
O    -1.196018  3.021398  0.390000
H    -1.471858  2.400517  1.079227
H    -1.585820  2.631408 -0.402007
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          zpe= -762.456526
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  th enthalpy= -762.435930
  free energy= -762.506375

TS2
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C    -2.741759  0.014961  0.030178
O    -3.639075 -0.972444  0.094826
C    -5.000680 -0.574829 -0.099749
C    -0.332803  0.337243  0.199068
C     1.061342 -0.156512  0.418973
O     1.780270  0.759648  1.094255
C     3.103781  0.362415  1.469074
O    -3.028208  1.173828 -0.175001
O     1.346263 -1.383621  0.456389
H    -1.232805 -1.561277  0.421248
H    -5.590921 -1.484184 -0.015878
H    -5.294895  0.146773  0.664166
H    -5.124272 -0.125606 -1.086545
H    -0.452459  1.399282  0.007223
H     3.542032  1.224193  1.966552
H     3.067061 -0.493060  2.144866
H     3.679814  0.106145  0.577514
O     1.647170 -0.105551 -1.287939
H     4.647544 -1.633311 -0.947562
H     2.493123 -0.633500 -1.294264
O     3.713429 -1.831075 -1.084102
H     3.397014 -2.206536 -0.250889
O     1.347029  2.823735 -0.901688
H     1.557657  1.978452 -1.322354
H     1.618123  2.665078  0.011065
    el energy= -762.634208849
          zpe= -762.432333
    th energy= -762.413813
  th enthalpy= -762.412869
  free energy= -762.479960

5
C    -1.395498 -0.516023  0.137615
C    -2.761564  0.037098 -0.048052
O    -3.691823 -0.905892  0.133606
C    -5.045292 -0.468470 -0.025424
C    -0.339855  0.276839 -0.003913
C     1.080121 -0.206401  0.158445
O     1.630941  0.569458  1.184272
C     3.040406  0.428299  1.364228
O    -3.018315  1.187818 -0.327560
O     1.186687 -1.552221  0.476835
H    -1.300558 -1.567797  0.383212
H    -5.664340 -1.344069  0.155320
H    -5.274192  0.319152  0.694423
H    -5.202586 -0.088784 -1.036416
```

```
H    -0.450034  1.328387 -0.257432
H     3.282232  0.956095  2.285095
H     3.316930 -0.623960  1.460324
H     3.582217  0.883622  0.529539
O     1.730605 -0.084148 -1.057682
H     4.696514 -1.356138 -0.781452
H     2.566151 -0.630270 -1.053827
O     3.828745 -1.685495 -1.045141
H     3.653720 -2.443575 -0.473355
O     1.580827  2.815272 -0.673100
H     1.781046  2.009519 -1.169633
H     1.561652  2.491418  0.236972
    el energy= -762.658825275
          zpe= -762.454177
    th energy= -762.436023
  th enthalpy= -762.435079
  free energy= -762.501527

TS3
C    -1.363535 -0.553852  0.047851
C    -2.733476 -0.005760 -0.129179
O    -3.656141 -0.858752  0.324350
C    -5.011876 -0.415692  0.199812
C    -0.310611  0.159161 -0.336018
C     1.078377 -0.370957 -0.174016
O     1.528275  0.453370  1.290520
C     2.916635  0.536851  1.500419
O    -2.994257  1.071798 -0.617279
O     1.300586 -1.489820  0.402762
H    -1.254203 -1.535391  0.496272
H    -5.625010 -1.216289  0.606600
H    -5.159748  0.506721  0.763929
H    -5.255436 -0.239391 -0.849207
H    -0.413599  1.145007 -0.780573
H     3.060937  1.460120  2.075198
H     3.283632 -0.302081  2.096503
H     3.468770  0.621358  0.559543
O     1.888111  0.056869 -1.154050
H     4.671202 -1.483338 -0.585858
H     2.703471 -0.527061 -1.168332
O     3.794842 -1.704154 -0.924279
H     3.325899 -2.143518 -0.198674
O     1.472304  2.850821 -0.464404
H     1.837245  2.084178 -0.927620
H     1.234009  2.490117  0.398050
    el energy= -762.645575827
          zpe= -762.443200
    th energy= -762.425071
  th enthalpy= -762.424127
  free energy= -762.490663

6
C    -1.338462 -0.658955  0.049605
C    -2.698769 -0.101035 -0.178606
O    -3.596313 -0.685139  0.617712
C    -4.940924 -0.213335  0.474062
C    -0.303713 -0.199445 -0.649787
C     1.057580 -0.755250 -0.420289
O     1.374434  1.176405  1.553734
C     2.746875  1.092481  1.619594
O    -2.966086  0.768323 -0.977832
O     1.327445 -1.542389  0.469810
H    -1.217960 -1.438390  0.794684
H    -5.534076 -0.786538  1.182393
H    -4.991456  0.852405  0.702932
H    -5.290788 -0.380734 -0.545870
H    -0.418043  0.590273 -1.385289
H     3.064660  2.024615  2.121634
H     3.080940  0.257845  2.246144
H     3.217249  1.079705  0.627974
O     1.952269 -0.295202 -1.288039
H     4.750421 -1.173916 -0.005762
H     2.839599 -0.724398 -1.074603
O     3.997747 -1.615369 -0.417859
H     3.450830 -1.960163  0.305610
O     1.293235  2.528910 -1.048442
H     1.727288  1.772215 -1.462340
H     1.123968  2.216009 -0.147643
    el energy= -762.675738784
          zpe= -762.474033
    th energy= -762.454521
  th enthalpy= -762.453576
  free energy= -762.525110

7
C     1.695558 -0.490414 -0.037722
C     3.053859  0.099311  0.127993
O     3.963145 -0.593582 -0.556221
C     5.305844 -0.101232 -0.462656
C     0.661966  0.078366  0.582082
C    -0.710202 -0.487109  0.508064
O    -3.583523  0.636397 -0.996011
C    -4.260454  1.044093  0.183817
O     3.300954  1.078463  0.794911
O    -0.975597 -0.956197 -0.699532
H     1.599705 -1.376447 -0.655767
H     5.909857 -0.770399 -1.070275
H     5.357668  0.919465 -0.844678
H     5.638884 -0.116671  0.576227
H     0.775342  0.962530  1.200674
H    -4.430355  2.120700  0.114770
H    -5.229776  0.543926  0.281544
H    -3.663965  0.838621  1.081171
O    -1.494591 -0.571068  1.431625
H    -2.925344 -1.705048  0.714090
H    -3.462295 -0.329806 -0.916314
O    -3.442838 -1.935038 -0.075011
H    -3.003689 -2.703440 -0.458380
O    -1.206695  1.929719 -0.498501
H    -1.507114  2.555046  0.170095
H    -2.025185  1.493882 -0.812705
    el energy= -762.658337636
          zpe= -762.455587
    th energy= -762.435984
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th enthalpy= -762.435039
free energy= -762.505939

8
C 1.807624 -0.630713 -0.254050
C 3.276577 -0.306803 0.031440
O 3.998545 -1.305096 0.255091
C 0.908076 0.309016 -0.548363
C -0.498446 -0.040511 -0.812577
O -1.237221 1.043786 -1.093563
C -2.642091 0.820250 -1.254057
O 3.595548 0.903456 0.007840
O -0.970122 -1.164404 -0.783305
H 1.505006 -1.675370 -0.214662
H 1.193693 1.354709 -0.581172
H -3.073682 1.790206 -1.488900
H -2.824651 0.111611 -2.063384
H -3.057218 0.431937 -0.321689
O -1.436019 -0.297956 1.848592
H -4.084642 -1.750025 0.421139
H -2.177431 -0.880573 1.527523
O -3.182580 -1.997666 0.654615
H -2.661575 -1.917706 -0.160945
O -0.766398 2.503313 1.353213
H -1.068781 1.608660 1.571770
H -0.875182 2.535647 0.396100
el energy= -722.899911016
zpe= -722.739509
th energy= -722.721808
th enthalpy= -722.720863
free energy= -722.787832

TS4
C -1.829546 -0.683174 0.186470
C -3.295729 -0.299695 -0.021015
O -4.097548 -1.262582 -0.013940
C -0.848564 0.213935 0.183443
C 0.571848 -0.171872 0.400204
O 1.222308 0.783428 1.104135
C 2.573737 0.490879 1.463889
O -3.542046 0.918501 -0.178872
O 0.965675 -1.375986 0.427394
H -1.604342 -1.737485 0.334062
H -1.050799 1.269511 0.032779
H 2.941041 1.371940 1.985476
H 2.616396 -0.382698 2.116415
H 3.169941 0.309839 0.566673
O 1.209691 -0.060548 -1.280284
H 4.300039 -1.445685 -0.804146
H 2.090079 -0.518751 -1.271054
O 3.390901 -1.684646 -1.019185
H 3.010942 -2.037236 -0.202133
O 0.794853 2.837138 -0.887575
H 0.988087 1.980476 -1.294190
H 0.957469 2.647217 0.044787
el energy= -722.873434559
zpe= -722.712947
th energy= -722.696291
th enthalpy= -722.695347
free energy= -722.758548

9
C -1.644884 -0.705571 -0.203298
C -3.042591 -0.292812 -0.081856
O -4.032454 -1.008757 -0.044396
C -0.653448 0.182806 -0.272195
C 0.804391 -0.262166 -0.349761
O 1.406851 0.285676 0.901267
C 1.213841 -0.557314 2.017653
O -3.317624 0.997575 -0.001524
O 1.007642 -1.530822 -0.499037
H -1.441704 -1.770869 -0.242845
H -0.830506 1.257438 -0.232320
H 0.146972 -0.727910 2.217345
H 1.694984 -1.528021 1.866331
H 1.658326 -0.057588 2.881071
O 1.391594 0.578274 -1.351006
H 3.546503 -0.479884 0.213851
H 2.299587 0.234206 -1.431463
O 3.595737 -1.070270 -0.549963
H 2.678239 -1.466799 -0.535912
O 0.940942 2.954384 0.104367
H 1.170532 2.416089 -0.670437
H 1.071717 2.285207 0.793466
el energy= -722.893956684
zpe= -722.731628
th energy= -722.715601
th enthalpy= -722.714657
free energy= -722.776030

TS5
C -1.586434 -0.613647 -0.462020
C -2.937971 -0.176537 0.009412
O -3.503791 -0.389191 1.061106
C -0.558502 0.268975 -0.561244
C 0.819413 -0.224981 -0.828490
O 1.096172 0.037151 1.007895
C 0.644696 -1.047152 1.761149
O -3.309751 0.445115 -1.049359
O 1.059239 -1.407870 -1.108831
H -1.457014 -1.644683 -0.781587
H -0.682891 1.327881 -0.355885
H -0.394026 -0.918478 2.105783
H 0.691956 -1.975636 1.169250
H 1.277290 -1.184037 2.649088
O 1.637053 0.790391 -1.263832
H 2.850240 -0.370467 0.632596
H 2.545891 0.441861 -1.178855
O 3.557616 -0.725941 0.053102
H 3.062705 -1.422532 -0.406956
O 0.911357 2.758777 0.753729
H 1.306714 2.579947 -0.110003
H 0.928753 1.858735 1.133241
el energy= -722.884398558

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          zpe= -722.722753
    th energy= -722.707210
  th enthalpy= -722.706265
  free energy= -722.765973

10
C    -1.867165 -0.800593  0.131087
C    -3.262631 -0.174806  0.073156
O    -4.155261 -0.828105  0.660888
C    -0.797235 -0.226922 -0.420584
C     0.538625 -0.851268 -0.343352
O     1.049656  1.344382  1.437873
C     2.423532  1.268958  1.381407
O    -3.363549  0.909702 -0.544352
O     0.814428 -1.852296  0.299362
H    -1.763236 -1.750357  0.652481
H    -0.884910  0.722649 -0.939092
H     2.783075  1.756517  2.304736
H     2.763135  0.225615  1.432517
H     2.846311  1.791156  0.515922
O     1.455598 -0.193892 -1.066119
H     4.206055 -1.491016  0.106722
H     2.332345 -0.657910 -0.956576
O     3.485383 -1.764848 -0.472888
H     2.835470 -2.216689  0.090624
O     0.821533  2.642232 -1.130829
H     1.148148  1.779484 -1.420838
H     0.660530  2.490930 -0.188271
    el energy= -722.917309676
          zpe= -722.756780
    th energy= -722.739205
  th enthalpy= -722.738260
  free energy= -722.804773

11
C     1.916822 -0.774619 -0.088487
C     3.322136 -0.158416 -0.088514
O     4.209456 -0.892959 -0.576885
C     0.856970 -0.125397  0.394456
C    -0.472099 -0.771354  0.361718
O    -1.219251  1.224819 -1.421248
C    -2.594154  0.911188 -1.488754
O     3.424631  0.991400  0.392237
O    -0.804256 -1.760870 -0.271135
H     1.802466 -1.772795 -0.506230
H     0.942890  0.867897  0.822846
H    -2.788238  0.455035 -2.462888
H    -2.896102  0.196427 -0.710654
H    -3.226653  1.803896 -1.400228
O    -1.331029 -0.182081  1.183406
H    -4.101506 -1.786831 -0.087245
H    -1.680887  2.190866  1.541464
O    -3.484980 -1.899669  0.644586
H    -2.630245 -2.062074  0.213437
O    -0.970220  2.562152  1.004729
H    -1.110405  3.516384  1.019375
H    -1.084179  1.760462 -0.617907
    el energy= -722.895908917
          zpe= -722.736238
    th energy= -722.717475
  th enthalpy= -722.716531
  free energy= -722.786136

12
C     0.425113 -0.159658 -0.213577
C     1.661062  0.669473 -0.455216
O     2.770632  0.087697 -0.377062
C    -0.739951  0.073840 -0.822008
C    -1.968735 -0.794261 -0.608743
O    -2.794600 -0.817874 -1.544762
O     1.501186  1.896879 -0.722899
O    -2.041488 -1.414803  0.491293
H     0.520049 -1.008895  0.458745
H    -0.825156  0.886428 -1.542484
O    -0.710668  2.589927  0.430006
H    -0.918251  1.170062  1.834286
H     0.169961  2.370068 -0.040862
O    -1.151614  0.425179  2.409469
H    -1.428893 -0.265081  1.771946
O     2.602837 -2.448019  0.567147
H     2.697150 -1.533180  0.210544
H     2.109907 -2.907648 -0.120444
    el energy= -683.156740946
          zpe= -683.036645
    th energy= -683.021941
  th enthalpy= -683.020997
  free energy= -683.080317

TS6
C    -0.463780 -0.028100 -0.216190
C    -1.718455 -0.869093 -0.234973
O    -2.815220 -0.252473 -0.311966
C     0.711443 -0.480790 -0.724888
C     1.972761  0.374063 -0.775013
O     2.847443 -0.004163 -1.579919
O    -1.567849 -2.114485 -0.160337
O     2.014088  1.385569 -0.019382
H    -0.500804  0.947025  0.260132
H     0.723786 -1.391126 -1.316792
O     0.963768 -1.709305  1.007772
H     0.827282 -0.201169  2.178777
H     0.101039 -2.106172  0.750200
O     0.963974  0.721533  2.454446
H     1.339435  1.085876  1.626163
O    -2.515628  2.426942 -0.210050
H    -2.661999  1.450697 -0.257981
H    -1.965162  2.609439 -0.978634
    el energy= -683.150402231
          zpe= -683.029392
    th energy= -683.015450
  th enthalpy= -683.014505
  free energy= -683.071859

13
```

```
C     1.245858  0.150906  0.298752
C     1.960360 -1.079663 -0.122544
O     3.155441 -0.974925 -0.471416
C    -0.215145  0.152193  0.624291
C    -0.951710  0.670890 -0.663019
O    -0.801630  1.900532 -0.899907
O     1.288819 -2.174133 -0.092712
O    -1.576039 -0.152242 -1.363182
H     1.747026  1.107525  0.212981
H    -0.423519  0.901807  1.403014
O    -0.653714 -1.106635  1.073482
H    -2.500034 -1.361177  0.908191
H    -0.010090 -1.741174  0.610257
O    -3.358300 -1.276644  0.456400
H    -3.025036 -0.898198 -0.374275
O     0.828945  3.376317  0.643874
H     0.698049  3.059263  1.543373
H     0.209249  2.827863  0.099266
    el energy= -683.202422181
          zpe= -683.080074
    th energy= -683.066117
  th enthalpy= -683.065173
  free energy= -683.125439

TS7
C     1.073324  0.295186 -0.408055
C     2.198638 -0.712157 -0.100580
O     3.365279 -0.284826 -0.122037
C    -0.320978 -0.109580  0.070797
C    -1.417800  0.899434 -0.352773
O    -1.162790  2.117894 -0.129821
O     1.836895 -1.908373  0.134011
O    -2.476902  0.462339 -0.851638
H     1.077329  0.552355 -1.473988
H    -0.310498 -0.099779  1.176044
O    -0.610491 -1.413156 -0.402319
H    -2.142224 -1.908844  0.632143
H     0.253959 -1.880346 -0.216885
O    -3.021437 -1.620576  0.928310
H    -3.115778 -0.858335  0.329239
O     1.239213  2.424319  0.888309
H     1.397795  1.286024  0.152726
H     0.282177  2.450656  0.585862
    el energy= -683.160757805
          zpe= -683.041997
    th energy= -683.029549
  th enthalpy= -683.028605
  free energy= -683.083047

14
C    -0.689749 -0.096454 -0.585920
C    -2.117305  0.305228 -0.163015
O    -3.070749 -0.160720 -0.809637
C     0.299197 -0.113199  0.590401
C     1.694689 -0.532270  0.090451
O     1.794227 -1.755959 -0.232649
O    -2.204440  1.117787  0.815980
O     2.610184  0.310640 -0.002463
H    -0.325226  0.649497 -1.305587
H    -0.022962 -0.895177  1.297228
O     0.302457  1.147875  1.229622
H     0.780025  2.397911 -0.158628
H    -0.685448  1.337600  1.258876
O     1.341034  2.607363 -0.924588
H     1.984010  1.884906 -0.803276
O    -0.353916 -3.149800  0.078530
H    -0.721479 -1.067159 -1.087106
H     0.519713 -2.624893 -0.031372
    el energy= -683.176411970
          zpe= -683.052738
    th energy= -683.039908
  th enthalpy= -683.038964
  free energy= -683.093663

15
C     0.339136 -0.565370 -0.835805
C     1.852419 -0.705215 -0.602817
O     2.358329 -1.808041 -0.861690
C    -0.372917  0.564838 -0.100539
C    -1.832035  0.633505 -0.607329
O    -2.005487  1.297137 -1.651547
O     2.511395  0.322294 -0.223046
O    -2.707053 -0.024092  0.022924
H    -0.138479 -1.509543 -0.555597
H     0.103181  1.520665 -0.357138
O    -0.310638  0.366672  1.308588
H    -0.862801 -1.563555  1.694763
H     0.434789  0.914416  1.612827
O    -1.624745 -2.090782  1.417480
H    -2.107100 -1.391452  0.915876
O     1.823586  2.124689  1.343048
H     0.190508 -0.431675 -1.914948
H     2.097177  1.391585  0.637103
    el energy= -683.170174468
          zpe= -683.046871
    th energy= -683.033974
  th enthalpy= -683.033030
  free energy= -683.088248

TS8
C     0.421651 -0.864744  0.415926
C     1.958671 -0.752666  0.381163
O     2.570337 -1.359357  1.276957
C    -0.374732 -0.058994 -0.607160
C    -1.830428 -0.631534 -0.643239
O    -1.994372 -1.594982 -1.414624
O     2.501968 -0.103602 -0.570738
O    -2.676701 -0.123415  0.139553
H     0.065230 -0.592522  1.415579
H     0.052284 -0.198643 -1.607450
O    -0.408843  1.316631 -0.293836
H    -0.834502  1.549529  1.742819
H     0.303491  1.830159 -0.946969
O    -1.548082  1.160138  2.264634
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H    -2.031808  0.693265  1.543937
O     1.465793  2.113551 -1.238252
H     0.189765 -1.927836  0.277893
H     1.923763  1.221967 -1.015496
    el energy= -683.155423835
          zpe= -683.038049
    th energy= -683.025358
  th enthalpy= -683.024413
  free energy= -683.080427

16
C    -0.300725  0.741764 -0.687224
C    -1.847251  0.861988 -0.580940
O    -2.307447  2.001674 -0.795858
C     0.246383 -0.539355 -0.074649
C     1.988762 -0.491010 -0.761778
O     2.062019 -1.261268 -1.701520
O    -2.511236 -0.182343 -0.334768
O     2.701069  0.310427 -0.176426
H     0.155791  1.602024 -0.190765
H    -0.102513 -1.445523 -0.594411
O     0.325761 -0.618350  1.212153
H     0.925974  0.979747  1.873850
H    -0.971992 -2.074501  1.435361
O     1.483096  1.780957  1.942351
H     2.117606  1.572459  1.240680
O    -1.814002 -2.430280  1.111295
H    -0.051642  0.794493 -1.754517
H    -2.110311 -1.675551  0.559526
    el energy= -683.201125043
          zpe= -683.077800
    th energy= -683.063818
  th enthalpy= -683.062874
  free energy= -683.120453

18
P    -2.701052 -0.089151 -0.257743
O    -2.942061  1.037329  0.854762
O    -1.906412 -1.265026  0.486387
C    -1.834100  1.580077  1.604684
H    -1.263843  0.773653  2.076027
H    -1.196568  2.171244  0.939062
H    -2.275597  2.229117  2.358309
C    -2.523489 -1.885927  1.636239
H    -3.450262 -2.376763  1.331841
H    -1.804501 -2.611922  2.005609
H    -2.715328 -1.137076  2.406198
S    -4.360379 -0.521009 -1.155263
S    -1.215425  0.567792 -1.580603
C     0.351945  0.118654 -0.703811
C     1.314821  1.243102 -1.050929
O     1.261998  2.238901 -0.156431
C     2.179146  3.320242 -0.401217
C     0.867747 -1.226438 -1.206342
C     2.073284 -1.658018 -0.401999
O     3.092729 -2.028553 -1.157735
C     4.266899 -2.459280 -0.448936
O     1.999876  1.257200 -2.041119
O     2.099184 -1.674912  0.815677
H     0.174968  0.083381  0.374638
H     2.014186  4.035774  0.400752
H     3.200215  2.934480 -0.378710
H     1.972573  3.771462 -1.371539
H     0.086474 -1.976988 -1.055710
H     1.118637 -1.169220 -2.265512
H     4.996903 -2.705986 -1.215716
H     4.623380 -1.648713  0.187657
H     4.034010 -3.334589  0.158871
O     3.567769  0.510922  0.546667
H     3.056383  0.693657  1.372599
O     0.092664 -0.888420  2.691779
H     0.690683 -0.145436  2.875026
H     0.588653 -1.390327  2.027588
O     1.774920  1.355518  2.486174
H     2.046978  1.940312  3.204450
H     1.327836  1.914514  1.833139
    el energy= -2131.16928230
          zpe= -2130.858769
    th energy= -2130.829975
  th enthalpy= -2130.829031
  free energy= -2130.918999

TS9
P    -2.613949 -0.211305 -0.143500
O    -2.920978  1.042449  0.802602
O    -1.705090 -1.199610  0.736217
C    -1.844706  1.840474  1.347891
H    -1.095134  1.207639  1.833727
H    -1.380876  2.420588  0.547294
H    -2.312112  2.504447  2.072935
C    -2.136005 -1.560903  2.063866
H    -3.121723 -2.029761  2.023609
H    -1.397052 -2.269855  2.431112
H    -2.155571 -0.677959  2.704729
S    -4.263124 -0.915750 -0.878193
S    -1.221648  0.348257 -1.609401
C     0.375158 -0.010385 -0.747994
C     1.324833  1.143456 -1.033781
O     0.925055  2.257087 -0.382990
C     1.537984  3.479342 -0.815588
C     0.928486 -1.355382 -1.209078
C     1.912116 -1.939569 -0.220976
O     2.991994 -2.428398 -0.817469
C     3.975092 -2.997582  0.057241
O     2.041616  1.218125 -2.058912
O     1.725549 -2.010893  0.977644
H     0.193672 -0.012767  0.327458
H     1.082751  4.263763 -0.213834
H     2.617159  3.451533 -0.646417
H     1.339434  3.649342 -1.874014
H     0.103567 -2.070604 -1.271913
H     1.388730 -1.265109 -2.194067
H     4.781656 -3.339149 -0.586825
H     4.332189 -2.236717  0.753411
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H     3.547587 -3.831066  0.615975
O     2.771009  0.532505 -0.117730
H     2.951067  1.343694  0.416645
O     0.668561  0.083515  2.582313
H     1.370600  0.731799  2.408476
H     0.968793 -0.723079  2.134869
O     2.538537  2.256318  1.948485
H     3.169049  2.595209  2.595851
H     1.854045  2.932007  1.864196
    el energy= -2131.14179671
          zpe= -2130.832092
    th energy= -2130.803906
  th enthalpy= -2130.802962
  free energy= -2130.892039

19
P    -2.584148 -0.166029 -0.265669
O    -2.952094  0.843358  0.922469
O    -1.742721 -1.345658  0.424566
C    -1.907778  1.406485  1.748371
H    -1.303401  0.609165  2.191986
H    -1.280178  2.069875  1.145506
H    -2.418815  1.978106  2.520752
C    -2.346604 -2.071143  1.516890
H    -3.240251 -2.589754  1.163187
H    -1.597973 -2.783920  1.853414
H    -2.593695 -1.386244  2.329562
S    -4.177895 -0.642921 -1.258844
S    -1.097696  0.707185 -1.452726
C     0.450606  0.175515 -0.606386
C     1.503197  1.327264 -0.692769
O     1.002633  2.392225  0.062736
C     1.763383  3.595317 -0.083909
C     0.974358 -1.121522 -1.222687
C     2.113786 -1.701820 -0.417873
O     3.143814 -2.052843 -1.175172
C     4.265825 -2.605635 -0.473495
O     1.607718  1.611908 -2.024083
O     2.082851 -1.868339  0.785923
H     0.258222  0.035506  0.463911
H     1.278479  4.342233  0.542140
H     2.794281  3.443038  0.247089
H     1.752862  3.925554 -1.126119
H     0.165332 -1.857461 -1.199857
H     1.281067 -0.969009 -2.258060
H     5.002638 -2.844319 -1.236377
H     4.661115 -1.868797  0.227816
H     3.966997 -3.502815  0.069916
O     2.741360  0.907816 -0.234428
H     2.691918  0.882653  0.746932
O     0.216835 -0.934789  2.709334
H     0.859538 -0.223073  2.862124
H     0.661900 -1.465014  2.030201
O     2.049593  1.212473  2.401071
H     2.650483  1.560074  3.072177
H     1.480609  1.950422  2.135681
    el energy= -2131.17568445
          zpe= -2130.862851
    th energy= -2130.835285
  th enthalpy= -2130.834340
  free energy= -2130.920932

TS10
P    -2.592279 -0.169114 -0.246912
O    -2.986283  0.661032  1.066380
O    -1.733287 -1.418685  0.285872
C    -1.954602  1.146242  1.954841
H    -1.314478  0.320887  2.279708
H    -1.361938  1.911934  1.445413
H    -2.477558  1.585050  2.802601
C    -2.332592 -2.285361  1.272785
H    -3.277716 -2.681117  0.894152
H    -1.622963 -3.093676  1.433600
H    -2.485018 -1.737843  2.203808
S    -4.181819 -0.548134 -1.292497
S    -1.143427  0.892172 -1.311819
C     0.430299  0.299502 -0.560200
C     1.454935  1.432210 -0.706134
O     0.739599  2.648009  0.341223
C     1.608424  3.707149  0.644147
C     0.921973 -0.934939 -1.334594
C     2.118673 -1.565875 -0.666339
O     3.144668 -1.727878 -1.482430
C     4.324168 -2.304724 -0.900315
O     1.407918  2.188527 -1.711468
O     2.133874 -1.904432  0.505628
H     0.281968  0.051569  0.495353
H     1.401668  3.941099  1.697481
H     2.654687  3.406932  0.545614
H     1.387093  4.591594  0.042433
H     0.123703 -1.681973 -1.333753
H     1.159153 -0.670140 -2.366544
H     5.036215 -2.401878 -1.715573
H     4.714012 -1.640828 -0.126544
H     4.092319 -3.278223 -0.467703
O     2.663448  1.157121 -0.185232
H     2.603936  0.759795  0.724821
O     0.197414 -1.274256  2.567307
H     0.907426 -0.661860  2.811732
H     0.575427 -1.722911  1.796297
O     2.674724  0.089492  2.248316
H     3.019335 -0.796114  2.056128
H     3.306562  0.513132  2.843784
    el energy= -2131.15592580
          zpe= -2130.845653
    th energy= -2130.818111
  th enthalpy= -2130.817167
  free energy= -2130.903909

20
P    -2.376277 -0.331668 -0.228848
O    -3.074843  0.668464  0.765064
O    -1.624122 -1.439147  0.604131
C    -2.250819  1.444054  1.699550
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H    -1.489267  0.798390  2.147335
H    -1.779136  2.261153  1.152957
H    -2.947972  1.809722  2.449011
C    -2.229275 -2.020020  1.792523
H    -3.271254 -2.277297  1.595193
H    -1.652468 -2.918513  1.995651
H    -2.134566 -1.314210  2.616101
S    -3.906192 -1.023720 -1.381050
S    -1.008072  0.466918 -1.518164
C     0.568782  0.019008 -0.671979
C     1.629069  0.998958 -1.240974
O     0.289672  2.874346  0.524982
C     1.061079  3.884298 -0.097277
C     1.003422 -1.417197 -0.990291
C     2.224013 -1.737794 -0.157776
O     3.293805 -2.007390 -0.894797
C     4.501010 -2.245474 -0.159885
O     1.367635  1.568276 -2.307244
O     2.223563 -1.760577  1.057144
H     0.435582  0.152232  0.404211
H     0.530072  4.209294 -0.994636
H     1.199452  4.753770  0.558768
H     2.043956  3.505462 -0.400654
H     0.222273 -2.127327 -0.710754
H     1.226586 -1.521843 -2.053631
H     5.265191 -2.453625 -0.904731
H     4.758133 -1.356782  0.419195
H     4.374643 -3.095531  0.511761
O     2.698787  1.026740 -0.569772
H     2.466531  1.184150  1.034611
O     0.259195 -0.454930  2.688723
H     0.934354  0.247852  2.642967
H     0.686303 -1.163493  2.183252
O     2.144233  1.437818  1.946997
H     2.880580  1.860879  2.401715
H     0.856317  2.465757  1.206664
    el energy= -2131.16082240
          zpe= -2130.849706
    th energy= -2130.820801
  th enthalpy= -2130.819857
  free energy= -2130.910787

21
P    -2.446288 -0.437486 -0.240072
O    -2.946819  0.586087  0.886713
O    -1.494012 -1.472266  0.533587
C    -1.983816  1.285153  1.705426
H    -1.266733  0.581392  2.139597
H    -1.464026  2.031040  1.098178
H    -2.559996  1.777298  2.486831
C    -2.036202 -2.196004  1.658654
H    -2.894118 -2.789656  1.335693
H    -1.236475 -2.841366  2.013108
H    -2.322847 -1.498766  2.447295
S    -3.966571 -1.150268 -1.209765
S    -1.060263  0.530477 -1.478007
C     0.548809  0.163462 -0.663514
C     1.525946  1.225420 -1.163686
O     0.512736  3.061830  0.515823
C     0.571284  4.155674 -0.314498
C     1.077262 -1.210889 -1.103220
C     2.309129 -1.604675 -0.320919
O     3.131763 -2.364253 -1.028635
C     4.296937 -2.836229 -0.333517
O     1.421958  1.732737 -2.256687
O     2.512125 -1.288138  0.835486
H     0.442049  0.194709  0.424779
H     0.643718  5.103175  0.228276
H     1.498471  4.013742 -0.902419
H    -0.250723  4.149722 -1.041151
H     0.316120 -1.970238 -0.900529
H     1.291071 -1.220522 -2.173986
H     4.840207 -3.444908 -1.051661
H     4.902787 -1.990368 -0.006577
H     4.000510 -3.429976  0.531944
O     2.567315  1.484001 -0.383216
H     2.425154  1.209663  0.556638
O     0.414470 -0.764111  2.767197
H     0.931665  0.056226  2.826300
H     0.924876 -1.263679  2.114865
O     1.981988  1.506991  2.230296
H     2.740403  1.721235  2.788440
H     1.493255  2.335718  2.096952
    el energy= -2131.18148415
          zpe= -2130.872567
    th energy= -2130.843153
  th enthalpy= -2130.842209
  free energy= -2130.935914

22
P    -2.390973 -0.230627 -0.248108
O    -2.762092  0.372974  1.190792
O    -1.289005 -1.365002  0.041827
C    -1.734321  0.945640  2.033204
H    -0.936754  0.222194  2.216721
H    -1.312861  1.838170  1.562046
H    -2.229376  1.210876  2.965869
C    -1.596104 -2.406254  0.987492
H    -2.554131 -2.871188  0.741421
H    -0.792106 -3.134126  0.893271
H    -1.623528 -1.996527  1.999898
S    -4.011691 -0.779977 -1.170801
S    -1.255192  1.140609 -1.321904
C     0.407157  0.987660 -0.534150
C     1.025963  2.420039 -0.528024
O     0.650776  3.161398  0.419602
C     1.256595 -0.022901 -1.276083
C     2.535217 -0.266229 -0.516798
O     3.356482 -1.092266 -1.181526
C     4.566846 -1.440910 -0.492154
O     1.807912  2.685814 -1.455159
O     2.803954  0.179117  0.578947
H     0.270299  0.663036  0.496438
H     0.736119 -0.981692 -1.372329
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H     1.510156  0.342209 -2.274104
H     5.109034 -2.101759 -1.164093
H     5.149360 -0.544760 -0.277318
H     4.324797 -1.952241  0.441828
O     0.973219 -1.212300  1.988173
H     1.202760 -1.828467  1.248331
O     1.552380 -3.046057 -0.013775
H     1.958583 -3.830163  0.375809
H     2.105585 -2.822642 -0.774960
O     1.146327  1.688337  2.710939
H     0.967171  2.277974  1.949436
H     1.561870  0.919990  2.297160
    el energy= -2091.42178000
          zpe= -2091.152922
    th energy= -2091.126048
  th enthalpy= -2091.125104
  free energy= -2091.210164

TS11
P    -2.409908 -0.472374 -0.187799
O    -2.790789 -0.111633  1.331260
O    -1.115760 -1.414592 -0.072195
C    -1.806263  0.468698  2.213241
H    -0.912507 -0.156799  2.268343
H    -1.522156  1.466694  1.867326
H    -2.280473  0.531671  3.191091
C    -1.161298 -2.616358  0.715427
H    -1.778987 -3.365149  0.214928
H    -0.129627 -2.958657  0.789517
H    -1.560962 -2.407010  1.710568
S    -3.966599 -1.188275 -1.104320
S    -1.569800  1.187800 -1.119149
C     0.143479  1.178085 -0.419150
C     0.531203  2.680190 -0.290808
O     0.429453  3.169280  0.865677
C     1.078317  0.372080 -1.304228
C     2.336048  0.008745 -0.552180
O     3.093891 -0.859791 -1.260109
C     4.465015 -0.959361 -0.854681
O     0.861354  3.253614 -1.343574
O     2.868416  0.756837  0.313832
H     0.096999  0.737039  0.571577
H     0.620117 -0.555547 -1.650242
H     1.366317  0.977315 -2.170069
H     4.906213 -1.718185 -1.498522
H     4.970840 -0.002955 -0.993737
H     4.543925 -1.262883  0.190958
O     1.650280 -0.943151  0.838704
H     2.338591 -1.647008  0.939172
O     2.865669 -3.284044  0.459189
H     3.696815 -3.730112  0.659743
H     2.843305 -3.198433 -0.502890
O     1.088489  1.301766  2.788815
H     0.872486  2.007755  2.141457
H     1.533080  0.636705  2.244757
    el energy= -2091.39520251
          zpe= -2091.126314
    th energy= -2091.100312
  th enthalpy= -2091.099368
  free energy= -2091.183589

23
P    -2.428434 -0.271596 -0.205486
O    -2.921976  0.465233  1.133506
O    -1.306768 -1.315386  0.285007
C    -1.978695  1.134601  1.997444
H    -1.210199  0.444236  2.351349
H    -1.496327  1.965019  1.471968
H    -2.560927  1.510086  2.837100
C    -1.690984 -2.361645  1.199573
H    -2.486571 -2.967453  0.759536
H    -0.795793 -2.961495  1.345343
H    -2.029575 -1.929373  2.144019
S    -3.957003 -0.988888 -1.166463
S    -1.273465  1.036487 -1.335310
C     0.347557  0.980892 -0.445829
C     0.872274  2.445748 -0.469182
O     0.681137  3.107321  0.585680
C     1.263332 -0.015490 -1.128676
C     2.515599 -0.312968 -0.264437
O     3.214275 -1.328968 -0.938882
C     4.455926 -1.667593 -0.321989
O     1.394492  2.819726 -1.533368
O     3.207710  0.855064 -0.192432
H     0.161693  0.674433  0.581238
H     0.769048 -0.985702 -1.245817
H     1.579928  0.359948 -2.103095
H     4.940228 -2.389875 -0.977562
H     5.089333 -0.780362 -0.225386
H     4.294186 -2.111375  0.664091
O     2.194852 -0.710786  1.034824
H     1.767725 -1.594745  0.962456
O     1.367897 -3.168510  0.224392
H     1.735451 -3.926050  0.696152
H     1.966933 -3.016768 -0.523165
O     1.067135  1.404198  2.733750
H     0.928189  2.073031  2.029707
H     1.560582  0.704393  2.281484
    el energy= -2091.42617722
          zpe= -2091.154616
    th energy= -2091.129003
  th enthalpy= -2091.128059
  free energy= -2091.211232

TS12
P    -2.440863 -0.173963 -0.065738
O    -2.553043 -0.011433  1.528794
O    -1.401934 -1.382326 -0.261346
C    -1.384589  0.027854  2.374699
H    -0.581426 -0.593803  1.966266
H    -1.035335  1.056742  2.477878
H    -1.698528 -0.356800  3.344194
C    -1.738747 -2.681723  0.269559
H    -2.604685 -3.082239 -0.261857
```

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H    -0.855645 -3.293750  0.098768
H    -1.958249 -2.607847  1.337702
S    -4.214159 -0.384564 -0.833219
S    -1.441957  1.442030 -0.915056
C     0.289214  1.234251 -0.332875
C     0.993150  2.593580 -0.467548
O     0.372224  3.611387 -0.768527
C     1.095312  0.156596 -1.057491
C     2.178329 -0.295353 -0.085536
O     3.008083 -1.374035 -1.140956
C     4.284212 -1.705793 -0.599146
O     2.258103  2.558329 -0.249271
O     3.043420  0.625180  0.266749
H     0.270107  1.005948  0.734540
H     0.478278 -0.709834 -1.295812
H     1.545923  0.552121 -1.969673
H     4.725824 -2.494232 -1.211198
H     4.917288 -0.819003 -0.622809
H     4.179950 -2.051799  0.434886
O     1.771475 -1.086211  0.908503
H     1.447778 -2.134422  0.379907
O     1.412651 -3.004075 -0.445876
H     1.791948 -3.813769 -0.082341
H     2.321350 -2.272323 -0.990579
O     1.596267  1.230066  2.627502
H     2.105583  1.686858  1.940968
H     1.701386  0.306624  2.343090
    el energy= -2091.38449298
          zpe= -2091.119148
    th energy= -2091.094716
  th enthalpy= -2091.093772
  free energy= -2091.174286

24
P    -2.124962  0.367190  0.245683
O    -1.425713  0.471568  1.686017
O    -1.745846 -1.090862 -0.313216
C    -0.480717 -0.481621  2.226943
H    -0.246183 -1.270099  1.509166
H     0.429643  0.051990  2.510556
H    -0.937430 -0.917585  3.116744
C    -2.477100 -2.244860  0.148846
H    -3.519262 -2.167084 -0.164831
H    -1.992860 -3.103359 -0.309860
H    -2.415475 -2.329885  1.236764
S    -4.020176  0.789926  0.286791
S    -1.074783  1.660352 -1.009436
C     0.616723  1.432459 -0.343857
C     1.481739  2.579640 -0.868361
O     1.020775  3.509747 -1.517249
C     1.258643  0.086665 -0.694836
C     2.388623 -0.192476  0.277472
O     0.298334 -2.557027 -2.364644
C     1.671689 -2.795704 -2.586309
O     2.741418  2.469389 -0.600035
O     3.080031  0.806152  0.668629
H     0.550962  1.548823  0.742386
H     0.542817 -0.735922 -0.661124
H     1.657391  0.115251 -1.715422
H     1.910895 -3.867938 -2.611521
H     1.942251 -2.365709 -3.554248
H     2.301515 -2.329721 -1.815189
O     2.584050 -1.347946  0.709410
H     1.322269 -2.530451  0.469545
O     0.506522 -3.061803  0.323789
H     0.724013 -3.961923  0.591402
H     0.144325 -2.796300 -1.431770
O     2.742909 -0.204495  3.345130
H     3.000557  0.577115  2.838952
H     2.800920 -0.891909  2.663483
    el energy= -2091.42620442
          zpe= -2091.157145
    th energy= -2091.129631
  th enthalpy= -2091.128687
  free energy= -2091.217384

25
P    -2.558442 -0.317281  0.050509
O    -2.823845  0.576808  1.344307
O    -1.503855 -1.387460  0.614373
C    -1.755741  1.135113  2.129501
H    -1.054287  0.350752  2.425869
H    -1.251339  1.923268  1.562610
H    -2.224545  1.562240  3.013275
C    -1.328071 -2.643874 -0.076215
H    -1.308008 -2.490755 -1.158906
H    -0.375876 -3.052475  0.258757
H    -2.150683 -3.311651  0.181745
S    -4.199385 -0.966995 -0.731988
S    -1.455858  0.812455 -1.345497
C     0.255624  0.734329 -0.656725
C     0.828120  2.134856 -0.785619
O     0.720748  2.818114  0.358748
C     1.187249  4.178692  0.308438
C     1.109239 -0.280506 -1.404396
C     2.444234 -0.409654 -0.713888
O     3.009922 -1.595664 -0.917418
C     4.245852 -1.825311 -0.217321
O     1.285891  2.584152 -1.805998
O     2.954571  0.466907 -0.045270
H     0.204037  0.463228  0.396331
H     1.011760  4.585975  1.300670
H     2.249842  4.194052  0.064246
H     0.626363  4.733395 -0.444051
H     0.624986 -1.257103 -1.430528
H     1.273201  0.049598 -2.435522
H     4.530457 -2.847061 -0.454637
H     5.003447 -1.118419 -0.554842
H     4.083906 -1.710226  0.856313
O     1.176490 -1.492213  1.469940
H     1.248035 -0.654799  2.004745
O     1.881667 -3.997814  0.374680
H     1.698792 -3.438951  1.141294
H     2.023586 -3.350664 -0.328469
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O     1.700434  0.983233  2.428119
H     1.123841  1.740602  2.260940
H     2.387778  1.070476  1.747783
    el energy= -2131.16654662
          zpe= -2130.856559
    th energy= -2130.827356
  th enthalpy= -2130.826412
  free energy= -2130.917003

TS13
P    -2.607277 -0.418836  0.020135
O    -3.036110  0.615863  1.153067
O    -1.533205 -1.319318  0.798333
C    -2.060944  1.368164  1.904756
H    -1.335495  0.700304  2.371226
H    -1.553003  2.081228  1.248992
H    -2.624267  1.906252  2.664325
C    -1.173878 -2.626146  0.301087
H    -1.231051 -2.659417 -0.790487
H    -0.150229 -2.818955  0.622499
H    -1.859468 -3.362466  0.721615
S    -4.130015 -1.294126 -0.785133
S    -1.465203  0.611124 -1.424929
C     0.198064  0.648858 -0.623083
C     0.753763  2.045015 -0.843261
O     0.648558  2.805204  0.254166
C     1.108361  4.161859  0.107936
C     1.120724 -0.396209 -1.230197
C     2.413150 -0.467032 -0.446171
O     3.178951 -1.481822 -0.880112
C     4.474657 -1.582036 -0.270757
O     1.207248  2.431137 -1.890900
O     2.909420  0.542237  0.123075
H     0.069102  0.460803  0.442258
H     0.940819  4.632639  1.073032
H     2.168016  4.165042 -0.148806
H     0.535820  4.661540 -0.673515
H     0.659040 -1.383951 -1.228832
H     1.361752 -0.128727 -2.263774
H     4.894900 -2.520657 -0.625025
H     5.099662 -0.742535 -0.576459
H     4.371139 -1.592391  0.815565
O     1.875678 -1.063913  1.172778
H     1.621638 -0.281690  1.742925
O     2.111112 -3.802013  0.503713
H     2.183595 -3.071187  1.132239
H     2.307191 -3.362484 -0.333844
O     1.065067  1.083792  2.538219
H     1.191381  1.840726  1.945085
H     1.564964  1.282294  3.339369
    el energy= -2131.14542511
          zpe= -2130.835684
    th energy= -2130.807520
  th enthalpy= -2130.806575
  free energy= -2130.895222
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P    -2.498058 -0.213137 -0.199650
O    -3.006500  0.695880  1.017010
O    -1.421614 -1.214892  0.446072
C    -2.067847  1.422421  1.838369
H    -1.309539  0.758011  2.259437
H    -1.582572  2.204080  1.245719
H    -2.658057  1.875849  2.632132
C    -1.870836 -2.163607  1.436861
H    -2.552237 -2.881488  0.976360
H    -0.975003 -2.668697  1.789405
H    -2.367412 -1.642163  2.258062
S    -3.997282 -0.972739 -1.157398
S    -1.231148  0.929500 -1.419502
C     0.386864  0.730167 -0.547807
C     1.103153  2.060262 -0.704307
O     0.956217  2.823387  0.382822
C     1.562684  4.125774  0.307328
C     1.178047 -0.419068 -1.149896
C     2.347668 -0.841510 -0.221875
O     2.988786 -1.898973 -0.870440
C     4.143902 -2.375070 -0.177150
O     1.710503  2.392682 -1.692031
O     3.122921  0.273365 -0.088583
H     0.196265  0.550670  0.510480
H     1.343614  4.606397  1.257112
H     2.638588  4.024156  0.161821
H     1.129286  4.686682 -0.521132
H     0.546159 -1.308472 -1.228552
H     1.565820 -0.155538 -2.135393
H     4.619733 -3.100170 -0.835162
H     4.835740 -1.550474  0.020348
H     3.864156 -2.854273  0.764540
O     1.911357 -1.214535  1.047472
H     1.415489 -2.061423  0.934543
O     0.825582 -3.488410  0.139210
H     0.907456 -4.324028  0.615057
H     1.502688 -3.515403 -0.553467
O     0.996597  0.902341  2.733342
H     1.196241  1.674726  2.188553
H     1.436737  0.167476  2.277171
    el energy= -2131.17045430
          zpe= -2130.858617
    th energy= -2130.830393
  th enthalpy= -2130.829449
  free energy= -2130.918763

TS14
P    -2.562164 -0.190375 -0.252120
O    -3.003064  0.962586  0.764978
O    -1.612300 -1.161252  0.626919
C    -2.038982  1.849755  1.371257
H    -1.239890  1.286426  1.862035
H    -1.622282  2.513226  0.609438
H    -2.594630  2.432017  2.103508
C    -2.034022 -1.542152  1.959930
H    -3.076133 -1.867209  1.948585
H    -1.386714 -2.370283  2.242805
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H    -1.890054 -0.703981  2.641537
S    -4.101796 -0.990988 -1.101255
S    -1.167387  0.566527 -1.620240
C     0.382174  0.535055 -0.621000
C     1.019289  1.913521 -0.675734
O     1.073574  2.475099  0.535979
C     1.723362  3.756111  0.588222
C     1.364154 -0.515583 -1.151867
C     2.420283 -0.697208 -0.072717
O     3.714769 -1.421902 -1.025803
C     4.730832 -1.985184 -0.241642
O     1.425984  2.433434 -1.685022
O     3.152687  0.279055  0.250309
H     0.119150  0.300267  0.410326
H     1.667896  4.072009  1.626723
H     2.761207  3.652074  0.268633
H     1.205657  4.462356 -0.061245
H     0.849790 -1.456681 -1.350417
H     1.838462 -0.159433 -2.067791
H     5.003269 -2.912909 -0.763810
H     5.611866 -1.340193 -0.201847
H     4.370542 -2.235448  0.759520
O     2.115020 -1.582161  0.898093
H     1.442737 -2.253945  0.595438
O     0.190469 -3.252924  0.251348
H    -0.605927 -2.751060  0.019772
H     0.297454 -3.933778 -0.423762
O     0.714096  0.316402  2.590449
H     1.165569  1.080641  2.205161
H     1.249002 -0.439695  2.304418
    el energy= -2131.15135951
          zpe= -2130.840987
    th energy= -2130.813167
  th enthalpy= -2130.812223
  free energy= -2130.900428

27
P     1.161017 -1.285399  0.171551
O     0.814145 -2.548585  1.061338
O     0.928067  0.019287  1.035497
C    -0.538411 -2.720954  1.572273
H    -0.895421 -1.799099  2.040882
H    -1.195327 -3.008895  0.749334
H    -0.468746 -3.524024  2.301560
C     1.527989  0.181405  2.347300
H     2.614230  0.153919  2.255626
H     1.198265  1.164814  2.674677
H     1.167162 -0.604173  3.012219
S     3.067778 -1.552797 -0.398311
S    -0.191316 -1.051667 -1.383937
C    -1.234273  0.266300 -0.597026
C    -2.624364  0.158049 -1.200612
O    -3.376131 -0.697082 -0.499843
C    -4.706927 -0.899847 -1.001500
C    -0.625613  1.666526 -0.718749
C    -0.845649  2.372541  0.625499
O     2.647468  0.631473 -1.216110
C     3.708896  0.938075 -2.108554
O    -3.007184  0.755574 -2.175177
O    -2.004370  2.308720  1.093270
H    -1.339967 -0.018541  0.447465
H    -5.169771 -1.615867 -0.327271
H    -5.253329  0.044009 -0.998628
H    -4.664346 -1.295900 -2.016804
H     0.432871  1.620263 -0.971773
H    -1.145833  2.214654 -1.510063
H     3.680979  0.230532 -2.937907
H     3.559532  1.952109 -2.493560
H     4.681839  0.883811 -1.611456
O     0.141368  2.938343  1.178892
H     1.508126  2.608453  0.747005
O     2.494306  2.356918  0.536300
H     2.943473  3.170045  0.275861
H     2.630375  1.335922 -0.423726
O    -2.429056 -0.101703  2.404534
H    -3.049734 -0.459231  1.755711
H    -2.311824  0.823489  2.112148
    el energy= -2131.16545439
          zpe= -2130.855477
    th energy= -2130.827423
  th enthalpy= -2130.826479
  free energy= -2130.915722

28
P    -2.359096 -0.701241 -0.233543
O    -3.130765  0.317789  0.730112
O    -1.176281 -1.311774  0.687820
C    -2.489147  1.477792  1.301489
H    -1.607040  1.193767  1.882709
H    -2.209092  2.175226  0.507488
H    -3.234684  1.937003  1.947213
C    -1.503724 -1.753169  2.028457
H    -2.341964 -2.452364  1.999694
H    -0.610805 -2.253734  2.398497
H    -1.738545 -0.893300  2.655946
S    -3.586379 -1.954668 -1.042820
S    -1.238564  0.383815 -1.632149
C     0.210113  0.845152 -0.593994
C     0.542669  2.305932 -0.837432
O     0.446258  3.013622  0.290915
C     0.810548  4.399262  0.176513
C     1.423310 -0.039938 -0.907530
C     2.424090  0.206851  0.207448
O     3.339300 -2.460044 -1.036169
C     4.601498 -2.738378 -0.564504
O     0.860277  2.763412 -1.907354
O     3.000238  1.267850  0.315325
H    -0.058046  0.715512  0.453070
H     0.667709  4.823952  1.166690
H     1.853499  4.478606 -0.133384
H     0.169747  4.893144 -0.554343
H     1.117864 -1.082750 -0.955160
H     1.866291  0.248890 -1.863174
H     4.744401 -3.801627 -0.341349
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H     5.387104 -2.345008 -1.219184
H     4.666900 -2.189369  0.393917
O     2.562696 -0.742035  1.129742
H     1.988713 -1.547455  0.949770
O     1.183702 -2.908655  0.650574
H     0.302092 -2.742546  0.284826
H     1.723218 -3.272290 -0.070468
O     0.599861  0.980911  2.542653
H     0.940251  1.793800  2.143465
H     1.359489  0.383179  2.564814
    el energy= -2131.17559136
          zpe= -2130.866549
    th energy= -2130.836973
  th enthalpy= -2130.836029
  free energy= -2130.929883

29
P     2.060919 -0.770868  0.104558
O     1.920460 -1.286362  1.616276
O     1.615111  0.760006  0.108277
C     0.690702 -1.058542  2.335488
H     0.464349  0.010762  2.362462
H    -0.120873 -1.620123  1.859492
H     0.856643 -1.442105  3.340471
C     2.439524  1.804275  0.663286
H     3.481542  1.649767  0.374619
H     2.056781  2.723823  0.221272
H     2.320902  1.815489  1.746564
S     3.809897 -1.227245 -0.595552
S     0.472282 -1.561769 -1.011888
C    -0.824498 -0.241404 -0.849430
C    -2.135459 -1.008759 -0.918674
O    -2.494790 -1.463211  0.289276
C    -3.740941 -2.175369  0.329926
C    -0.705309  0.841248 -1.932705
C    -0.197412  2.178219 -1.367897
O     0.734055  2.760003 -1.921931
O    -2.766428 -1.208015 -1.926288
O    -0.834980  2.609047 -0.333197
H    -0.741888  0.197199  0.150120
H    -3.885508 -2.459651  1.369493
H    -4.546989 -1.522140 -0.007756
H    -3.689378 -3.057806 -0.308533
H    -0.057744  0.516697 -2.746632
H    -1.704676  1.016738 -2.346269
O    -3.033105  1.443545 -0.013332
H    -2.140696  1.992373 -0.143761
O    -0.124012  2.164758  2.326841
H    -0.902087  1.607711  2.507146
H    -0.222837  2.386886  1.382543
O    -2.362824  0.459790  2.473655
H    -2.784765  0.863622  1.687763
H    -2.198956 -0.446484  2.185093
    el energy= -2091.42582338
          zpe= -2091.156629
    th energy= -2091.130700
  th enthalpy= -2091.129756
  free energy= -2091.212986

TS15
P     2.213070 -0.594388  0.044944
O     2.140741 -0.829122  1.630964
O     1.772464  0.926907 -0.188058
C     0.924968 -0.549536  2.358458
H     0.620901  0.490493  2.204334
H     0.135091 -1.236673  2.036958
H     1.159538 -0.727716  3.406364
C     2.525733  1.996527  0.413449
H     3.579392  1.911481  0.136722
H     2.096232  2.909846  0.006950
H     2.403387  1.972389  1.497300
S     3.948273 -1.155684 -0.622554
S     0.609990 -1.557897 -0.875088
C    -0.739210 -0.297530 -0.669104
C    -2.013419 -1.148347 -0.631654
O    -2.147036 -1.673426  0.641220
C    -3.242544 -2.576980  0.775069
C    -0.727984  0.734496 -1.811744
C    -0.917183  2.140414 -1.255549
O    -0.046607  2.995316 -1.343293
O    -2.432182 -1.732308 -1.622307
O    -2.042778  2.368148 -0.627248
H    -0.600063  0.194231  0.295366
H    -3.267337 -2.873461  1.822519
H    -4.171571 -2.072007  0.499408
H    -3.097163 -3.449576  0.136285
H     0.223656  0.721662 -2.338741
H    -1.529670  0.483531 -2.514064
O    -3.256158  0.276151 -0.365781
H    -2.642227  1.463713 -0.569420
O    -0.206860  2.496011  1.702899
H    -1.056577  2.020893  1.743030
H    -0.206135  2.932528  0.840497
O    -2.420417  0.780269  2.115790
H    -3.231419  1.060695  1.670718
H    -2.295812 -0.126757  1.786860
    el energy= -2091.40737389
          zpe= -2091.138231
    th energy= -2091.113340
  th enthalpy= -2091.112396
  free energy= -2091.192215

30
P     2.256172 -0.521301  0.000140
O     2.221439 -0.839811  1.573376
O     1.785691  1.004938 -0.133880
C     1.007153 -0.653731  2.332186
H     0.658978  0.381025  2.247497
H     0.239652 -1.348848  1.974953
H     1.264097 -0.886959  3.363896
C     2.480057  2.043693  0.579726
H     3.541442  2.030519  0.320562
H     2.019781  2.973969  0.252731
H     2.340945  1.915975  1.654362
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S     3.991355 -1.000077 -0.728789
S     0.650226 -1.472006 -0.932376
C    -0.687354 -0.228725 -0.651892
C    -2.043368 -0.968357 -0.573086
O    -1.950491 -1.794908  0.576638
C    -3.159262 -2.479057  0.882827
C    -0.681556  0.839933 -1.759808
C    -1.124033  2.170960 -1.175028
O    -0.389754  3.146845 -1.134382
O    -2.285727 -1.716699 -1.707434
O    -2.326836  2.186423 -0.648818
H    -0.514449  0.241823  0.319004
H    -2.913742 -3.218821  1.645088
H    -3.913180 -1.788114  1.272043
H    -3.553903 -2.981033 -0.004069
H     0.317965  0.976223 -2.165286
H    -1.360390  0.525502 -2.559488
O    -3.101472 -0.134647 -0.556148
H    -2.736342  1.205456 -0.687404
O    -0.362168  2.334166  1.788864
H    -1.216684  1.865582  1.841033
H    -0.398743  2.850772  0.972522
O    -2.538510  0.574936  2.103420
H    -2.983145  0.458098  1.242883
H    -2.067356 -0.266561  2.183562
   el energy= -2091.43794397
         zpe= -2091.166613
   th energy= -2091.141786
 th enthalpy= -2091.140842
 free energy= -2091.220689

TS16
P     2.208710 -0.561337  0.012651
O     2.129491 -0.932589  1.574154
O     1.773085  0.979926 -0.071231
C     0.899481 -0.736194  2.303098
H     0.571658  0.306158  2.225078
H     0.130784 -1.414110  1.915496
H     1.123877 -0.987725  3.338196
C     2.486154  1.975653  0.683803
H     3.551651  1.934294  0.445249
H     2.063207  2.929066  0.373249
H     2.320760  1.822920  1.751454
S     3.957549 -1.043553 -0.683941
S     0.614771 -1.460757 -0.989326
C    -0.691081 -0.186371 -0.748247
C    -2.077091 -0.857019 -0.838352
O    -1.994211 -1.873736  0.595029
C    -3.262443 -2.377883  0.938480
C    -0.572318  0.953214 -1.787528
C    -0.982705  2.265134 -1.140225
O    -0.229351  3.219877 -1.048163
O    -2.173859 -1.959218 -1.523593
O    -2.192054  2.291124 -0.618768
H    -0.585804  0.231128  0.255910
H    -3.313372 -2.375231  2.034869
H    -4.059060 -1.733608  0.549969
H    -3.399418 -3.404192  0.587414
H     0.453459  1.065028 -2.128961
H    -1.214800  0.741842 -2.649042
O    -3.065456 -0.032567 -0.742482
H    -2.636083  1.350796 -0.711314
O    -0.359866  2.322775  1.847959
H    -1.230795  1.884060  1.832812
H    -0.342055  2.883496  1.060985
O    -2.573008  0.588949  1.985158
H    -2.949415  0.430968  1.099488
H    -2.090539 -0.231394  2.150969
   el energy= -2091.42047458
         zpe= -2091.150523
   th energy= -2091.125911
 th enthalpy= -2091.124967
 free energy= -2091.203602

31
P    -2.321479  0.053502 -0.221617
O    -2.319329  1.481611  0.508793
O    -1.728669 -0.969252  0.868953
C    -1.078358  2.048307  0.988058
H    -0.576955  1.350894  1.667143
H    -0.431543  2.294054  0.144152
H    -1.350197  2.963597  1.510853
C    -2.352765 -1.014308  2.168694
H    -3.427331 -1.180748  2.061690
H    -1.895604 -1.850811  2.692874
H    -2.151308 -0.087950  2.707290
S    -4.096572 -0.322223 -0.919244
S    -0.830875  0.028380 -1.681792
C     0.659546 -0.487880 -0.736639
C     1.917349  0.016871 -1.493692
O     1.689340  3.388220  0.708809
C     1.987082  3.209472 -0.659256
C     0.730164 -2.021788 -0.671708
C     1.894920 -2.440488  0.210067
O     2.785617 -3.120882 -0.474519
O     1.800498  0.316955 -2.685871
O     2.006174 -2.226741  1.399072
H     0.617400 -0.086577  0.279938
H     1.992766  4.189453 -1.144605
H     2.965269  2.736926 -0.810466
H     1.240934  2.584422 -1.175948
H    -0.165206 -2.435752 -0.199640
H     0.829301 -2.437684 -1.678403
O     2.974359 -0.017894 -0.795256
H     2.818400  0.512349  0.676381
O     0.520785 -0.230816  2.820125
H     1.326255  0.229669  2.513843
H     0.635143 -1.101972  2.415924
O     2.667223  0.974515  1.561492
H     3.525405  1.018405  1.998306
H     1.992989  2.573849  1.155561
   el energy= -2091.42935798
         zpe= -2091.160835
   th energy= -2091.133927
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th enthalpy= -2091.132983
free energy= -2091.219379

32

P	2.175701	-0.656208	-0.038172
O	2.022803	-1.288041	1.430182
O	1.811042	0.894246	0.140774
C	0.782875	-1.132589	2.154117
H	0.489315	-0.078096	2.193481
H	0.003271	-1.734623	1.678292
H	0.976009	-1.509469	3.157209
C	2.542734	1.708364	1.074598
H	3.614349	1.638447	0.873069
H	2.188494	2.723705	0.907292
H	2.318233	1.395690	2.095570
S	3.927910	-1.094353	-0.756222
S	0.580780	-1.294830	-1.230467
C	-0.649517	0.031458	-0.910428
C	-2.056353	-0.498663	-1.264189
O	-2.240097	-2.270866	0.994795
C	-3.575123	-2.521614	0.749202
C	-0.344917	1.335446	-1.689078
C	-0.734472	2.531615	-0.838293
O	0.059462	3.395807	-0.507020
O	-2.201275	-1.634287	-1.709097
O	-1.985198	2.551383	-0.423446
H	-0.640919	0.246077	0.163520
H	-4.023306	-2.682352	1.746243
H	-4.070954	-1.647096	0.308251
H	-3.732350	-3.419828	0.145150
H	0.714329	1.424463	-1.913901
H	-0.910174	1.350390	-2.626895
O	-2.991057	0.357695	-1.047991
H	-2.474620	1.684381	-0.734029
O	-0.345678	1.996379	2.150532
H	-1.224789	1.603339	1.990788
H	-0.245416	2.685735	1.480928
O	-2.655457	0.446629	1.791245
H	-3.007935	0.543452	0.890645
H	-2.335806	-0.469826	1.788615

el energy= -2091.45002793
zpe= -2091.180639
th energy= -2091.154601
th enthalpy= -2091.153657
free energy= -2091.236633

33

P	0.763617	-1.271638	-0.516664
O	1.871892	-0.212820	-0.963480
O	-0.086899	-1.389032	-1.870818
C	1.695568	0.734513	-2.041140
H	0.651599	1.031133	-2.147575
H	2.298892	1.601035	-1.772617
H	2.043976	0.274771	-2.966726
C	-1.274996	-2.209464	-1.901334
H	-1.048993	-3.202649	-1.504323
H	-2.074892	-1.724272	-1.332658
H	-1.549133	-2.289927	-2.952101
S	1.563133	-2.927160	0.141101
S	-0.480697	-0.443652	0.920497
C	-1.257032	0.945279	-0.005085
C	-0.368796	2.197860	-0.175966
O	-0.815343	3.039857	-0.965459
C	-2.566572	1.281334	0.705423
C	-3.670056	0.207239	0.516990
O	-4.499353	0.106644	1.446750
O	0.712939	2.291342	0.485210
O	-3.652838	-0.423078	-0.570972
H	-1.529358	0.565908	-0.994148
H	-2.408227	1.469722	1.772105
H	-2.927765	2.214756	0.257850
O	2.674934	0.860524	1.341159
H	1.801585	1.292912	1.047834
O	3.145868	3.254659	-0.348107
H	3.472840	2.481500	0.132774
H	2.190388	3.193693	-0.154736
O	2.009192	-1.311720	3.156055
H	2.227985	-0.555551	2.586246
H	1.846018	-2.017048	2.516442

el energy= -2051.66267239
zpe= -2051.435568
th energy= -2051.410644
th enthalpy= -2051.409700
free energy= -2051.491633

TS17

P	-1.456738	-0.978053	0.060963
O	-1.921705	-0.120978	1.339093
O	-0.406051	-1.887224	0.931635
C	-1.150975	1.006204	1.798342
H	-0.140195	0.698293	2.074366
H	-1.118659	1.785921	1.031356
H	-1.675431	1.383617	2.675010
C	0.425772	-2.869832	0.307282
H	0.283158	-2.896269	-0.778669
H	1.467647	-2.623833	0.538775
H	0.162055	-3.848980	0.711907
S	-2.779039	-2.163534	-0.773592
S	0.010268	-0.074503	-1.249668
C	1.475019	0.209671	-0.181958
C	1.669792	1.726028	0.113030
O	2.010446	2.001271	1.273769
C	2.683304	-0.360507	-0.927810
C	3.818759	-0.662834	0.106808
O	4.942779	-0.195639	-0.160311
O	1.499071	2.495929	-0.869152
O	3.474803	-1.369764	1.083736
H	1.324859	-0.356411	0.737007
H	2.434122	-1.316060	-1.404924
H	3.020502	0.339340	-1.695219
O	-2.125424	0.735115	-0.967622
H	-2.455494	0.472059	-1.843011
O	-1.113604	3.408496	-0.724806
H	-1.531045	2.562725	-0.950619

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H    -0.160482  3.205030 -0.795593
O    -4.059366  1.722444  0.875664
H    -3.446031  1.506451  0.154113
H    -3.951205  0.957938  1.452992
    el energy= -2051.63612520
          zpe= -2051.408474
    th energy= -2051.384203
  th enthalpy= -2051.383259
  free energy= -2051.463924

37
P    -1.104796 -1.102427 -0.047638
O    -1.902410 -0.685310  1.328457
O     0.102088 -1.799176  0.921303
C    -1.803679  0.658197  1.798474
H    -0.792551  0.858382  2.165629
H    -2.042156  1.379859  1.012461
H    -2.519062  0.755437  2.616435
C     1.142299 -2.554540  0.328838
H     1.265297 -2.329016 -0.738409
H     2.078130 -2.298789  0.835820
H     0.932082 -3.626113  0.421833
S    -1.750181 -2.770196 -1.008479
S     0.279755  0.403028 -0.817119
C     1.778725  0.305543  0.042710
C     0.354568  3.429047  0.241748
O     0.019558  3.194477  1.329246
C     3.088991  0.259578 -0.656631
C     4.223666 -0.452517  0.144981
O     5.286878 -0.620853 -0.494561
O     0.724780  3.702187 -0.828557
O     3.982444 -0.769948  1.333708
H     1.758163  0.203816  1.120225
H     2.993854 -0.231785 -1.633096
H     3.463047  1.272242 -0.881073
O    -2.263852 -0.037610 -0.970527
H    -2.538144 -0.552645 -1.741544
O    -2.066858  2.753533 -1.134865
H    -2.158674  1.780434 -1.111315
H    -1.305616  2.888660 -1.710594
O    -4.595441 -0.100096  0.625698
H    -3.853797  0.014447  0.003365
H    -4.186739 -0.673322  1.284460
    el energy= -2051.66959669
          zpe= -2051.445019
    th energy= -2051.419448
  th enthalpy= -2051.418504
  free energy= -2051.503079

38
P    -1.728764 -0.195621  0.886927
O    -2.870754 -1.295615  0.612072
O    -2.401145  1.069724  0.191340
C    -4.252670 -0.944348  0.854559
H    -4.582609 -0.239777  0.091480
H    -4.810309 -1.876104  0.786694
H    -4.364377 -0.517051  1.853368
C    -2.092956  2.445836  0.475579
H    -3.042476  2.948958  0.655720
H    -1.454469  2.525395  1.357336
H    -1.594163  2.846351 -0.405430
S    -1.141901  0.064752  2.715191
S    -0.347933 -1.083447 -0.426330
C     1.237212 -0.362044  0.139683
C     1.421080  0.984432 -0.536382
O     0.955433  1.977259  0.209302
C     1.073389  3.286052 -0.372483
C     2.359082 -1.311708 -0.255966
C     3.684321 -0.742639  0.198053
O     4.691484 -1.566784 -0.077920
C     5.991849 -1.102951  0.311227
O     1.905983  1.119083 -1.638143
O     3.814555  0.330651  0.743676
H     1.194073 -0.231409  1.223382
H     0.657302  3.972158  0.362118
H     2.124516  3.512000 -0.557012
H     0.509183  3.318981 -1.305387
H     2.217496 -2.296013  0.196539
H     2.396305 -1.442564 -1.341579
H     6.685647 -1.885826  0.014966
H     6.225088 -0.167933 -0.200106
H     6.026761 -0.945794  1.390174
O    -3.131297 -0.240872 -2.141237
H    -2.956303 -1.217956 -2.050887
O    -0.937297  1.691295 -2.343469
H    -1.604889  0.990888 -2.247410
H    -0.121177  1.233521 -2.577980
O    -2.738929 -2.908771 -1.712143
H    -1.929800 -3.306944 -2.055354
H    -2.639110 -2.910986 -0.749736
    el energy= -2131.16691779
          zpe= -2130.857619
    th energy= -2130.828234
  th enthalpy= -2130.827290
  free energy= -2130.918973

TS21
P    -1.876301 -0.234890  0.664939
O    -3.309089 -0.930140  0.446675
O    -1.913925  1.305934  0.187788
C    -4.242552 -0.458326 -0.551763
H    -4.003134  0.561814 -0.851159
H    -4.217220 -1.124516 -1.413995
H    -5.222316 -0.492321 -0.077693
C    -1.975714  2.398558  1.120681
H    -1.103137  2.392046  1.773464
H    -1.984344  3.292067  0.496887
H    -2.888227  2.341829  1.714951
S    -1.527114 -0.298549  2.616596
S    -0.263685 -1.541305 -0.091466
C     1.218670 -0.538651  0.280895
C     1.175461  0.804605 -0.439423
O     0.952566  1.798134  0.404440
C     0.955807  3.114929 -0.175449
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C     2.430266 -1.345533 -0.181465
C     3.703612 -0.592412  0.133025
O     4.777435 -1.353546 -0.050376
C     6.037740 -0.710057  0.188799
O     1.340220  0.922242 -1.632563
O     3.739117  0.563941  0.490236
H     1.223662 -0.372936  1.361427
H     0.796760  3.799469  0.654702
H     1.922653  3.300253 -0.646773
H     0.154493  3.189077 -0.912850
H     2.461273 -2.326036  0.298975
H     2.388128 -1.502373 -1.264074
H     6.795827 -1.462758 -0.012487
H     6.155088  0.143952 -0.479649
H     6.095005 -0.372848  1.224603
O    -1.624858 -0.361083 -1.400704
H    -2.012086 -1.204403 -1.730692
O    -1.122753  2.233087 -2.576772
H    -1.516942  1.539595 -2.025053
H    -0.212606  1.919240 -2.663136
O    -2.679380 -2.919197 -1.568483
H    -2.132773 -3.678320 -1.804046
H    -2.997193 -3.095480 -0.673294
    el energy= -2131.13854688
          zpe= -2130.827597
    th energy= -2130.799450
  th enthalpy= -2130.798506
  free energy= -2130.887175

39
P    -2.639626  0.029387 -0.434246
O    -4.122873 -0.081598 -1.015418
O    -2.199131 -1.467126 -0.107968
C    -5.117359 -0.775024 -0.230539
H    -4.862413 -1.833941 -0.153458
H    -5.184156 -0.330584  0.763891
H    -6.058641 -0.653363 -0.761438
C    -2.070876 -2.378068 -1.216543
H    -1.108933 -2.215135 -1.706746
H    -2.122475 -3.380502 -0.795771
H    -2.888840 -2.237066 -1.927957
S    -1.534356  1.026038 -1.712492
S     0.429411  1.809334  0.422791
C     1.676164  0.620593 -0.170864
C     1.520298 -0.651295  0.632411
O     0.810798 -1.576257 -0.000210
C     0.573708 -2.780548  0.748903
C     3.074910  1.198357  0.018427
C     4.121113  0.207546 -0.437849
O     5.345203  0.731451 -0.396864
C     6.405802 -0.147629 -0.794500
O     1.953367 -0.781499  1.761184
O     3.883292 -0.926757 -0.790114
H     1.475970  0.417896 -1.225255
H     0.127773 -3.481975  0.047972
H     1.518224 -3.172063  1.128443
H    -0.104459 -2.558789  1.574556
H     3.190450  2.130273 -0.539384
H     3.256748  1.419603  1.075002
H     7.321830  0.429616 -0.694699
H     6.430796 -1.024325 -0.145573
H     6.262812 -0.465654 -1.828284
O    -2.720114  0.612778  1.024423
H    -2.624140  1.638542  1.038228
O    -0.800064 -0.679179  2.908252
H    -1.237088 -0.181082  2.203263
H     0.144160 -0.532677  2.765234
O    -2.405622  3.110357  0.873670
H    -2.137881  3.265115 -0.045079
H    -3.187640  3.658417  1.023667
    el energy= -2131.23865486
          zpe= -2130.928049
    th energy= -2130.898821
  th enthalpy= -2130.897877
  free energy= -2130.991103

41
H     1.420688  2.816409 -0.368964
S     2.133961  1.766444 -0.816558
C     0.787981  0.579867 -0.423199
C     1.398330 -0.807348 -0.340618
O     1.915435 -1.035140  0.869583
C     2.482766 -2.338248  1.054614
C    -0.340375  0.632171 -1.459057
C    -1.612151  0.093306 -0.849856
O    -1.960005 -1.095689 -1.306867
C    -3.098289 -1.695527 -0.672734
O     1.432514 -1.598704 -1.252107
O    -2.250643  0.700329 -0.003891
H     0.417207  0.852773  0.564423
H     2.844910 -2.360216  2.079663
H     1.715071 -3.098363  0.901077
H     3.302913 -2.496191  0.352831
H    -0.526855  1.673306 -1.728652
H    -0.058027  0.066811 -2.347358
H    -3.241781 -2.652390 -1.168165
H    -2.887805 -1.837856  0.389403
H    -3.975912 -1.059666 -0.793722
O    -0.596902 -1.592919  1.315324
H    -0.627882 -0.796499  1.901334
O    -0.620660  3.088348  0.669756
H    -0.505428  2.662302  1.532244
H    -1.346010  2.570746  0.288933
O    -1.065437  0.881180  2.487862
H    -1.878243  0.893047  1.958171
H    -1.340212  0.938129  3.411515
    el energy= -1162.04627974
          zpe= -1161.818986
    th energy= -1161.798539
  th enthalpy= -1161.797594
  free energy= -1161.867733

TS22
H     1.673019  2.803829 -0.690560
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S     2.072990  1.609382 -1.152772
C     0.653093  0.686653 -0.451910
C     1.121927 -0.752547 -0.263399
O     1.945741 -0.775317  0.965099
C     2.794569 -1.909999  1.104454
C    -0.554893  0.736475 -1.395808
C    -1.759008  0.106198 -0.739575
O    -2.093307 -1.060060 -1.265680
C    -3.153630 -1.762780 -0.600713
O     1.424451 -1.463445 -1.211252
O    -2.351928  0.606116  0.203868
H     0.404754  1.144207  0.504388
H     2.722695 -2.256850  2.134095
H     2.511589 -2.681593  0.390218
H     3.813278 -1.568613  0.896506
H    -0.797234  1.782054 -1.599628
H    -0.314201  0.223834 -2.327627
H    -3.300018 -2.678884 -1.167002
H    -2.854932 -1.986778  0.425330
H    -4.061680 -1.159260 -0.596227
O     0.053385 -1.454548  0.757026
H    -0.232780 -0.806243  1.460882
O    -0.892479  2.955329  1.148974
H    -0.664147  2.433189  1.930730
H    -1.570906  2.401242  0.734003
O    -0.884620  0.376564  2.503992
H    -1.799410  0.386902  2.182698
H    -0.920157  0.111746  3.432046
    el energy= -1162.01019358
          zpe= -1161.783633
    th energy= -1161.764014
  th enthalpy= -1161.763070
  free energy= -1161.832325

42
H    -1.254470 -2.246582  2.258517
S    -1.819807 -1.950284  1.078522
C    -0.508580 -0.785584  0.545930
C    -0.954317 -0.103699 -0.781537
O    -2.125798  0.611999 -0.504166
C    -2.724106  1.185290 -1.668837
C     0.845027 -1.480476  0.381656
C     1.958505 -0.488609  0.129146
O     2.696894 -0.813545 -0.924593
C     3.752442  0.102170 -1.243592
O    -1.156487 -1.123101 -1.671006
O     2.182438  0.483423  0.824311
H    -0.430320  0.019516  1.284727
H    -3.648867  1.655622 -1.338880
H    -2.064843  1.933396 -2.117246
H    -2.950251  0.406011 -2.402329
H     1.089867 -1.994868  1.316099
H     0.809965 -2.220292 -0.418513
H     4.253095 -0.314951 -2.113904
H     3.331593  1.082672 -1.473642
H     4.444312  0.190302 -0.405006
O     0.040461  0.719719 -1.290601
H     0.068835  1.515268 -0.715880
O     0.430513  1.395015  2.901533
H     0.067609  2.043504  2.278221
H     1.170461  1.027792  2.393918
O    -0.557705  2.673039  0.558383
H    -0.598641  3.618018  0.366527
H    -1.467783  2.342192  0.503535
    el energy= -1162.05064254
          zpe= -1161.821164
    th energy= -1161.801826
  th enthalpy= -1161.800882
  free energy= -1161.869148

TS23
H     1.479430  3.026597 -0.021540
S     1.975257  1.970531 -0.684597
C     0.605987  0.846513 -0.233362
C     1.002610 -0.582470 -0.607043
O     2.412432 -0.823767  0.409927
C     2.805889 -2.166911  0.505026
C    -0.675693  1.226093 -1.000351
C    -1.868663  0.436225 -0.517535
O    -2.444221 -0.274598 -1.473410
C    -3.548613 -1.093188 -1.061282
O     1.664613 -0.801468 -1.656783
O    -2.266251  0.449903  0.635545
H     0.428922  0.914985  0.842631
H     3.657210 -2.383484 -0.144828
H     3.125442 -2.289271  1.548948
H     1.971839 -2.845230  0.307657
H    -0.895109  2.281336 -0.815218
H    -0.532494  1.083108 -2.072828
H    -3.900500 -1.588364 -1.962611
H    -3.208499 -1.825394 -0.326568
H    -4.334285 -0.474784 -0.626114
O     0.111453 -1.517651 -0.220102
H    -0.194267 -1.346922  0.708638
O    -0.643848  1.792389  2.647592
H    -0.498102  0.883785  2.947639
H    -1.342291  1.662345  1.988741
O    -0.712544 -1.057653  2.286445
H    -1.666473 -0.946731  2.157909
H    -0.597113 -1.815277  2.874662
    el energy= -1162.03069904
          zpe= -1161.804626
    th energy= -1161.784702
  th enthalpy= -1161.783758
  free energy= -1161.854368

43
H     1.841162  0.011516 -2.374546
S     1.661442 -0.965465 -1.467204
C     0.195571 -0.280023 -0.649084
C     0.186060 -0.884633  0.788668
O     2.954577  0.414344 -0.051007
C     3.590896 -0.419391  0.919513
C    -1.105120 -0.663606 -1.372672
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C    -2.235730 -0.055413 -0.566243
O    -2.946161 -0.976794  0.070392
C    -3.944230 -0.471406  0.968872
O     0.632939 -2.032688  0.900576
O    -2.446628  1.136571 -0.479465
H     0.291363  0.807136 -0.662594
H     4.335987 -1.021712  0.400497
H     4.087240  0.216353  1.658101
H     2.867252 -1.072306  1.416166
H    -1.127936 -0.236087 -2.377787
H    -1.217943 -1.747383 -1.425148
H    -4.420432 -1.346885  1.403119
H    -3.463761  0.132237  1.740408
H    -4.670113  0.134067  0.425123
O    -0.318936 -0.131927  1.665693
H     0.555108  1.223111  1.559878
O    -0.225794  2.976434 -0.929742
H     0.240203  2.874543 -0.085017
H    -1.069665  2.520211 -0.791812
O     1.241870  1.895741  1.268598
H     1.593598  2.320590  2.060387
H     2.315238  1.025448  0.433810
    el energy= -1162.04761940
          zpe= -1161.819098
    th energy= -1161.799447
  th enthalpy= -1161.798503
  free energy= -1161.868445

44
H     3.221865 -2.681380 -0.091888
S     3.294744 -1.413239  0.345156
C     1.733801 -0.846314 -0.415269
C     1.651803  0.699402 -0.326868
O     2.211665  1.249180  0.645161
C     0.508332 -1.457515  0.299319
C    -0.736790 -0.797215 -0.233780
O    -1.106957  0.232242  0.529501
C    -1.949333  1.247139 -0.047468
O     0.953383  1.227869 -1.229738
O    -1.312554 -1.137458 -1.250552
H     1.717823 -1.133838 -1.467478
H     0.453609 -2.531298  0.110998
H     0.587646 -1.270908  1.371722
H    -1.490169  2.195731  0.230455
H    -1.966741  1.142941 -1.132640
H    -2.951750  1.149194  0.372272
O    -4.026415 -0.708789 -1.066762
H    -3.088098 -0.907734 -1.312966
O    -3.686307 -0.724062  1.831931
H    -2.726118 -0.638593  1.862519
H    -3.879836 -0.876387  0.893812
O     0.527084  3.508864  0.251664
H     1.145861  3.008705  0.807771
H     0.533951  2.899641 -0.512321
    el energy= -1122.28882539
          zpe= -1122.103982
    th energy= -1122.085018
  th enthalpy= -1122.084074
  free energy= -1122.153060

TS24
H    -3.179602 -2.419472 -0.112819
S    -3.098386 -1.171134 -0.602697
C    -1.632648 -0.663263  0.365310
C    -1.467147  0.873322  0.256918
O    -1.795122  1.400825 -0.830428
C    -0.363080 -1.363420 -0.152437
C     0.848742 -0.766310  0.530190
O     1.311812  0.293321 -0.141625
C     2.222638  1.140183  0.563006
O    -0.951699  1.416881  1.264387
O     1.057712 -0.909868  1.769741
H    -1.785860 -0.922241  1.413930
H    -0.398039 -2.430973  0.068352
H    -0.267467 -1.216217 -1.230245
H     2.376622  2.000127 -0.083667
H     1.770883  1.455511  1.504138
H     3.162104  0.612182  0.744892
O     2.082962 -2.099864  0.257483
H     2.731061 -2.006297  0.980913
O     3.423984 -0.533284 -1.865843
H     2.701752  0.082815 -2.033013
H     3.029420 -1.128475 -1.211153
O     0.157123  3.379564 -0.368250
H    -0.491289  2.910235 -0.919204
H    -0.020616  2.897255  0.459391
    el energy= -1122.26475912
          zpe= -1122.080507
    th energy= -1122.062109
  th enthalpy= -1122.061165
  free energy= -1122.127729

45
H    -2.777059 -2.614219  0.341103
S    -2.832268 -1.428242 -0.288383
C    -1.394782 -0.682792  0.564293
C    -1.332070  0.822176  0.216541
O    -1.839672  1.197033 -0.861729
C    -0.090309 -1.394991  0.188401
C     1.140454 -0.609665  0.632578
O     1.412041  0.338292 -0.363580
C     2.213600  1.449369  0.021712
O    -0.732839  1.526176  1.073923
O     1.025344 -0.050520  1.887144
H    -1.545741 -0.760531  1.641837
H    -0.053379 -2.375497  0.671336
H    -0.018165 -1.541239 -0.891970
H     2.304962  2.072466 -0.865961
H     1.721324  2.011117  0.815492
H     3.211203  1.132709  0.349086
O     2.207370 -1.520702  0.777535
H     2.992426 -1.028875  1.063336
O     2.226261 -1.778566 -2.147954
H     2.006757 -0.869975 -1.895992
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H     2.438238 -2.161862 -1.286551
O    -0.196712  3.482247 -0.846605
H    -0.836359  2.871064 -1.248293
H    -0.163623  3.060459  0.029673
    el energy= -1122.29110645
          zpe= -1122.103559
    th energy= -1122.085737
  th enthalpy= -1122.084793
  free energy= -1122.149269

TS25
H    -1.958530 -2.570078  1.153604
S    -2.569476 -1.830682  0.215221
C    -1.352741 -0.457299  0.256691
C    -1.994630  0.697744 -0.517291
O    -1.817249  1.913663 -0.046428
C    -0.014738 -0.859206 -0.380804
C     0.998752  0.264323 -0.170801
O     2.301040 -0.346470 -1.216902
C     3.505718  0.313000 -0.930136
O    -2.635822  0.493307 -1.528946
O     0.930034  1.276357 -0.999331
H    -1.190550 -0.167261  1.297665
H     0.360926 -1.759937  0.110963
H    -0.158725 -1.054096 -1.446125
H     4.297383 -0.448121 -0.946581
H     3.743292  1.077537 -1.676684
H     3.475488  0.755985  0.072105
O     1.424429  0.414256  1.035256
H     0.527178  1.514906  1.670065
O     2.700432 -2.054952  1.122272
H     2.282589 -1.195586  1.326897
H     2.708115 -2.024281  0.157214
O    -0.242557  2.107945  1.953030
H    -1.208786  1.966728  0.771565
H     0.096599  3.010909  1.968203
    el energy= -1122.28567305
          zpe= -1122.100452
    th energy= -1122.083693
  th enthalpy= -1122.082748
  free energy= -1122.145340

46
H     1.239571 -1.864660  0.736522
S     0.052209 -2.332692  0.290894
C    -0.689030 -0.650005  0.166123
C    -2.028775 -0.794656 -0.518069
O    -3.107101 -0.972967  0.013299
C     0.232339  0.323061 -0.558329
C    -0.303918  1.759265 -0.464282
O     3.053699 -0.751895  0.921549
C     3.623828 -1.211491 -0.288918
O    -1.983444 -0.802055 -1.839373
O    -1.552455  1.886133 -0.394026
H    -0.927537 -0.290524  1.169861
H     1.228545  0.266703 -0.124292
H     0.328709  0.044980 -1.615607
H     3.682057 -2.301722 -0.244063
H     3.012534 -0.938771 -1.160740
H     4.636729 -0.818583 -0.439857
O     0.541933  2.688428 -0.481393
H     2.068285  2.219284 -0.055465
O     2.973291  1.899499  0.222572
H     3.502996  1.926662 -0.582265
H     3.014006  0.226096  0.842517
O    -2.694765  1.109743  2.041623
H    -3.137643  0.323914  1.696189
H    -2.339527  1.517564  1.229744
    el energy= -1122.29971982
          zpe= -1122.114754
    th energy= -1122.095637
  th enthalpy= -1122.094693
  free energy= -1122.165512

47
H     0.004306 -2.584501  0.830272
S    -1.181141 -2.464680  0.199749
C    -1.034897 -0.642203  0.128477
C    -2.369249 -0.078968 -0.344845
O    -2.582799  1.213076 -0.143847
C     0.100954 -0.163074 -0.801995
C     0.663021  1.179742 -0.312432
O     3.375193 -1.105600 -0.778533
C     3.733003  0.211772 -0.612369
O    -3.190754 -0.753696 -0.927769
O     0.637691  2.161470 -1.072568
H    -0.823667 -0.284496  1.139520
H     0.908514 -0.899145 -0.756387
H    -0.242612 -0.089270 -1.836506
H     3.597269  0.572237  0.412940
H     4.743430  0.400869 -0.997206
H     3.045436  0.792717 -1.258780
O     1.080793  1.182564  0.894546
H    -0.221899  2.333473  1.461961
O     1.707289 -1.394776  1.625419
H     1.465496 -0.453308  1.477864
H     2.330990 -1.568446  0.905498
O    -1.013549  2.843992  1.187089
H    -1.912644  1.709529  0.412926
H    -0.664266  3.285371  0.396193
    el energy= -1122.31335383
          zpe= -1122.129016
    th energy= -1122.110505
  th enthalpy= -1122.109561
  free energy= -1122.178895
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