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

Towards a Comprehensive Understanding of Malathion Degradation: Theoretical Investigation of Degradation Pathways and Related Kinetics under Alkaline Conditions

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

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

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

Supporting Information

Table of Contents

Malathion and Trimmed Structure

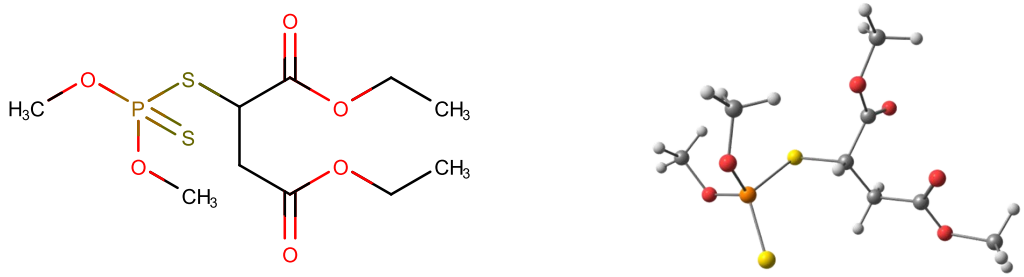

Figure S1. Schematic of malathion (left) and the trimmed structure used for computational studies (right).

Thiol-Thiolate Deprotonation

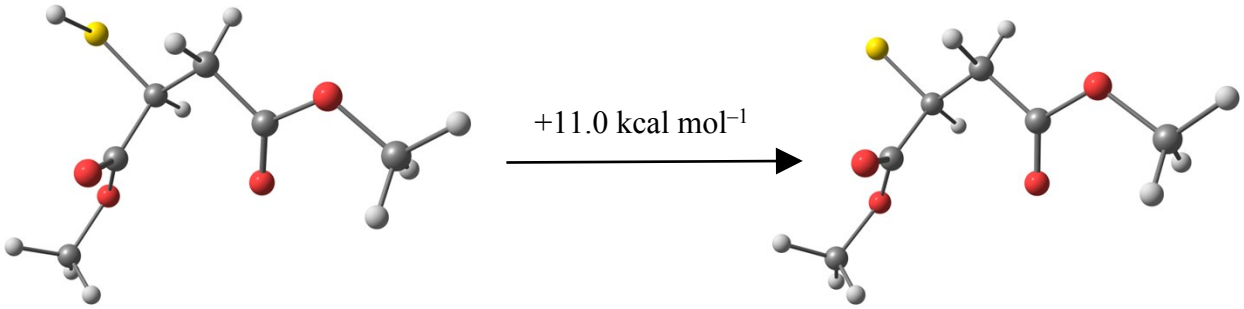

Figure S2. Deprotonation of the bis-ester thiol at the M06-2X/aug-cc-pVTZ//6-31G(d,p) level of theory.

Tabulated Relative Energies with Various Methodologies

Table S1. Relative free energies (kcal mol^{-1}) of intramolecular (I.M.) and base-assisted (B.A.) elimination from various levels of theory. 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. Where relevant, TS energies with tunneling corrections are noted in parentheses.

	M06-2X/6-31G(d,p) (w/ tunneling)	**M06-2X/aug-cc-pVTZ// M06-2X/6-31G(d,p) (w/ tunneling)**	**MP2/aug-cc-pVTZ// M06-2X/6-31G(d,p) (w/ tunneling)**
I.M.			
1	0.0	0.0	0.0
TS1	35.1 (34.7)	34.5 (34.1)	50.2 (49.8)
2	12.3	10.3	9.0
3	4.6	1.9	6.4
B.A.			
1	0.0	0.0	0.0
4	–16.0	11.4	38.9
TS2	–15.8 (–15.8)	14.9 (14.9)	46.7 (46.7)
5	–64.9	–26.5	–11.0

For the intramolecular elimination, all methodologies provide qualitatively similar results (Table S1): a highly endergonic transition state (**TS1**). For the base-assisted mechanism, the data are more interesting. Optimizations with M06-2X/6-31G(d,p) indicate that association of the hydroxide ion and explicit water molecules from solution, **4**, is exergonic. The transition state to extract the proton (**TS2**) is easily accessible (<1 kcal mol^{-1} with M06-2X/6-31G(d,p)) and the formation of **5** is highly exergonic. The story is slightly different from single-point computations M06-2X/aug-cc-pVTZ//6-31G(d,p) and MP2/aug-cc-pVTZ//M06-2X/6-31G(d,p). With these single-point computations, association of the hydroxide ion and explicit water molecules from solution is rather endergonic (11.4 kcal mol^{-1} with M06-2X/aug-cc-pVTZ//6-31G(d,p) and 38.9 kcal mol^{-1} with MP2/aug-cc-pVTZ//M06-2X/6-31G(d,p)). Otherwise, the elimination pathway to M06-2X/6-31G(d,p): proceeds through a relatively low transition state (less than 10 kcal mol^{-1} for **TS2** with

either methodology) leading to a highly exergonic product, **5**. This discrepancy is likely related to incorrectly predicting the stabilization of the hydroxide ion by the solvent when using an implicit solvation model. Because M06-2X/aug-cc-pVTZ//6-31G(d,p) qualitatively agrees with MP2/aug-cc-pVTZ//M06-2X/6-31G(d,p) (Table S1), we will believe that assignment that bringing the hydroxide ion proximal to malathion in the configuration shown in Figure 1 in the main text is truly endergonic.

Table S2. Relative free energies (kcal mol^{-1}) for the hydrolysis of fumarate to malate. 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. Where relevant, TS energies with tunneling corrections are noted in parentheses.

	M06-2X/6-31G(d,p) (w/ tunneling)	**M06-2X/aug-cc-pVTZ// M06-2X/6-31G(d,p) (w/ tunneling)**	**MP2/aug-cc-pVTZ// M06-2X/6-31G(d,p) (w/ tunneling)**
6	0.0	0.0	0.0
TS3	3.5	7.0	9.1
7	–5.6	–0.2	1.3
TS4	4.7	8.7	10.8
8	4.2 (3.8)	8.0 (7.6)	8.8 (8.4)
9	–25.6	–21.4	–30.9
10	–47.9	–29.6	–32.1
TS5	–41.2	–18.6	–18.0
11	–48.2	–24.8	–24.7
TS6	–39.4	–16.6	–16.6
12	–41.8	–20.0	–22.6
13	–73.5	–50.8	–60.8
14	–80.7	–52.1	–60.6
TS7	–58.6	–24.3	–21.6
15	–70.6	–31.9	–29.3
TS8	–69.4	–32.9	–30.2
16	–74.1	–45.2	–53.7
17	–95.3	–56.6	–59.1

Table S2 shows the methodological comparison for dimethyl fumarate hydrolysis. In this case, all three methodologies provide qualitatively similar in terms of the relative placement of transition state energies and minima. The largest differences in these pathways can be highlighted by

examining the energy differences between **8** and **9** across each level of theory (Table S2 here and Figure 2 in the main text). Between these two structures, a MeOH is exchanged for a hydroxide ion from solution with energy differences ranging from ~35 to ~50 kcal mol^{-1}. As discussed previously, these gaps in energy are likely related to correctly predicting the energy of the hydroxide ion in an implicit solvent as opposed to having explicit hydrogen bonding present. It is therefore not surprising that there are significant differences between methodologies.

Table S3. Relative free energies (kcal mol^{-1}) for the hydrolysis of the ester groups from malathion. 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)**
α First			
1	0.0	0.0	0.0
18	–28.6	5.8	38.2
TS9	–25.6	11.1	43.3
19	–37.4	3.0	35.0
TS10	–34.0	8.4	47.8
20	–57.1	–17.8	7.9
21	–85.3	–26.5	5.8
TS11	–78.1	–17.9	16.9
22	–83.8	–23.4	7.8
TS12	–79.8	–19.1	15.9
23	–106.1	–46.6	–21.0
ß First			
1	0.0	0.0	0.0
24	–33.0	3.5	37.7
TS13	–26.4	12.2	48.4
25	–33.4	6.2	38.2
TS14	–27.0	12.0	48.2
26	–52.8	–16.0	5.8
27	–77.1	–22.8	7.5
TS15	–74.1	–13.9	19.5
28	–87.9	–26.1	6.5
TS16	–83.0	–20.4	16.2
29	–105.4	–46.3	–22.9

Table S4. Relative free energies (kcal mol^{-1}) for the hydrolysis of the P-S bond in the malathion diacid. 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)**
30	–124.6	–54.2	–28.5
TS17	–121.7	–48.0	–20.2
31	–131.5	–51.2	–22.7
32	–133.2	–53.3	–30.8
TS18	–129.5	–52.6	–35.8
33	–143.2	–70.2	–69.1

These data have similar trends to the previously discussed pathways wherein M06-2X/6-31G(d,p) predicts the association of hydroxide ion from solution to be exergonic where M06-2X/aug-cc-pVTZ//6-31G(d,p) and MP2/aug-cc-pVTZ//M06-2X/6-31G(d,p) predict the association to be endergonic. Otherwise, the data in both Table S3 and Table S4 are qualitatively consistent across methodologies.

Table S5. Relative free energies (kcal mol^{-1}) for the conversion of malathion to malaoxon vs hydrolysis of P-S bond. 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. Where relevant, TS energies with tunneling corrections are noted in parentheses.

	M06-2X/6-31G(d,p) (w/ tunneling)	**M06-2X/aug-cc-pVTZ// M06-2X/6-31G(d,p) (w/ tunneling)**	**MP2/aug-cc-pVTZ// M06-2X/6-31G(d,p) (w/ tunneling)**
Hydrolyze P-S-C			
1	0.0	0.0	0.0
34	–28.9	3.9	32.0
TS19	–19.5	15.3	45.9
35	–47.4	–4.1	24.7
TS20	–48.1	–4.9	22.9
36	–75.6	–33.9	–16.7
Convert to Malaoxon			
34	–28.9	3.9	32.0
TS19	–19.5	15.3	45.9
35	–47.4	–4.1	24.7
37	–31.8	7.1	35.1
TS21	–18.6 (–20.2)	20.2 (18.6)	57.3 (55.7)
38	–56.8	–19.5	–12.2

These data have trends similar to the previously discussed pathways wherein M06-2X/6-31G(d,p) predicts the association of hydroxide ion from solution to be exergonic where M06-2X/aug-cc-pVTZ//6-31G(d,p) and MP2/aug-cc-pVTZ//M06-2X/6-31G(d,p) predict the association to be endergonic. Otherwise, the data in Table S5 are qualitatively consistent across methodologies.

Table S6. Relative free energies (kcal mol^{-1}) for the hydrolysis of the bisester thiol. 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)
39	0.0	0.0	0.0
TS22	1.7	4.4	5.3
40	–7.8	–2.7	–3.4
TS23	–5.2	1.3	7.7
41	–30.0	–26.3	–33.5
42	–72.4	–35.8	–40.0
TS24	–66.4	–25.4	–25.8
43	–73.1	–30.5	–33.1
TS25	–70.0	–26.1	–24.1
44	–95.4	–53.6	–61.8

These data have similar trends to the previously discussed pathways wherein exchanging the MeOH for a hydroxide ion from solution is predicted to be highly exergonic. Overall, the data in Table S5 are qualitatively consistent across methodologies.

Application of Tunneling Corrections

Some of the transition state computed herein involved proton abstraction as the primary imaginary vibrational mode. Accordingly, tunneling corrections were applied according to the equations below.

The rate constant of the forward reaction, $k_{\mathrm{BS1,TS}}$, is converted to a $\Delta\Delta G^{\ddagger}$ relative to the reactant side of that transition state.

$$\Delta\Delta G^{\ddagger}_{BS1,TS} = -ln\left(\frac{k_{BS1,TS}h}{k_B T}\right)RT$$

The relative free energy of the transition state for BS1, $^{\Delta G^{\ddagger}_{BS1,tunnel}}$, with respect to the zero each reaction sequence is then determined by applying the $^{\Delta\Delta G^{\ddagger}_{BS1,TS}}$ to the relative free energy of the reactant.

$$\Delta G^{\ddagger}_{BS1,tunnel} = \Delta G_{BS1,\,reactant} + \Delta\Delta G^{\ddagger}_{BS1,TS}$$

Tunneling corrections for transition states at higher levels of theory were applied by applying the difference between the canonical transition state energy, $^{\Delta G^{\ddagger}_{BS1}}$, and transition state energy with tunneling, $^{\Delta G^{\ddagger}_{BS1,tunnel}}$, at the M06-2X/6-31G(d,p) level of theory to the canonical transition state

state energy at the M06-2X/aug-cc-pVTZ//M06-2X/6-31G(d,p) or MP2/aug-cc-pVTZ//M06-2x/6-31G(d,p) level of theory.

$$\Delta G_{BS2,tunnel}^{\ddagger} = \Delta G_{BS1,tunnel}^{\ddagger} - \Delta G_{BS1}^{\ddagger} + \Delta G_{BS2}^{\ddagger}$$

Table S7. Computed forward rate constants relative to the reactant side for transition states in which proton abstraction is the primary vibrational mode.

	Forward rate constant M06-2X/6-31G(d,p)
TS1	2.15×10^{-13}
TS2	4.79×10^{12}
TS8	1.64×10^{12}
TS21	2.04×10^{04}

System of Equations for Kinetics

$$
\begin{aligned}
&= +k_{-1} \cdot \mathrm{INT2}(t) \cdot \mathrm{DF}(t) + k_{-2} \cdot \mathrm{INT5}(t) \cdot \mathrm{DF}(t) && (1)\\
&\quad + k_{-9} \cdot \mathrm{INT19}(t) + k_{-13} \cdot \mathrm{INT25}(t) + k_{-19} \cdot \mathrm{INT35}(t)\\
&\quad - k_{1} \cdot \mathrm{MAL}(t) - k_{2} \cdot \mathrm{MAL}(t) \cdot \mathrm{OH}(t)\\
&\quad - k_{9} \cdot \mathrm{MAL}(t) \cdot \mathrm{OH}(t) - k_{13} \cdot \mathrm{MAL}(t) \cdot \mathrm{OH}(t)\\
&\quad - k_{19} \cdot \mathrm{MAL}(t) \cdot \mathrm{OH}(t)\\
&= +k_{-2} \cdot \mathrm{INT5}(t) \cdot \mathrm{DF}(t) + k_{-3} \cdot \mathrm{INT7}(t) + k_{-5} \cdot \mathrm{INT11}(t) && (2)\\
&\quad + k_{-7} \cdot \mathrm{INT15}(t) + k_{-9} \cdot \mathrm{INT19}(t) + k_{-11} \cdot \mathrm{INT22}(t)\\
&\quad + k_{-13} \cdot \mathrm{INT25}(t) + k_{-15} \cdot \mathrm{INT28}(t) + k_{-17} \cdot \mathrm{INT32}(t)\\
&\quad + k_{-19} \cdot \mathrm{INT35}(t) + k_{-23} \cdot \mathrm{INT40}(t) + k_{-25} \cdot \mathrm{INT43}(t)\\
&\quad - k_{2} \cdot \mathrm{MAL}(t) \cdot \mathrm{OH}(t) - k_{3} \cdot \mathrm{DF}(t) \cdot \mathrm{OH}(t)\\
&\quad - k_{5} \cdot \mathrm{MF}(t) \cdot \mathrm{OH}(t) - k_{7} \cdot \mathrm{F}(t) \cdot \mathrm{OH}(t)\\
&\quad - k_{9} \cdot \mathrm{MAL}(t) \cdot \mathrm{OH}(t) - k_{11} \cdot \mathrm{INT20}(t) \cdot \mathrm{OH}(t)\\
&\quad - k_{13} \cdot \mathrm{MAL}(t) \cdot \mathrm{OH}(t) - k_{15} \cdot \mathrm{INT26}(t) \cdot \mathrm{OH}(t)\\
&\quad - k_{17} \cdot \mathrm{INT23}(t) \cdot \mathrm{OH}(t) - k_{19} \cdot \mathrm{MAL}(t) \cdot \mathrm{OH}(t)\\
&\quad - k_{23} \cdot \mathrm{INT39a}(t) \cdot \mathrm{OH}(t) - k_{25} \cdot \mathrm{INT41}(t) \cdot \mathrm{OH}(t)
\end{aligned}
$$

)(
4)

)(
3)

)(
5)

)(
6)

(7
)

$$= +k_{21} \cdot \mathrm{INT35}(t) - k_{-21} \cdot \mathrm{HS}(t) \cdot \mathrm{MALO}(t) \tag{8}$$

$$= +k_{1} \cdot \mathrm{MAL}(t) - k_{-1} \cdot \mathrm{INT2}(t) \cdot \mathrm{DF}(t) \tag{9}$$

$$= +k_{26} \cdot \mathrm{INT43}(t) - k_{-26} \cdot \mathrm{MEOH}(t) \cdot \mathrm{INT44}(t) \tag{10}$$

$$\begin{aligned} = {} & +k_{9} \cdot \mathrm{MAL}(t) \cdot \mathrm{OH}(t) + k_{-10} \cdot \mathrm{MEOH}(t) \cdot \mathrm{INT20}(t) \\ & - k_{-9} \cdot \mathrm{INT19}(t) - k_{10} \cdot \mathrm{INT19}(t) \end{aligned} \tag{11}$$

$$\begin{aligned} = {} & +k_{4} \cdot \mathrm{INT7}(t) + k_{6} \cdot \mathrm{INT11}(t) + k_{10} \cdot \mathrm{INT19}(t) \\ & + k_{12} \cdot \mathrm{INT22}(t) + k_{14} \cdot \mathrm{INT25}(t) + k_{16} \cdot \mathrm{INT28}(t) \\ & + k_{24} \cdot \mathrm{INT40}(t) + k_{26} \cdot \mathrm{INT43}(t) - k_{-4} \cdot \mathrm{MEOH}(t) \cdot \mathrm{MF}(t) \\ & - k_{-6} \cdot \mathrm{MEOH}(t) \cdot \mathrm{F}(t) - k_{-10} \cdot \mathrm{MEOH}(t) \cdot \mathrm{INT20}(t) \\ & - k_{-12} \cdot \mathrm{MEOH}(t) \cdot \mathrm{INT23}(t) - k_{-14} \cdot \mathrm{MEOH}(t) \cdot \mathrm{INT26}(t) \\ & - k_{-16} \cdot \mathrm{MEOH}(t) \cdot \mathrm{INT23}(t) - k_{-24} \cdot \mathrm{MEOH}(t) \cdot \mathrm{INT41}(t) \\ & - k_{-26} \cdot \mathrm{MEOH}(t) \cdot \mathrm{INT44}(t) \end{aligned} \tag{12}$$

$$\frac{d}{dt}\mathrm{DF}(t) = +k_1 \cdot \mathrm{MAL}(t) + k_2 \cdot \mathrm{MAL}(t) \cdot \mathrm{OH}(t) + k_{-3} \cdot \mathrm{INT7}(t) \tag{13}$$
$$- k_{-1} \cdot \mathrm{INT2}(t) \cdot \mathrm{DF}(t) - k_{-2} \cdot \mathrm{INT5}(t) \cdot \mathrm{DF}(t)$$
$$- k_3 \cdot \mathrm{DF}(t) \cdot \mathrm{OH}(t)$$

$$\frac{d}{dt}\mathrm{INT41}(t) = +k_{24} \cdot \mathrm{INT40}(t) + k_{-25} \cdot \mathrm{INT43}(t) \tag{14}$$
$$- k_{-24} \cdot \mathrm{MEOH}(t) \cdot \mathrm{INT41}(t) - k_{25} \cdot \mathrm{INT41}(t) \cdot \mathrm{OH}(t)$$

$$\frac{d}{dt}\mathrm{INT32}(t) = +k_{17} \cdot \mathrm{INT23}(t) \cdot \mathrm{OH}(t) + k_{-18} \cdot \mathrm{INT33a}(t) \cdot \mathrm{INT33b}(t) \tag{15}$$
$$- k_{-17} \cdot \mathrm{INT32}(t) - k_{18} \cdot \mathrm{INT32}(t)$$

$$\frac{d}{dt}\mathrm{INT40}(t) = +k_{23} \cdot \mathrm{INT39a}(t) \cdot \mathrm{OH}(t) + k_{-24} \cdot \mathrm{MEOH}(t) \cdot \mathrm{INT41}(t) \tag{16}$$
$$- k_{-23} \cdot \mathrm{INT40}(t) - k_{24} \cdot \mathrm{INT40}(t)$$

$$\frac{d}{dt}\mathrm{INT17}(t) = +k_8 \cdot \mathrm{INT15}(t) - k_{-8} \cdot \mathrm{INT17}(t) \tag{17}$$

$$\frac{d}{dt}\mathrm{INT26}(t) = +k_{14} \cdot \mathrm{INT25}(t) + k_{-15} \cdot \mathrm{INT28}(t) - k_{-14} \cdot \mathrm{MEOH}(t) \cdot \mathrm{INT26}(t) \tag{18}$$
$$- k_{15} \cdot \mathrm{INT26}(t) \cdot \mathrm{OH}(t)$$

$$\frac{d}{dt}\mathrm{INT5}(t) = +k_2 \cdot \mathrm{MAL}(t) \cdot \mathrm{OH}(t) - k_{-2} \cdot \mathrm{INT5}(t) \cdot \mathrm{DF}(t) \tag{19}$$

$$\mathrm{INT33a}(t) = +k_{18} \cdot \mathrm{INT32}(t) + k_{20} \cdot \mathrm{INT35}(t) + k_{-22} \cdot \mathrm{INT39a}(t) \cdot \mathrm{INT39b}(t) \tag{20}$$
$$- k_{-18} \cdot \mathrm{INT33a}(t) \cdot \mathrm{INT33b}(t) - k_{-20} \cdot \mathrm{INT36a}(t) \cdot \mathrm{INT33a}(t)$$
$$- k_{22} \cdot \mathrm{INT36a}(t) \cdot \mathrm{INT33a}(t)$$

$$+k_{12} \cdot \mathrm{INT22}(t) + k_{16} \cdot \mathrm{INT28}(t) + k_{-17} \cdot \mathrm{INT32}(t) - k_{-12} \cdot \mathrm{MEOH}(t) \cdot \mathrm{INT23}(t) \tag{21}$$
$$- k_{-16} \cdot \mathrm{MEOH}(t) \cdot \mathrm{INT23}(t) - k_{17} \cdot \mathrm{INT23}(t) \cdot \mathrm{OH}(t)$$

$$+k_{3} \cdot \mathrm{DF}(t) \cdot \mathrm{OH}(t) + k_{-4} \cdot \mathrm{MEOH}(t) \cdot \mathrm{MF}(t) \tag{22}$$
$$- k_{-3} \cdot \mathrm{INT7}(t) - k_{4} \cdot \mathrm{INT7}(t)$$

$$+k_{22} \cdot \mathrm{INT36a}(t) \cdot \mathrm{INT33a}(t) + k_{-23} \cdot \mathrm{INT40}(t) \tag{23}$$
$$- k_{-22} \cdot \mathrm{INT39a}(t) \cdot \mathrm{INT39b}(t) - k_{23} \cdot \mathrm{INT39a}(t) \cdot \mathrm{OH}(t)$$

$$+k_{15} \cdot \mathrm{INT26}(t) \cdot \mathrm{OH}(t) + k_{-16} \cdot \mathrm{MEOH}(t) \cdot \mathrm{INT23}(t) \tag{24}$$
$$- k_{-15} \cdot \mathrm{INT28}(t) - k_{16} \cdot \mathrm{INT28}(t)$$

$$+k_{22} \cdot \mathrm{INT36a}(t) \cdot \mathrm{INT33a}(t) - k_{-22} \cdot \mathrm{INT39a}(t) \cdot \mathrm{INT39b}(t) \tag{25}$$

$$\tag{26}$$

$$\frac{d}{dt}\mathrm{MF}(t) = +k_4 \cdot \mathrm{INT7}(t) + k_{-5} \cdot \mathrm{INT11}(t) - k_{-4} \cdot \mathrm{MEOH}(t) \cdot \mathrm{MF}(t) \tag{27}$$
$$- k_5 \cdot \mathrm{MF}(t) \cdot \mathrm{OH}(t)$$

$$\frac{d}{dt}\mathrm{INT20}(t) = +k_{10} \cdot \mathrm{INT19}(t) + k_{-11} \cdot \mathrm{INT22}(t) - k_{-10} \cdot \mathrm{MEOH}(t) \cdot \mathrm{INT20}(t) \tag{28}$$
$$- k_{11} \cdot \mathrm{INT20}(t) \cdot \mathrm{OH}(t)$$

$$\frac{d}{dt}\mathrm{INT25}(t) = +k_{13} \cdot \mathrm{MAL}(t) \cdot \mathrm{OH}(t) + k_{-14} \cdot \mathrm{MEOH}(t) \cdot \mathrm{INT26}(t) \tag{29}$$
$$- k_{-13} \cdot \mathrm{INT25}(t) - k_{14} \cdot \mathrm{INT25}(t)$$

$$\frac{d}{dt}\mathrm{INT43}(t) = +k_{25} \cdot \mathrm{INT41}(t) \cdot \mathrm{OH}(t) + k_{-26} \cdot \mathrm{MEOH}(t) \cdot \mathrm{INT44}(t) \tag{30}$$
$$- k_{-25} \cdot \mathrm{INT43}(t) - k_{26} \cdot \mathrm{INT43}(t)$$

$$\mathrm{INT36a}(t) = +k_{20} \cdot \mathrm{INT35}(t) + k_{-22} \cdot \mathrm{INT39a}(t) \cdot \mathrm{INT39b}(t) \tag{31}$$
$$- k_{-20} \cdot \mathrm{INT36a}(t) \cdot \mathrm{INT33a}(t) - k_{22} \cdot \mathrm{INT36a}(t) \cdot \mathrm{INT33a}(t)$$

$$\frac{d}{dt}\mathrm{INT35}(t) = +k_{19} \cdot \mathrm{MAL}(t) \cdot \mathrm{OH}(t) + k_{-20} \cdot \mathrm{INT36a}(t) \cdot \mathrm{INT33a}(t) \tag{32}$$
$$+ k_{-21} \cdot \mathrm{HS}(t) \cdot \mathrm{MALO}(t) - k_{-19} \cdot \mathrm{INT35}(t)$$
$$- k_{20} \cdot \mathrm{INT35}(t) - k_{21} \cdot \mathrm{INT35}(t)$$

$$\frac{}{t}\mathrm{MALO}(t) = +k_{21} \cdot \mathrm{INT35}(t) - k_{-21} \cdot \mathrm{HS}(t) \cdot \mathrm{MALO}(t) \tag{33}$$

$$\frac{d}{dt}\mathrm{INT11}(t) = +k_5 \cdot \mathrm{MF}(t) \cdot \mathrm{OH}(t) + k_{-6} \cdot \mathrm{MEOH}(t) \cdot \mathrm{F}(t) \tag{34}$$
$$- k_{-5} \cdot \mathrm{INT11}(t) - k_6 \cdot \mathrm{INT11}(t)$$

Molecular Coordinates

```
1
P    -2.135421 -0.794709  0.129112
O    -3.467321 -0.933894 -0.746127
O    -2.487672  0.179232  1.349381
C    -4.390958  0.164360 -0.887555
H    -4.753366  0.475491  0.093575
H    -3.916323  1.000830 -1.406993
H    -5.215367 -0.214949 -1.486975
C    -2.375191  1.618678  1.348372
H    -2.896505  2.056219  0.496164
H    -2.842680  1.944191  2.275513
H    -1.323979  1.910260  1.330310
S    -1.465469 -2.502721  0.743316
S    -0.902893  0.269448 -1.200113
C     0.673123  0.228109 -0.238751
C     1.297232  1.606981 -0.385157
O     0.907914  2.427618  0.586556
C     1.410889  3.769165  0.498113
C     1.603499 -0.847077 -0.774624
C     2.886890 -0.854237  0.023544
O     3.713946 -1.814747 -0.381216
C     4.964487 -1.887345  0.317310
O     2.028209  1.917195 -1.294631
O     3.134593 -0.078753  0.921005
H     0.443953  0.060362  0.816337
H     0.995099  4.296354  1.352917
H     2.500652  3.759781  0.542057
H     1.085714  4.229055 -0.436027
H     1.131187 -1.830988 -0.709356
H     1.844232 -0.656990 -1.824518
H     5.508782 -2.712157 -0.136000
H     5.514687 -0.952564  0.200126
H     4.791842 -2.076897  1.377671
    el energy= -1902.63611600
          zpe= -1902.389196
    th energy= -1902.367687
  th enthalpy= -1902.366743
  free energy= -1902.442919

TS1
P    -1.859168 -0.172429 -0.235033
O    -3.177678  0.376695 -0.943206
O    -2.478121 -1.360905  0.646399
C    -4.316313  0.754966 -0.138167
H    -4.686922 -0.111715  0.409437
H    -4.040180  1.554050  0.553072
H    -5.067287  1.114466 -0.837773
C    -1.617336 -2.152038  1.482326
H    -1.088628 -1.512708  2.193700
H    -2.264579 -2.849771  2.009377
H    -0.892687 -2.694250  0.869713
S    -0.703073 -0.884605 -1.718769
S    -0.963052  1.189979  0.912496
C     1.454589  0.733993  0.743347
C     1.686714  2.200091  0.554134
O     1.807664  2.527776 -0.728971
C     2.010162  3.923897 -0.987653
C     1.818812 -0.190132 -0.240244
C     2.042953 -1.586038  0.220245
O     2.663140 -2.311629 -0.710558
C     2.843692 -3.696429 -0.387573
O     1.754587  2.979513  1.475999
O     1.649205 -2.028314  1.278756
H     1.383769  0.410760  1.775287
H     2.086602  4.015533 -2.068007
H     1.162339  4.497718 -0.609950
H     2.926671  4.265210 -0.504673
H     0.676539 -0.438393 -0.931786
H     2.383429  0.160679 -1.100593
H     3.357444 -4.134272 -1.239908
H     3.444611 -3.797385  0.517280
H     1.874381 -4.174432 -0.235146
    el energy= -1902.57270276
          zpe= -1902.333227
    th energy= -1902.311715
  th enthalpy= -1902.310771
  free energy= -1902.386971

2
P     1.873525 -0.546707  0.111114
O     3.311691 -1.171100  0.427470
O     1.843667 -0.704089 -1.484402
C     4.482023 -0.438318  0.007263
H     4.462990 -0.294949 -1.074493
H     4.522375  0.525486  0.518575
H     5.335131 -1.050236  0.291599
C     0.727994 -0.205332 -2.241997
H     0.574476  0.858029 -2.036613
H     0.985746 -0.351676 -3.288953
H    -0.174838 -0.773172 -1.995518
S     0.587428 -2.075146  0.733673
S     1.523845  1.228042  0.809857
C    -1.931357  1.107921 -0.728581
C    -1.394682  2.464407 -0.451822
O    -1.505049  2.823751  0.826664
C    -0.898507  4.076979  1.160628
C    -2.128521  0.189299  0.214974
C    -2.533114 -1.186540 -0.181383
O    -2.787260 -1.943787  0.886441
C    -3.128356 -3.305773  0.602298
O    -0.891365  3.154770 -1.311589
O    -2.607899 -1.580425 -1.325462
H    -2.080449  0.867860 -1.776956
H    -1.068770  4.214443  2.225708
H     0.171090  4.042283  0.942655
H    -1.359732  4.883772  0.588966
```

```
H     0.273202 -1.495890  1.902291
H    -1.975368  0.397292  1.268577
H    -3.295489 -3.777686  1.567394
H    -4.030332 -3.348664 -0.009977
H    -2.306432 -3.791450  0.072304
    el energy= -1902.61179855
          zpe= -1902.369321
    th energy= -1902.346799
  th enthalpy= -1902.345855
  free energy= -1902.423292

3
P    -1.788581 -0.731723 -0.171732
O    -3.253755 -1.384235 -0.450478
O    -1.860784 -0.772501  1.462267
C    -4.415450 -0.717637  0.051813
H    -4.385026 -0.668177  1.142805
H    -4.485953  0.293004 -0.359511
H    -5.274282 -1.306798 -0.268983
C    -0.761920 -0.253419  2.206710
H    -0.628979  0.814945  2.003837
H    -0.998566 -0.400323  3.260829
H     0.160956 -0.789913  1.957558
S    -0.454063 -2.036708 -0.847642
S    -1.695713  1.153018 -0.801039
C     1.845244  1.187561  0.740032
C     1.243489  2.513494  0.457965
O     1.342164  2.876512 -0.821632
C     0.653220  4.082061 -1.164133
C     2.115298  0.285851 -0.201350
C     2.601541 -1.062059  0.195490
O     3.004618 -1.765804 -0.863629
C     3.413297 -3.107330 -0.582955
O     0.714561  3.189444  1.314783
O     2.642798 -1.473737  1.335536
H     1.982848  0.950176  1.790290
H     0.822493  4.229448 -2.228374
H    -0.412948  3.968970 -0.956077
H     1.050383  4.922144 -0.591938
H     1.970414  0.485676 -1.256967
H     3.702814 -3.537501 -1.538903
H     4.255105 -3.111438  0.111422
H     2.580749 -3.663915 -0.147322
    el energy= -1902.18212028
          zpe= -1901.948594
    th energy= -1901.926796
  th enthalpy= -1901.925852
  free energy= -1902.001889

1
P    -2.135421 -0.794709  0.129112
O    -3.467321 -0.933894 -0.746127
O    -2.487672  0.179232  1.349381
C    -4.390958  0.164360 -0.887555
H    -4.753366  0.475491  0.093575
H    -3.916323  1.000830 -1.406993
H    -5.215367 -0.214949 -1.486975
C    -2.375191  1.618678  1.348372
H    -2.896505  2.056219  0.496164
H    -2.842680  1.944191  2.275513
H    -1.323979  1.910260  1.330310
S    -1.465469 -2.502721  0.743316
S    -0.902893  0.269448 -1.200113
C     0.673123  0.228109 -0.238751
C     1.297232  1.606981 -0.385157
O     0.907914  2.427618  0.586556
C     1.410889  3.769165  0.498113
C     1.603499 -0.847077 -0.774624
C     2.886890 -0.854237  0.023544
O     3.713946 -1.814747 -0.381216
C     4.964487 -1.887345  0.317310
O     2.028209  1.917195 -1.294631
O     3.134593 -0.078753  0.921005
H     0.443953  0.060362  0.816337
H     0.995099  4.296354  1.352917
H     2.500652  3.759781  0.542057
H     1.085714  4.229055 -0.436027
H     1.131187 -1.830988 -0.709356
H     1.844232 -0.656990 -1.824518
H     5.508782 -2.712157 -0.136000
H     5.514687 -0.952564  0.200126
H     4.791842 -2.076897  1.377671
    el energy= -1902.63611600
          zpe= -1902.389196
    th energy= -1902.367687
  th enthalpy= -1902.366743
  free energy= -1902.442919

4
P    -2.262854 -0.329514  0.346500
O    -3.044324 -1.688378 -0.039057
O    -3.298714  0.844908  0.017514
C    -3.884736 -1.748097 -1.208138
H    -4.711268 -1.043115 -1.105825
H    -3.307466 -1.536988 -2.113042
H    -4.265948 -2.765793 -1.252835
C    -3.374819  1.578791 -1.219763
H    -3.694461  0.929652 -2.036807
H    -4.119607  2.354328 -1.051142
H    -2.408079  2.024684 -1.451605
S    -1.739052 -0.372288  2.216226
S    -0.735879 -0.346542 -1.092736
C     0.637179  0.491316 -0.208078
C     0.462797  2.001302 -0.168550
O    -0.747403  2.347257  0.275206
C    -1.002435  3.753709  0.384793
C     1.946764  0.090832 -0.864266
C     3.091672  0.421619  0.047567
O     4.258547  0.435365 -0.613000
C     5.416812  0.508499  0.222788
O     1.321554  2.793104 -0.472946
O     2.999429  0.642717  1.235390
H     0.622024  0.131955  0.826643
H    -2.025990  3.837703  0.743894
```

```
H    -0.306353  4.205452  1.092740
H    -0.894696  4.230825 -0.590663
H     1.956948 -1.018146 -1.021566
H     2.085427  0.593526 -1.824588
H     6.271603  0.523112 -0.450756
H     5.395803  1.412058  0.833814
H     5.445017 -0.374871  0.864896
O     1.806721 -2.877392 -1.111844
H     1.084662 -2.927857 -0.470046
O     3.844506 -2.376846  0.153252
H     2.911556 -2.646669 -0.388638
H     4.345326 -1.916046 -0.528398
O    -0.696336 -3.404255  0.911303
H    -1.512008 -3.205831  0.432914
H    -0.642042 -2.683644  1.552996
    el energy= -2131.32754281
          zpe= -2131.021381
    th energy= -2130.992133
  th enthalpy= -2130.991189
  free energy= -2131.082309

TS2
P    -2.272142 -0.391362  0.356567
O    -2.976009 -1.808977  0.031433
O    -3.380724  0.704863 -0.011338
C    -3.776706 -1.969257 -1.154782
H    -4.638276 -1.300725 -1.113621
H    -3.182897 -1.777259 -2.053497
H    -4.109054 -3.005012 -1.157389
C    -3.482648  1.399030 -1.269511
H    -3.726653  0.706250 -2.076985
H    -4.292601  2.114669 -1.140546
H    -2.548730  1.915964 -1.488558
S    -1.752907 -0.340411  2.229752
S    -0.748954 -0.369660 -1.078570
C     0.604372  0.527468 -0.206883
C     0.367542  2.031395 -0.180233
O    -0.885942  2.338094  0.170196
C    -1.184795  3.734563  0.285306
C     1.924138  0.136408 -0.830461
C     3.033520  0.432695  0.091890
O     4.217128  0.552947 -0.555038
C     5.358268  0.644583  0.298476
O     1.219196  2.857879 -0.401601
O     2.957302  0.514413  1.305048
H     0.588227  0.187950  0.835472
H    -2.230300  3.787010  0.582382
H    -0.545559  4.193475  1.040805
H    -1.031068  4.231176 -0.674189
H     1.916501 -1.110175 -0.981857
H     2.086405  0.609638 -1.800943
H     6.217311  0.757319 -0.361144
H     5.275872  1.504109  0.965762
H     5.446803 -0.270098  0.889401
O     1.859986 -2.516405 -1.110787
H     1.211500 -2.744355 -0.427973
O     4.197728 -2.394383 -0.125172
H     3.237725 -2.522358 -0.484378
H     4.530698 -1.694121 -0.696961
O    -0.397093 -3.279799  0.961484
H    -1.222099 -3.175640  0.469073
H    -0.426641 -2.546625  1.591122
    el energy= -2131.32568882
          zpe= -2131.021819
    th energy= -2130.993225
  th enthalpy= -2130.992281
  free energy= -2131.082071

5
P    -1.957139 -1.071712  0.075418
O    -1.168374 -2.492555 -0.074918
O    -3.453636 -1.643369 -0.235697
C    -1.070915 -3.121805 -1.361679
H    -2.050115 -3.152425 -1.844245
H    -0.352006 -2.583931 -1.982570
H    -0.717624 -4.135976 -1.176379
C    -4.540872 -0.720775 -0.279978
H    -4.400231  0.000232 -1.090362
H    -5.442329 -1.305601 -0.459337
H    -4.632258 -0.189544  0.672714
S    -1.767723 -0.549253  1.974972
S    -1.417622  0.208118 -1.352199
C     0.743239  1.957490  0.593522
C    -0.038872  3.004562 -0.115375
O    -1.174314  3.273987  0.532399
C    -2.028290  4.226796 -0.106070
C     1.987100  1.671729  0.215166
C     2.708610  0.562141  0.880114
O     3.868218  0.297346  0.282504
C     4.535601 -0.888790  0.731662
O     0.303840  3.554901 -1.138704
O     2.298675 -0.047930  1.848882
H     0.253790  1.417173  1.399098
H    -2.893945  4.334348  0.543353
H    -1.513143  5.181847 -0.221841
H    -2.329357  3.857002 -1.088576
H     0.863020 -0.666524 -1.164502
H     2.469486  2.184462 -0.610428
H     5.375535 -1.026906  0.056098
H     4.872920 -0.764259  1.761494
H     3.851560 -1.738153  0.667574
O     1.653687 -1.230641 -1.141271
H     1.557111 -1.793113 -0.345205
O     4.101276 -0.702081 -2.376462
H     3.237438 -0.911446 -1.974447
H     4.352220  0.102215 -1.909608
O     1.339212 -2.626898  1.231965
H     0.372906 -2.652303  1.140290
H     1.525350 -1.833432  1.757478
    el energy= -2131.40602658
          zpe= -2131.097009
    th energy= -2131.066671
  th enthalpy= -2131.065727
  free energy= -2131.160281
```

```
6
C     1.309402 -0.625272 -0.284043
C     2.625079  0.026777 -0.086721
O     3.599548 -0.881888  0.050001
C     4.911511 -0.345653  0.242138
C     0.212043  0.111907 -0.449052
C    -1.106323 -0.547288 -0.651652
O    -1.971753  0.268184 -1.261952
C    -3.303125 -0.245152 -1.380056
O     2.819670  1.223020 -0.052176
O    -1.341196 -1.713486 -0.405461
H     1.270732 -1.709442 -0.281433
H     5.574535 -1.203318  0.329649
H     5.195661  0.273563 -0.610562
H     4.943928  0.258387  1.150588
H     0.225183  1.197452 -0.441159
H    -3.891814  0.555265 -1.824121
H    -3.314434 -1.126401 -2.024937
H    -3.671323 -0.505913 -0.385140
O    -1.626069  0.700863  1.546271
H    -2.613348 -0.428963  1.745033
H    -0.827347  0.503625  2.048586
O    -3.256229 -1.230639  1.801397
H    -2.844005 -1.836573  1.174392
O    -1.325849  2.800587  0.155937
H    -1.446524  1.984597  0.774539
H    -1.677734  2.452674 -0.671256
    el energy= -762.850507519
          zpe= -762.648026
    th energy= -762.630078
  th enthalpy= -762.629133
  free energy= -762.694236

TS3
C     1.326993 -0.553772 -0.249139
C     2.667022  0.038681 -0.052723
O     3.620003 -0.905909 -0.040238
C     4.953827 -0.424928  0.140491
C     0.246368  0.223450 -0.304774
C    -1.117554 -0.366897 -0.484521
O    -1.909516  0.515962 -1.167225
C    -3.218833  0.031209 -1.445766
O     2.907086  1.220952  0.079546
O    -1.333250 -1.576889 -0.500654
H     1.249032 -1.631901 -0.339284
H     5.593453 -1.304665  0.126237
H     5.224005  0.257748 -0.667264
H     5.043229  0.097554  1.094733
H     0.308920  1.302906 -0.206027
H    -3.767078  0.866972 -1.879755
H    -3.180715 -0.798249 -2.157198
H    -3.696387 -0.309826 -0.524144
O    -1.647998  0.309189  1.344775
H    -2.847259 -0.812225  1.522521
H    -0.954016 -0.033628  1.922290
O    -3.466546 -1.592772  1.455226
H    -3.032589 -2.057212  0.726618
O    -1.409337  2.808670  0.587138
H    -1.497527  1.905590  1.007535
H    -1.673545  2.596873 -0.316229
    el energy= -762.847440156
          zpe= -762.644052
    th energy= -762.627009
  th enthalpy= -762.626064
  free energy= -762.688708

7
C    -1.344089 -0.486634  0.103042
C    -2.710677  0.057797 -0.033749
O    -3.638659 -0.887891  0.190749
C    -4.994171 -0.449826  0.082804
C    -0.279324  0.291236 -0.067417
C     1.142715 -0.240624  0.056467
O     1.696752  0.640801  1.096060
C     3.045856  0.350723  1.384303
O    -2.997940  1.204747 -0.310187
O     1.265343 -1.509879  0.334547
H    -1.224704 -1.536654  0.347831
H    -5.608877 -1.322462  0.293101
H    -5.196724  0.343209  0.805160
H    -5.194373 -0.075036 -0.922799
H    -0.389206  1.345653 -0.315342
H     3.361229  1.015266  2.191178
H     3.162677 -0.689988  1.705924
H     3.686785  0.527009  0.509550
O     1.776422  0.151105 -1.180339
H     4.128228 -1.876635 -0.323825
H     2.479194 -0.509264 -1.335868
O     3.391702 -2.098392 -0.903801
H     2.556869 -2.000613 -0.320275
O     1.702398  2.886704 -0.590247
H     1.850751  2.107832 -1.150468
H     1.658131  2.438095  0.268877
    el energy= -762.862861903
          zpe= -762.657920
    th energy= -762.640766
  th enthalpy= -762.639822
  free energy= -762.703110

TS4
C    -1.363614  0.664253  0.022237
C    -2.696830  0.030469  0.099432
O    -3.658451  0.868446 -0.316661
C    -4.986871  0.342322 -0.274058
C    -0.275556 -0.011037  0.390107
C     1.071958  0.611123  0.320317
O     1.433208 -1.022554 -1.203524
C     2.753437 -0.795592 -1.496631
O    -2.924155 -1.096666  0.487309
O     1.313174  1.651083 -0.288465
H    -1.300576  1.681384 -0.348983
H    -5.634137  1.134601 -0.643622
H    -5.065151 -0.542880 -0.907861
```

```
H    -5.256281  0.074296  0.749249
H    -0.319529 -1.032865  0.753778
H     3.093145 -1.305617 -2.421744
H     2.977114  0.282473 -1.659925
H     3.453814 -1.131697 -0.698414
O     1.910162  0.110341  1.243471
H     4.470780  1.219941 -0.168128
H     2.770384  0.584790  1.150870
O     3.954919  1.723423  0.473566
H     3.161880  2.009792 -0.020506
O     1.407778 -2.712657  0.682690
H     1.735302 -2.106050  1.356647
H     1.405018 -2.088725 -0.136877
   el energy= -762.843789158
         zpe= -762.641158
   th energy= -762.623877
 th enthalpy= -762.622933
 free energy= -762.686821

8
C    -1.339207 -0.705634  0.012302
C    -2.670344 -0.073760 -0.114027
O    -3.634344 -0.868643  0.373375
C    -4.959873 -0.338859  0.293773
C    -0.249634 -0.061497 -0.405168
C     1.091340 -0.688066 -0.292614
O     1.368280  1.247530  1.207762
C     2.713705  1.115159  1.430075
O    -2.891765  1.018717 -0.593075
O     1.338252 -1.652051  0.419832
H    -1.280814 -1.690810  0.462220
H    -5.610006 -1.093336  0.731040
H    -5.028821  0.596388  0.852329
H    -5.232907 -0.154764 -0.746931
H    -0.288206  0.929340 -0.846394
H     3.014336  1.307557  2.482603
H     3.105680  0.094682  1.205450
H     3.336159  1.799915  0.812530
O     1.960733 -0.205610 -1.182015
H     4.601022 -1.448127  0.160902
H     2.817964 -0.683414 -1.055784
O     3.956993 -1.863927 -0.424879
H     3.207028 -2.103524  0.150631
O     1.262299  2.673079 -0.846116
H     1.683162  2.041467 -1.440675
H     1.275896  2.127796  0.046969
   el energy= -762.844168144
         zpe= -762.641417
   th energy= -762.623472
 th enthalpy= -762.622527
 free energy= -762.687562

9
C     1.790693  0.641445 -0.040267
C     3.020541 -0.184571  0.016740
O     4.100381  0.570500  0.260078
C     5.338786 -0.140614  0.336088
C     0.603441  0.081755 -0.264038
C    -0.667164  0.900449 -0.340177
O    -3.219136 -0.975084  1.161889
C    -4.382187 -1.108282  0.364339
O     3.070255 -1.387010 -0.132086
O    -0.632933  2.091982  0.012316
H     1.883701  1.711973  0.109006
H     6.102060  0.608992  0.532186
H     5.305320 -0.873779  1.143986
H     5.538982 -0.654162 -0.605966
H     0.512588 -0.992701 -0.408105
H    -5.070460 -1.781684  0.879993
H    -4.882610 -0.143556  0.218445
H    -4.146830 -1.538101 -0.617621
O    -1.688830  0.264900 -0.766175
H    -3.237023  1.506087 -0.565489
H    -2.645608 -0.354448  0.674018
O    -3.469248  2.282310 -0.032420
H    -2.565695  2.558043  0.196453
O    -1.588561 -2.500619 -0.657674
H    -1.559690 -1.572105 -0.955730
H    -2.034826 -2.391468  0.195287
   el energy= -762.888366886
         zpe= -762.684306
   th energy= -762.665049
 th enthalpy= -762.664105
 free energy= -762.735048

10
C     1.810331 -0.726262 -0.155735
C     3.200894 -0.135512  0.074171
O     4.091820 -0.974050  0.349276
C     0.742497  0.015363 -0.450204
C    -0.585112 -0.604221 -0.662716
O    -1.408303  0.210025 -1.339398
C    -2.759624 -0.245347 -1.454986
O     3.310825  1.108271 -0.032112
O    -0.901068 -1.733807 -0.338077
H     1.707934 -1.806543 -0.066783
H     0.803905  1.095557 -0.530478
H    -3.299287  0.553030 -1.961594
H    -2.802706 -1.163099 -2.045571
H    -3.162391 -0.426138 -0.455637
O    -1.312109  0.862978  1.650106
H    -2.267740 -0.277751  1.722037
H    -0.444130  0.473318  1.805574
O    -2.908224 -1.095698  1.743532
H    -2.453337 -1.700496  1.145644
O    -0.914803  2.761896  0.015447
H    -1.075177  2.002834  0.701018
H    -1.126101  2.308234 -0.807592
   el energy= -723.086825991
         zpe= -722.925665
   th energy= -722.909610
 th enthalpy= -722.908665
 free energy= -722.970430
```

TS5

C	1.808224	-0.678823	-0.168445
C	3.241068	-0.200090	0.031633
O	4.117169	-1.100320	0.002630
C	0.760162	0.139835	-0.214613
C	-0.638252	-0.360437	-0.410455
O	-1.335354	0.553608	-1.185512
C	-2.661399	0.154593	-1.496168
O	3.415759	1.031577	0.202863
O	-0.929572	-1.562452	-0.453818
H	1.652221	-1.750570	-0.280300
H	0.888093	1.211940	-0.100905
H	-3.142851	1.015824	-1.961379
H	-2.664202	-0.688494	-2.193922
H	-3.195359	-0.140067	-0.588910
O	-1.276512	0.323377	1.294034
H	-2.527795	-0.768482	1.458102
H	-0.607866	-0.027251	1.896056
O	-3.142778	-1.543169	1.342338
H	-2.664758	-1.971600	0.617046
O	-0.934781	2.831048	0.559274
H	-1.061346	1.933424	0.975346
H	-1.046396	2.585461	-0.367306

el energy= -723.079265559
zpe= -722.917121
th energy= -722.901904
th enthalpy= -722.900960
free energy= -722.959712

11

C	-1.823849	-0.637684	0.128239
C	-3.276810	-0.197832	0.010222
O	-4.131235	-1.101180	0.199494
C	-0.788217	0.175341	-0.047777
C	0.663088	-0.259008	0.056038
O	1.187774	0.664094	1.088334
C	2.560728	0.480269	1.334746
O	-3.497505	1.009115	-0.262179
O	0.896354	-1.515812	0.338760
H	-1.638018	-1.683040	0.369078
H	-0.958923	1.222485	-0.293139
H	2.849793	1.163881	2.136531
H	2.770101	-0.549136	1.647976
H	3.163172	0.709029	0.444207
O	1.270393	0.166695	-1.190050
H	3.763737	-1.661523	-0.293327
H	2.027040	-0.433554	-1.328867
O	3.054907	-1.961686	-0.872373
H	2.199817	-1.899008	-0.298064
O	1.151243	2.891187	-0.599779
H	1.291699	2.101318	-1.148242
H	1.066507	2.443737	0.257392

el energy= -723.091908359
zpe= -722.928166
th energy= -722.912991
th enthalpy= -722.912046
free energy= -722.970944

TS6

C	-1.861652	0.727938	-0.080689
C	-3.290658	0.198166	-0.046825
O	-4.167069	1.000044	-0.455409
C	-0.803039	0.009993	0.286796
C	0.574800	0.561785	0.257220
O	1.096220	-0.986161	-1.175094
C	2.432770	-0.780082	-1.396599
O	-3.459535	-0.970529	0.378695
O	0.891076	1.610842	-0.316071
H	-1.720274	1.747665	-0.434794
H	-0.906340	-1.011746	0.637387
H	2.833182	-1.364062	-2.250721
H	2.666245	0.281776	-1.632512
H	3.076967	-1.048366	-0.527472
O	1.334518	0.069751	1.268539
H	3.972631	1.198446	-0.023917
H	2.202541	0.526504	1.230753
O	3.443265	1.722193	0.589316
H	2.627402	1.931868	0.083982
O	0.959429	-2.740444	0.656804
H	1.157793	-2.117768	1.365743
H	0.993300	-2.096692	-0.142126

el energy= -723.076258298
zpe= -722.914469
th energy= -722.899294
th enthalpy= -722.898350
free energy= -722.956901

12

C	-1.889959	-0.755087	0.106520
C	-3.296523	-0.164478	0.072425
O	-4.193092	-0.902982	0.548350
C	-0.810777	-0.104501	-0.325320
C	0.528177	-0.731593	-0.300055
O	1.164997	1.291062	1.236720
C	2.499184	1.014737	1.296301
O	-3.421137	0.982906	-0.417948
O	0.845493	-1.678576	0.410459
H	-1.786158	-1.759365	0.514026
H	-0.869719	0.899369	-0.731815
H	3.054655	1.574313	2.085548
H	2.719819	-0.059226	1.511532
H	3.051087	1.237992	0.351104
O	1.336936	-0.257072	-1.254529
H	3.976777	-1.160153	0.098595
H	2.215042	-0.698236	-1.156254
O	3.463328	-1.746874	-0.470914
H	2.709056	-2.021828	0.085219
O	0.887220	2.615252	-0.857378
H	1.096925	1.903593	-1.472219
H	0.981933	2.099342	0.056963

el energy= -723.077777893
zpe= -722.917222
th energy= -722.901691
th enthalpy= -722.900747

```
  free energy= -722.960662

13
C     2.349744  0.489483 -0.096080
C     3.781863 -0.034206 -0.167328
O     4.618129  0.766246 -0.653823
C     1.323916 -0.224258  0.365945
C    -0.086532  0.293208  0.423590
O    -3.371546 -0.269427 -0.003604
C    -3.050901 -0.115234 -1.376861
O     3.987442 -1.196459  0.258166
O    -0.323679  1.458712  0.036210
H     2.173144  1.503211 -0.451297
H     1.495974 -1.237738  0.719562
H    -3.981677 -0.024525 -1.942520
H    -2.447090  0.784779 -1.541845
H    -2.497545 -0.985932 -1.750352
O    -0.952274 -0.523902  0.880432
H    -3.371524  1.652807  0.456426
H    -2.480014 -0.278414  0.458142
O    -2.864555  2.476631  0.503117
H    -1.950093  2.153443  0.362639
O    -2.149884 -2.891175  0.031900
H    -1.465146 -2.262706  0.319233
H    -2.933627 -2.323897  0.055246
    el energy= -723.127292113
          zpe= -722.964118
    th energy= -722.947383
  th enthalpy= -722.946439
  free energy= -723.011289

14
C    -0.237772  0.965241 -0.290638
C    -1.664263  1.484601 -0.242574
O    -1.786791  2.722929 -0.073034
C     0.090234 -0.270656 -0.669876
C     1.506911 -0.795517 -0.768318
O     1.675792 -1.782787 -1.515666
O    -2.602267  0.650532 -0.375836
O     2.420496 -0.204844 -0.114178
H     0.540470  1.665496  0.006324
H    -0.694478 -0.973008 -0.936786
O    -2.257029 -2.200910  0.420239
H    -1.304436 -2.248974  0.942567
H    -2.347001 -1.258839  0.207675
O    -0.081700 -2.305192  1.623656
H     0.238751 -1.410954  1.461391
O     2.640315  2.118331  1.160493
H     2.844221  2.697864  0.419201
H     2.481279  1.241931  0.722668
    el energy= -683.296446003
          zpe= -683.177819
    th energy= -683.162863
  th enthalpy= -683.161919
  free energy= -683.222599

TS7
C    -0.778517  0.441790  0.129982
C    -2.235637  0.274173 -0.085256
O    -3.034102  0.821199  0.739190
C     0.139028 -0.195489 -0.698927
C     1.642083  0.010106 -0.528616
O     2.354711 -0.121385 -1.546268
O    -2.616101 -0.427688 -1.082501
O     2.079766  0.322043  0.630586
H    -0.453690  0.715292  1.132214
H    -0.147832 -0.298106 -1.742404
O     0.081403 -2.078238 -0.499463
H     0.441922 -2.012405  1.088456
H    -0.882446 -2.003156 -0.539140
O     0.803126 -1.803934  2.002849
H     1.229949 -0.957475  1.781011
O     1.008552  2.893936  0.343307
H     0.224925  2.384811  0.062659
H     1.566589  2.140088  0.612503
    el energy= -683.269152395
          zpe= -683.147178
    th energy= -683.134140
  th enthalpy= -683.133196
  free energy= -683.187270

15
C     0.594982  0.566407 -0.462083
C     1.991465  0.297439 -0.198417
O     2.883623  0.414382 -1.097370
C    -0.391924  0.113684  0.602761
C    -1.796521 -0.061065 -0.005727
O    -2.477596  0.995331 -0.143396
O     2.316359 -0.054535  1.027935
O    -2.191936 -1.205993 -0.358667
H     0.289071  0.368461 -1.494082
H    -0.515924  0.908229  1.365961
O     0.050382 -1.056218  1.315265
H     0.236714 -2.381026  0.059456
H     1.043267 -0.786451  1.377979
O    -0.109028 -2.949451 -0.658621
H    -0.949721 -2.455223 -0.749926
O    -0.611516  3.101001 -0.071247
H     0.036961  2.350431 -0.261109
H    -1.410679  2.540657 -0.028659
    el energy= -683.290358316
          zpe= -683.167124
    th energy= -683.154630
  th enthalpy= -683.153686
  free energy= -683.206422

TS8
C    -0.614738  0.426631  0.420098
C    -2.002340 -0.027918  0.089432
O    -2.892531  0.007974  0.979584
C     0.411763  0.128450 -0.668726
C     1.836618  0.262445 -0.100986
O     2.368508  1.397335 -0.187308
O    -2.239382 -0.413456 -1.121229
```

```
O     2.368537 -0.743889  0.454158
H    -0.307572 -0.013904  1.377780
H     0.326286  0.910386 -1.442503
O     0.204246 -1.141287 -1.311099
H     0.141182 -2.397824  0.150707
H    -0.786999 -1.061701 -1.443808
O     0.598010 -2.731182  0.942112
H     1.317381 -2.058203  0.921859
O    -0.234533  3.034499  0.410136
H    -0.539211  1.774200  0.502093
H     0.678267  2.829456  0.164132
    el energy= -683.283320617
          zpe= -683.164518
    th energy= -683.151900
  th enthalpy= -683.150956
  free energy= -683.204573

16
C     0.631745  0.318977 -0.336319
C     2.094813  0.001647  0.016764
O     2.992059  0.668358 -0.533458
C    -0.357519 -0.076250  0.764559
C    -1.807334  0.199518  0.307366
O    -2.390115  1.171194  0.837207
O     2.296248 -0.958513  0.836554
O    -2.289766 -0.545333 -0.595756
H     0.376828 -0.277328 -1.223547
H    -0.182787  0.560498  1.647279
O    -0.179530 -1.443770  1.124804
H    -0.224613 -2.495057 -0.586797
H     0.824281 -1.483814  1.154077
O    -0.695916 -2.551390 -1.432021
H    -1.342535 -1.826927 -1.248996
O    -0.062478  3.477833 -0.671682
H     0.517737  1.387680 -0.578312
H    -0.703168  2.924558 -0.203096
    el energy= -683.293769960
          zpe= -683.170383
    th energy= -683.156849
  th enthalpy= -683.155905
  free energy= -683.212077

17
C    -0.495173 -0.380588  0.653172
C    -1.822016 -0.993475  0.198046
O    -2.646097 -0.188709 -0.342961
C     0.370381  0.069243 -0.565373
C     1.405651  1.097029 -0.007416
O     0.936629  2.234116  0.319579
O    -2.022320 -2.218425  0.368144
O     2.614877  0.774832  0.122235
H     0.100401 -1.110720  1.209530
H    -0.310307  0.706153 -1.174787
O     0.861144 -0.988293 -1.273852
H     1.728341 -1.704612 -0.333197
H    -2.117373  1.522930 -0.127778
O     2.414090 -2.046277  0.387453
H     2.768398 -1.161212  0.565979
O    -1.827311  2.450582  0.018122
H    -0.718976  0.480898  1.293206
H    -0.851645  2.370692  0.106715
    el energy= -683.331498095
          zpe= -683.206648
    th energy= -683.194442
  th enthalpy= -683.193497
  free energy= -683.245844

1
P    -2.135421 -0.794709  0.129112
O    -3.467321 -0.933894 -0.746127
O    -2.487672  0.179232  1.349381
C    -4.390958  0.164360 -0.887555
H    -4.753366  0.475491  0.093575
H    -3.916323  1.000830 -1.406993
H    -5.215367 -0.214949 -1.486975
C    -2.375191  1.618678  1.348372
H    -2.896505  2.056219  0.496164
H    -2.842680  1.944191  2.275513
H    -1.323979  1.910260  1.330310
S    -1.465469 -2.502721  0.743316
S    -0.902893  0.269448 -1.200113
C     0.673123  0.228109 -0.238751
C     1.297232  1.606981 -0.385157
O     0.907914  2.427618  0.586556
C     1.410889  3.769165  0.498113
C     1.603499 -0.847077 -0.774624
C     2.886890 -0.854237  0.023544
O     3.713946 -1.814747 -0.381216
C     4.964487 -1.887345  0.317310
O     2.028209  1.917195 -1.294631
O     3.134593 -0.078753  0.921005
H     0.443953  0.060362  0.816337
H     0.995099  4.296354  1.352917
H     2.500652  3.759781  0.542057
H     1.085714  4.229055 -0.436027
H     1.131187 -1.830988 -0.709356
H     1.844232 -0.656990 -1.824518
H     5.508782 -2.712157 -0.136000
H     5.514687 -0.952564  0.200126
H     4.791842 -2.076897  1.377671
    el energy= -1902.63611600
          zpe= -1902.389196
    th energy= -1902.367687
  th enthalpy= -1902.366743
  free energy= -1902.442919

18
P     2.631629 -0.130114 -0.165799
O     2.767763 -0.380779  1.410430
O     1.923341  1.299739 -0.302118
C     1.598549 -0.352898  2.261546
H     0.954585  0.496212  2.017554
H     1.037607 -1.281422  2.144522
H     1.972316 -0.270271  3.280757
```

```
C     2.465254  2.431305  0.404083
H     3.414541  2.727554 -0.047275
H     1.726105  3.222938  0.305268
H     2.609176  2.188553  1.459044
S     4.350511 -0.377595 -1.033237
S     1.157088 -1.355695 -0.985169
C    -0.441320 -0.606900 -0.393084
C    -1.446710 -1.730362 -0.596169
O    -1.449443 -2.575520  0.440273
C    -2.408998 -3.633427  0.353132
C    -0.860863  0.656826 -1.138252
C    -1.147078  1.779907 -0.172154
O    -2.061553  2.626460 -0.680554
C    -2.354945  3.766837  0.130576
O    -2.107727 -1.893098 -1.592195
O    -0.589836  1.989724  0.881433
H    -0.381243 -0.425435  0.678772
H    -2.289214 -4.220533  1.261013
H    -3.414164 -3.211697  0.297957
H    -2.221345 -4.247550 -0.528910
H    -0.072833  1.008102 -1.810278
H    -1.762580  0.463327 -1.720764
H    -3.102123  4.338372 -0.415820
H    -2.748215  3.451575  1.099268
H    -1.454788  4.363832  0.287414
O    -2.938150 -0.003700  0.791078
H    -3.187996  0.845171  1.179117
O    -1.438785 -0.795707  2.716392
H    -1.298942 -1.720627  2.486875
H    -2.049070 -0.482407  1.951027
O    -4.139936  0.587837 -1.434926
H    -3.690932  0.248311 -0.592104
H    -3.785649  1.482971 -1.488522
    el energy= -2131.35385034
          zpe= -2131.043988
    th energy= -2131.015888
  th enthalpy= -2131.014944
  free energy= -2131.102444

TS9
P    -2.723462 -0.149395 -0.186170
O    -3.005412  0.540810  1.237120
O    -1.822609 -1.432405  0.151487
C    -1.909818  0.938209  2.086126
H    -1.242520  0.098445  2.295724
H    -1.341242  1.742135  1.608135
H    -2.362415  1.298951  3.008045
C    -2.297544 -2.421380  1.082197
H    -3.084229 -3.019055  0.617370
H    -1.431486 -3.036789  1.316725
H    -2.677360 -1.942237  1.987715
S    -4.400555 -0.438417 -1.120415
S    -1.340042  0.982145 -1.254277
C     0.260057  0.398025 -0.499443
C     1.182266  1.607110 -0.591156
O     0.911222  2.472008  0.435407
C     1.534716  3.745459  0.311862
C     0.809903 -0.815102 -1.239626
C     1.556641 -1.716538 -0.283277
O     2.708128 -2.145668 -0.803290
C     3.541122 -2.877226  0.094404
O     1.688824  1.985044 -1.633893
O     1.144363 -2.058755  0.802864
H     0.088664  0.159870  0.548735
H     1.226015  4.320406  1.183458
H     2.623906  3.643886  0.299147
H     1.217182  4.244017 -0.606154
H    -0.011902 -1.407963 -1.649019
H     1.459505 -0.494281 -2.055039
H     4.471772 -3.054908 -0.439077
H     3.726442 -2.274680  0.986069
H     3.067585 -3.818725  0.380147
O     2.664344  0.537608  0.438362
H     3.136354  1.324329  0.743205
O     1.190198  0.517336  2.632887
H     0.925339  1.428637  2.457079
H     1.777611  0.348435  1.840887
O     4.968013 -0.245180 -0.672207
H     5.440841 -0.496261  0.127658
H     4.050793 -0.040667 -0.339630
    el energy= -2131.34911780
          zpe= -2131.039486
    th energy= -2131.011838
  th enthalpy= -2131.010894
  free energy= -2131.097732

19
P    -2.526064 -0.161046 -0.336357
O    -2.887053  0.739217  0.946497
O    -1.763156 -1.444083  0.264826
C    -1.828617  1.200548  1.815695
H    -1.267708  0.349596  2.212910
H    -1.160063  1.869747  1.264927
H    -2.322006  1.742685  2.620961
C    -2.419264 -2.215773  1.288151
H    -3.347875 -2.638038  0.896354
H    -1.725460 -3.007789  1.559915
H    -2.619696 -1.591205  2.160349
S    -4.150132 -0.500133 -1.357940
S    -1.021363  0.759072 -1.427853
C     0.506242  0.204042 -0.552575
C     1.526175  1.375293 -0.712676
O     0.981352  2.397869  0.256158
C     1.642621  3.640868  0.134858
C     1.039692 -1.047942 -1.246122
C     2.177673 -1.656879 -0.467978
O     3.243325 -1.908392 -1.223974
C     4.372953 -2.449588 -0.531849
O     1.677430  1.797377 -1.901371
O     2.129183 -1.941713  0.714428
H     0.270210 -0.015066  0.492565
H     1.134373  4.352652  0.789049
H     2.694619  3.560106  0.437138
H     1.601496  3.990219 -0.899717
```

```
H     0.251513 -1.804484 -1.305850
H     1.370996 -0.784508 -2.251821
H     5.142287 -2.596061 -1.286547
H     4.711298 -1.744334  0.229760
H     4.113221 -3.397461 -0.058255
O     2.760927  0.930264 -0.106922
H     2.593526  0.771390  0.837076
O     0.200164 -1.297831  2.729008
H     0.661704 -0.447224  2.837005
H     0.661205 -1.681178  1.966749
O     1.491335  1.170203  2.540648
H     1.911306  1.740887  3.193236
H     1.187041  1.756022  1.802809
    el energy= -2131.37316262
          zpe= -2131.060567
    th energy= -2131.034103
  th enthalpy= -2131.033158
  free energy= -2131.116410

TS10
P    -2.522576 -0.212408 -0.314340
O    -2.906121  0.811605  0.857926
O    -1.740007 -1.408782  0.421891
C    -1.863365  1.362922  1.699853
H    -1.291765  0.556261  2.169101
H    -1.196635  1.996280  1.105979
H    -2.380920  1.953169  2.454801
C    -2.381276 -2.076762  1.525095
H    -3.297821 -2.562193  1.181453
H    -1.669515 -2.816590  1.883370
H    -2.600337 -1.363605  2.321475
S    -4.123192 -0.680891 -1.317695
S    -1.016770  0.603717 -1.496460
C     0.509755  0.112623 -0.594208
C     1.584173  1.159815 -0.927070
O     0.784193  2.523919  0.270497
C     1.487649  3.707180  0.053123
C     0.979645 -1.258612 -1.107239
C     2.177089 -1.737510 -0.323182
O     3.237164 -1.967742 -1.091604
C     4.426970 -2.358061 -0.396176
O     1.657633  1.628978 -2.057467
O     2.179735 -1.910684  0.880147
H     0.310838  0.059301  0.478303
H     0.850781  4.592030  0.201685
H     2.355395  3.810456  0.727809
H     1.869002  3.741374 -0.979637
H     0.179035 -1.987560 -0.959428
H     1.223666 -1.197741 -2.169160
H     5.182527 -2.510816 -1.163148
H     4.729217 -1.564122  0.289347
H     4.255626 -3.277741  0.164827
O     2.739058  0.965321 -0.215925
H     2.514651  0.915038  0.745508
O     0.266478 -0.946379  2.808410
H     0.755526 -0.099406  2.741676
H     0.707099 -1.481432  2.131801
O     1.628015  1.342927  2.200771
H     2.112725  1.907603  2.811973
H     1.175908  1.967705  1.425519
    el energy= -2131.36604641
          zpe= -2131.055813
    th energy= -2131.029565
  th enthalpy= -2131.028621
  free energy= -2131.111103

20
P    -2.547877 -0.188798 -0.287054
O    -2.895981  0.933670  0.805346
O    -1.803020 -1.345378  0.545962
C    -1.832264  1.512734  1.597431
H    -1.228066  0.725625  2.061019
H    -1.206849  2.151176  0.968003
H    -2.327682  2.110210  2.361627
C    -2.457383 -1.884943  1.709949
H    -3.449622 -2.256191  1.442243
H    -1.830077 -2.703877  2.055043
H    -2.527253 -1.122600  2.487132
S    -4.171863 -0.687878 -1.237530
S    -1.027670  0.495885 -1.537386
C     0.505637 -0.016452 -0.658005
C     1.671205  0.868872 -1.166756
O     0.739404  3.130871  0.554370
C     1.744770  3.920032 -0.048909
C     0.846869 -1.481166 -0.987189
C     2.083868 -1.889365 -0.224999
O     3.129286 -2.105497 -1.017884
C     4.363546 -2.371770 -0.343526
O     1.548829  1.433522 -2.258869
O     2.127577 -2.015041  0.983258
H     0.366100  0.094963  0.420483
H     1.267158  4.553753 -0.800581
H     2.242976  4.575180  0.678768
H     2.498645  3.299866 -0.546238
H     0.028296 -2.131085 -0.672713
H     1.012119 -1.590472 -2.060872
H     5.102723 -2.527582 -1.125860
H     4.632423 -1.513728  0.275424
H     4.272603 -3.260449  0.282563
O     2.701692  0.833036 -0.424984
H     2.393231  0.930211  1.101207
O     0.271238 -0.790594  2.785679
H     0.919503 -0.067419  2.685691
H     0.614604 -1.440200  2.154338
O     2.063106  1.192925  2.022041
H     2.837354  1.463706  2.528048
H     1.177979  2.525007  1.181801
    el energy= -2131.39938427
          zpe= -2131.087904
    th energy= -2131.059448
  th enthalpy= -2131.058504
  free energy= -2131.147832

21
```

```
P     2.365353  0.215194 -0.153223
O     2.558307  0.100832  1.434697
O     1.217824  1.324041 -0.354476
C     1.421400 -0.159227  2.295413
H     0.615151  0.556873  2.107021
H     1.054164 -1.176561  2.134823
H     1.794496 -0.058032  3.313576
C     1.409931  2.644887  0.203134
H     2.200953  3.156451 -0.349644
H     0.450749  3.151902  0.095410
H     1.677137  2.567734  1.259554
S     4.083496  0.551930 -1.002367
S     1.413393 -1.481091 -0.888425
C    -0.342577 -1.246791 -0.355329
C    -0.853487 -2.688254 -0.059056
O    -0.976368 -2.976698  1.155963
C    -1.137547 -0.526506 -1.437681
C    -2.492025 -0.144754 -0.885666
O    -2.888373  1.063165 -1.306483
C    -4.085591  1.544705 -0.687273
O    -1.040806 -3.410719 -1.057111
O    -3.163729 -0.852811 -0.170118
H    -0.354037 -0.676577  0.569421
H    -0.623591  0.368690 -1.791523
H    -1.282987 -1.217144 -2.275461
H    -4.255510  2.538064 -1.096281
H    -4.923415  0.881796 -0.909499
H    -3.918637  1.601527  0.389182
O    -1.321267  1.513773  1.293785
H    -0.757453  1.217503  0.570716
O    -1.852481  3.586362 -0.046763
H    -1.696079  2.771899  0.580895
H    -1.911260  3.146593 -0.903036
O    -1.539689 -0.655669  2.800883
H    -1.435090 -1.421579  2.210273
H    -1.533075  0.146967  2.201327
    el energy= -2091.60986289
          zpe= -2091.338720
    th energy= -2091.313590
  th enthalpy= -2091.312646
  free energy= -2091.392724

TS11
P    -2.389556 -0.274031 -0.139355
O    -2.673209  0.071537  1.404896
O    -1.206740 -1.369958 -0.089954
C    -1.603943  0.496755  2.276005
H    -0.764952 -0.202457  2.240976
H    -1.250131  1.491164  1.991009
H    -2.027018  0.522368  3.278761
C    -1.434611 -2.650417  0.537936
H    -2.219304 -3.188513  0.001908
H    -0.482015 -3.178150  0.464514
H    -1.722529 -2.509504  1.582753
S    -4.045420 -0.808614 -1.006933
S    -1.432137  1.309923 -1.077733
C     0.290737  1.194835 -0.399009
C     0.772978  2.670099 -0.317880
O     0.857861  3.148813  0.841872
C     1.162694  0.287558 -1.249942
C     2.442165 -0.068956 -0.498205
O     3.030325 -1.151333 -1.150009
C     4.267752 -1.545320 -0.587105
O     0.979513  3.240811 -1.406601
O     3.142703  0.790988  0.040539
H     0.225296  0.807438  0.610616
H     0.637065 -0.627339 -1.529387
H     1.445708  0.824203 -2.162570
H     4.617977 -2.401021 -1.166383
H     5.000766 -0.736224 -0.636655
H     4.131932 -1.844236  0.457105
O     1.654239 -1.052545  0.946470
H     0.725206 -1.128772  0.691275
O     1.912444 -3.520711  0.099365
H     1.899714 -2.620862  0.538915
H     2.065200 -3.252893 -0.815073
O     1.413088  1.057929  2.704911
H     1.314843  1.803785  2.082396
H     1.618076  0.298963  2.112094
    el energy= -2091.59875318
          zpe= -2091.327555
    th energy= -2091.303010
  th enthalpy= -2091.302066
  free energy= -2091.381194

22
P    -2.333391 -0.211057 -0.026638
O    -2.458871  0.221988  1.515556
O    -1.274366 -1.421404 -0.019199
C    -1.297474  0.582055  2.297597
H    -0.456448 -0.086136  2.089977
H    -1.003167  1.608951  2.073158
H    -1.603343  0.500129  3.339912
C    -1.534971 -2.561244  0.821246
H    -2.528867 -2.965002  0.611947
H    -0.768695 -3.289881  0.562609
H    -1.460946 -2.277631  1.873952
S    -4.109193 -0.609209 -0.727333
S    -1.345999  1.220022 -1.149134
C     0.395224  1.176149 -0.500314
C     0.886857  2.635329 -0.738297
O     0.835073  3.400210  0.260985
C     1.252900  0.091918 -1.136282
C     2.267696 -0.376014 -0.069046
O     3.056827 -1.408389 -0.815996
C     4.099160 -1.950681 -0.034261
O     1.231388  2.922703 -1.901129
O     2.996730  0.550532  0.459898
H     0.342326  1.012904  0.570370
H     0.647928 -0.754374 -1.476092
H     1.785587  0.511692 -1.993701
H     4.752162 -2.526055 -0.695448
H     4.668866 -1.147451  0.441300
H     3.708672 -2.613021  0.749946
```

```
O     1.556744 -1.118415  0.948208
H     1.052400 -1.810989  0.492808
O     1.170301 -3.366258 -0.907935
H     1.571557 -4.081559 -0.401234
H     1.903598 -2.725663 -1.048082
O     1.615037  1.810492  2.431307
H     1.284827  2.478061  1.799760
H     2.140222  1.242128  1.814444
    el energy= -2091.60810378
          zpe= -2091.335781
    th energy= -2091.310839
  th enthalpy= -2091.309895
  free energy= -2091.390211

TS12
P    -2.352443 -0.403322 -0.106399
O    -2.810840  0.337286  1.246605
O    -1.118788 -1.335835  0.324143
C    -1.891600  1.129158  2.025959
H    -1.017861  0.543619  2.322242
H    -1.560700  2.004101  1.457702
H    -2.447019  1.445261  2.907353
C    -1.310023 -2.382787  1.291600
H    -2.174674 -2.993971  1.020658
H    -0.400574 -2.979622  1.249498
H    -1.452721 -1.953111  2.285783
S    -3.891661 -1.282227 -0.911273
S    -1.396263  0.934177 -1.369259
C     0.245759  1.106149 -0.522405
C     0.631200  2.594558 -0.741737
O     0.561323  3.338118  0.275065
C     1.274287  0.102883 -1.041138
C     2.306056 -0.050121  0.066087
O     3.294550 -1.489567 -0.979714
C     4.423521 -1.785021 -0.231380
O     0.925805  2.920073 -1.906064
O     3.090589  0.864000  0.337004
H     0.087048  0.931880  0.538709
H     0.809719 -0.862489 -1.248874
H     1.747772  0.490415 -1.944048
H     5.284926 -2.062807 -0.863324
H     4.735480 -0.917028  0.376475
H     4.266392 -2.624515  0.473732
O     1.911860 -0.854022  1.098855
H     1.546525 -1.688818  0.713753
O     1.545052 -3.081221 -0.321903
H     1.969906 -3.800073  0.159305
H     2.341797 -2.475549 -0.706703
O     1.247584  1.861209  2.482717
H     0.965345  2.456205  1.753199
H     1.939808  1.335901  2.053450
    el energy= -2091.59812135
          zpe= -2091.329229
    th energy= -2091.304441
  th enthalpy= -2091.303496
  free energy= -2091.383965

23
P     2.285953 -0.056876 -0.212207
O     2.511951 -0.657421  1.258875
O     1.421041  1.276578  0.006318
C     1.385133 -0.993840  2.104503
H     0.690407 -0.151858  2.180134
H     0.864997 -1.865745  1.698143
H     1.809953 -1.226475  3.080148
C     1.902835  2.255906  0.946450
H     2.954568  2.481635  0.750098
H     1.292540  3.142719  0.789024
H     1.771967  1.887883  1.965315
S     4.012096  0.148486 -1.096633
S     0.979343 -1.230995 -1.306724
C    -0.675142 -0.978232 -0.498101
C    -1.295323 -2.406372 -0.437812
O    -0.955563 -3.110601  0.554355
C    -1.515206  0.026953 -1.261909
C    -2.895222  0.205420 -0.603835
O    -0.786682  3.284853 -0.416264
C    -2.158448  3.592943 -0.545450
O    -2.040466 -2.727531 -1.379222
O    -3.877938  0.382254 -1.335352
H    -0.502120 -0.628233  0.517319
H    -1.013205  1.003891 -1.257918
H    -1.659504 -0.296096 -2.293950
H    -2.253572  4.492062 -1.160742
H    -2.722600  2.784952 -1.032082
H    -2.628721  3.796039  0.426182
O    -2.921214  0.201959  0.678944
H    -1.693980  1.009514  1.322079
O    -0.931436  1.556421  1.680369
H    -1.294033  2.030314  2.437878
H    -0.722185  2.619219  0.302612
O    -1.671713 -1.467904  2.652650
H    -1.359048 -2.152962  2.028489
H    -2.163386 -0.879100  2.055629
    el energy= -2091.64131383
          zpe= -2091.369963
    th energy= -2091.344017
  th enthalpy= -2091.343073
  free energy= -2091.425853

1
P    -2.135421 -0.794709  0.129112
O    -3.467321 -0.933894 -0.746127
O    -2.487672  0.179232  1.349381
C    -4.390958  0.164360 -0.887555
H    -4.753366  0.475491  0.093575
H    -3.916323  1.000830 -1.406993
H    -5.215367 -0.214949 -1.486975
C    -2.375191  1.618678  1.348372
H    -2.896505  2.056219  0.496164
H    -2.842680  1.944191  2.275513
H    -1.323979  1.910260  1.330310
S    -1.465469 -2.502721  0.743316
S    -0.902893  0.269448 -1.200113
```

```
C     0.673123  0.228109 -0.238751
C     1.297232  1.606981 -0.385157
O     0.907914  2.427618  0.586556
C     1.410889  3.769165  0.498113
C     1.603499 -0.847077 -0.774624
C     2.886890 -0.854237  0.023544
O     3.713946 -1.814747 -0.381216
C     4.964487 -1.887345  0.317310
O     2.028209  1.917195 -1.294631
O     3.134593 -0.078753  0.921005
H     0.443953  0.060362  0.816337
H     0.995099  4.296354  1.352917
H     2.500652  3.759781  0.542057
H     1.085714  4.229055 -0.436027
H     1.131187 -1.830988 -0.709356
H     1.844232 -0.656990 -1.824518
H     5.508782 -2.712157 -0.136000
H     5.514687 -0.952564  0.200126
H     4.791842 -2.076897  1.377671
    el energy= -1902.63611600
          zpe= -1902.389196
    th energy= -1902.367687
  th enthalpy= -1902.366743
  free energy= -1902.442919

24
P     2.511005 -0.065557 -0.106191
O     2.633193 -0.321312  1.467313
O     1.615092  1.258777 -0.251411
C     1.457403 -0.376493  2.310585
H     0.807373  0.486473  2.137755
H     0.907694 -1.301293  2.119686
H     1.829322 -0.374432  3.333654
C     2.066891  2.501633  0.341567
H     2.966648  2.838921 -0.176286
H     1.240533  3.200469  0.208232
H     2.271440  2.352866  1.404007
S     4.261379 -0.073844 -0.935974
S     1.233707 -1.474981 -0.983255
C    -0.460224 -0.928134 -0.480331
C    -1.299141 -2.196779 -0.522609
O    -1.376683 -2.771667  0.674149
C    -2.119603 -3.997798  0.716180
C    -1.035520  0.127354 -1.415796
C    -2.320758  0.643787 -0.809985
O    -2.599507  1.883870 -1.201544
C    -3.678320  2.513751 -0.499454
O    -1.798395 -2.641128 -1.529345
O    -3.033903 -0.016007 -0.082439
H    -0.450872 -0.571406  0.551205
H    -2.084762 -4.328671  1.751128
H    -3.149274 -3.820479  0.402245
H    -1.660160 -4.737141  0.058472
H    -0.339480  0.953516 -1.559369
H    -1.254912 -0.320958 -2.390364
H    -3.753531  3.517810 -0.910297
H    -4.606082  1.960444 -0.649904
H    -3.421032  2.552487  0.560292
O    -0.867130  1.886310  1.300211
H    -0.256207  1.512522  0.656763
O    -0.989501  4.061100 -0.014504
H    -0.997622  3.226855  0.585204
H    -1.186902  3.678032 -0.876811
O    -1.644573 -0.194683  2.546775
H    -2.232322 -0.622108  1.912711
H    -1.389426  0.674650  2.067634
    el energy= -2131.36328640
          zpe= -2131.052007
    th energy= -2131.024485
  th enthalpy= -2131.023541
  free energy= -2131.109442

TS13
P    -2.536519 -0.000113 -0.087092
O    -2.678242  0.413713  1.454472
O    -1.587644 -1.300882 -0.070565
C    -1.513455  0.585827  2.289543
H    -0.827431 -0.257954  2.186097
H    -0.995352  1.511067  2.026664
H    -1.882345  0.643798  3.311647
C    -2.048702 -2.530762  0.537713
H    -2.939978 -2.884640  0.016479
H    -1.223053 -3.234059  0.417252
H    -2.268333 -2.363769  1.594728
S    -4.279545 -0.167577 -0.912528
S    -1.304998  1.351411 -1.099739
C     0.387861  0.890686 -0.509137
C     1.207817  2.164136 -0.628307
O     1.316106  2.786620  0.546497
C     2.055510  4.014489  0.520341
C     1.020776 -0.243667 -1.300096
C     2.222257 -0.733230 -0.500045
O     2.712538 -1.879902 -1.085452
C     3.844245 -2.421961 -0.423088
O     1.664811  2.586204 -1.664028
O     2.976317  0.076971  0.056365
H     0.343723  0.633268  0.547370
H     2.047059  4.386730  1.541854
H     3.077391  3.826957  0.186948
H     1.577497  4.726581 -0.154021
H     0.315474 -1.054377 -1.478739
H     1.374412  0.135498 -2.264662
H     4.118164 -3.327029 -0.965570
H     4.676535 -1.714669 -0.427393
H     3.586798 -2.675048  0.609721
O     1.252609 -1.574286  0.930987
H     0.324837 -1.484095  0.677855
O     1.109298 -4.043835  0.001959
H     1.239623 -3.179445  0.477293
H     1.367155 -3.787365 -0.891704
O     1.590717  0.459864  2.596348
H     2.069826  0.998347  1.951883
H     1.508542 -0.388277  2.084740
    el energy= -2131.35419634
```

```
          zpe= -2131.042552
    th energy= -2131.015679
  th enthalpy= -2131.014735
  free energy= -2131.098936

25
P     2.509212 -0.046286 -0.043299
O     2.564645 -0.504213  1.493350
O     1.650357  1.309024 -0.028487
C     1.369886 -0.563433  2.302381
H     0.712176  0.282443  2.084493
H     0.836213 -1.496744  2.113191
H     1.704056 -0.526997  3.338003
C     2.128432  2.435667  0.734209
H     3.128789  2.716315  0.396712
H     1.419862  3.237081  0.533906
H     2.147719  2.189517  1.798576
S     4.302407  0.023577 -0.783067
S     1.262270 -1.291689 -1.154835
C    -0.421258 -0.834647 -0.525830
C    -1.269969 -2.074201 -0.741633
O    -1.280979 -2.852202  0.342240
C    -2.036669 -4.060166  0.216630
C    -1.037698  0.386672 -1.187534
C    -2.085347  0.893754 -0.173317
O    -2.749740  1.994200 -0.891959
C    -3.797218  2.575407 -0.139337
O    -1.814536 -2.363774 -1.782009
O    -2.890399 -0.029832  0.261339
H    -0.359469 -0.675002  0.548621
H    -1.944147 -4.570365  1.172728
H    -3.082291 -3.828571  0.005859
H    -1.635032 -4.677853 -0.588677
H    -0.282163  1.145688 -1.398620
H    -1.530337  0.095974 -2.118783
H    -4.378386  3.208290 -0.813323
H    -4.434680  1.791380  0.277500
H    -3.405150  3.187149  0.682731
O    -1.376001  1.520214  0.928612
H    -0.832294  2.233373  0.553733
O    -0.583469  3.687462 -0.793039
H    -0.875504  4.503404 -0.370310
H    -1.410718  3.223949 -1.041329
O    -1.754291 -0.668219  2.612911
H    -2.231028 -0.595046  1.745194
H    -1.446263  0.244505  2.678650
    el energy= -2131.36499484
          zpe= -2131.051956
    th energy= -2131.024679
  th enthalpy= -2131.023735
  free energy= -2131.110166

TS14
P    -2.555899 -0.194506 -0.168308
O    -3.036831  0.672430  1.092980
O    -1.467149 -1.217337  0.410981
C    -2.083521  1.369093  1.920503
H    -1.308228  0.695420  2.292707
H    -1.620453  2.181781  1.351942
H    -2.654702  1.782499  2.749447
C    -1.854483 -2.254098  1.335723
H    -2.713685 -2.802797  0.943075
H    -0.986475 -2.907350  1.403425
H    -2.099162 -1.813804  2.304627
S    -4.089852 -0.923496 -1.102378
S    -1.327703  0.977347 -1.391179
C     0.291220  0.811258 -0.513070
C     1.039105  2.107832 -0.761548
O     1.265342  2.775382  0.375326
C     2.027227  3.984391  0.233922
C     1.106131 -0.384730 -1.008544
C     2.264264 -0.545460 -0.034806
O     2.880351 -2.225549 -1.015552
C     4.069548 -2.596201 -0.399701
O     1.376881  2.500181 -1.851871
O     3.173409  0.279157 -0.003126
H     0.101306  0.710172  0.555547
H     2.110904  4.399495  1.235120
H     3.012516  3.751154 -0.172361
H     1.509199  4.676190 -0.430811
H     0.479076 -1.275845 -1.021328
H     1.497290 -0.187305 -2.007619
H     4.770088 -3.073743 -1.104471
H     4.584717 -1.717618  0.026556
H     3.916030 -3.309851  0.431127
O     1.935454 -1.184149  1.135077
H     1.432340 -2.023853  0.907997
O     1.049748 -3.375432  0.092114
H     1.382103 -4.142432  0.571921
H     1.881309 -2.984068 -0.499123
O     1.049649  0.945996  2.736350
H     1.340819  1.643789  2.134200
H     1.412600  0.136195  2.336435
    el energy= -2131.34997153
          zpe= -2131.041106
    th energy= -2131.014068
  th enthalpy= -2131.013124
  free energy= -2131.099925

26
P     1.503184 -1.581373 -0.059082
O     0.963855 -2.741498  0.914435
O     1.483980 -0.256306  0.842839
C    -0.297835 -2.600952  1.595860
H    -0.338848 -1.669316  2.166785
H    -1.118132 -2.625313  0.871225
H    -0.373190 -3.455847  2.265100
C     2.363412 -0.186939  1.986729
H     3.401454 -0.273220  1.656640
H     2.184492  0.793552  2.421753
H     2.125246 -0.987589  2.690967
S     3.181877 -2.123128 -0.864379
S     0.027566 -1.131522 -1.466206
C    -1.048129  0.033638 -0.505454
```

```
C    -2.461776 -0.226093 -0.984999
O    -3.115434 -1.064224 -0.168366
C    -4.450772 -1.396184 -0.574479
C    -0.629459  1.477025 -0.712167
C    -1.378008  2.389790  0.270396
O     2.731469  1.926214 -0.907487
C     2.458892  3.167580 -1.523644
O    -2.930058  0.212256 -2.007666
O    -2.493580  1.980235  0.683582
H    -0.990685 -0.233423  0.548689
H    -4.828217 -2.081479  0.180580
H    -5.062001 -0.493520 -0.615974
H    -4.435854 -1.872607 -1.555557
H     0.449139  1.571385 -0.580765
H    -0.872278  1.786398 -1.735707
H     2.583953  3.049779 -2.603133
H     1.431019  3.503621 -1.327873
H     3.143274  3.958369 -1.185803
O    -0.823804  3.476890  0.576390
H     0.736426  3.131586  1.097153
O     1.626050  2.840686  1.428925
H     2.105678  3.654811  1.619369
H     2.437486  2.034572  0.018642
O    -2.279202 -0.111775  2.510117
H    -2.744426 -0.753395  1.958673
H    -2.377539  0.709610  1.989222
    el energy= -2131.39090727
          zpe= -2131.079938
    th energy= -2131.050986
  th enthalpy= -2131.050042
  free energy= -2131.140937

27
P     2.550717 -0.023001 -0.069865
O     2.692649 -0.789421  1.328361
O     1.750423  1.328059  0.262043
C     1.512628 -1.184448  2.068203
H     0.799989 -0.358387  2.168489
H     1.029828 -2.021244  1.557598
H     1.874675 -1.499922  3.045740
C     2.234706  2.180237  1.317596
H     3.241491  2.533293  1.082814
H     1.543627  3.019196  1.362755
H     2.235249  1.641091  2.267051
S     4.298893  0.158308 -0.899444
S     1.166980 -1.008741 -1.279851
C    -0.469998 -0.236389 -0.820863
C    -1.424427 -1.413429 -0.678796
O    -1.286011 -2.011274  0.508769
C    -2.243491 -3.040377  0.779688
C    -0.899182  0.749189 -1.900207
C    -2.074381  1.636951 -1.410277
O    -3.228180  1.329250 -1.797222
O    -2.160713 -1.806394 -1.551405
O    -1.746957  2.584377 -0.657115
H    -0.366570  0.251167  0.153309
H    -1.997087 -3.420316  1.769394
H    -3.237174 -2.590726  0.766597
H    -2.168583 -3.835619  0.036028
H    -0.049724  1.401798 -2.113716
H    -1.174684  0.197348 -2.801928
O    -3.050681  1.938075  1.908231
H    -2.706037  2.363661  1.108194
O    -1.144839  0.439174  2.413333
H    -1.470461 -0.316021  1.905175
H    -1.931554  1.149386  2.235602
O    -3.588801 -0.200152  0.628837
H    -3.442616  0.667357  1.174702
H    -3.605339  0.125934 -0.283835
    el energy= -2091.59333417
          zpe= -2091.324192
    th energy= -2091.298812
  th enthalpy= -2091.297868
  free energy= -2091.379638

TS15
P    -2.495487 -0.064137 -0.024151
O    -2.565219  0.414389  1.505087
O    -1.606941 -1.393389 -0.028090
C    -1.377976  0.814166  2.229808
H    -0.635226  0.009289  2.259313
H    -0.935840  1.695160  1.757405
H    -1.721790  1.058111  3.234047
C    -1.759281 -2.421712  0.961380
H    -2.699465 -2.955817  0.803950
H    -0.903898 -3.077095  0.810060
H    -1.735965 -1.993647  1.965800
S    -4.301754 -0.198600 -0.741173
S    -1.243281  1.191612 -1.111533
C     0.430140  0.457354 -0.671059
C     1.375141  1.650254 -0.545084
O     1.056797  2.402802  0.538701
C     1.989904  3.441598  0.799972
C     0.859762 -0.562309 -1.725867
C     1.767684 -1.671433 -1.144842
O     2.965297 -1.697897 -1.535889
O     2.024384  2.088675 -1.479465
O     1.231756 -2.474500 -0.341982
H     0.325083 -0.015613  0.301571
H     1.677478  3.909791  1.733117
H     2.983180  2.998294  0.902875
H     1.994767  4.179711 -0.005790
H    -0.033955 -1.060579 -2.106977
H     1.361244 -0.041004 -2.543961
O     2.824008  0.478620  0.575043
H     3.112095  0.030036 -0.229344
O     1.318632 -1.030724  2.061120
H     1.923840 -0.420006  1.513167
H     1.154032 -1.717396  1.392621
O     4.345027 -1.870952  0.910094
H     3.902616 -1.020330  1.096906
H     3.922522 -2.088752  0.058023
    el energy= -2091.59252713
          zpe= -2091.321553
```

th energy= -2091.297016
th enthalpy= -2091.296071
free energy= -2091.374800

28

P	2.276774	-0.322460	-0.163658
O	2.298225	-1.196076	1.188885
O	1.791675	1.137903	0.306697
C	1.084189	-1.338612	1.960594
H	0.705135	-0.355379	2.256127
H	0.326828	-1.866440	1.372720
H	1.358913	-1.923202	2.837607
C	2.482162	1.786460	1.387631
H	3.497633	2.045413	1.077494
H	1.910088	2.682666	1.615839
H	2.509134	1.138256	2.265832
S	4.035814	-0.426935	-1.005206
S	0.714464	-0.941784	-1.370889
C	-0.700078	0.050687	-0.699420
C	-1.949641	-0.865260	-0.885819
O	-1.722854	-1.905283	0.210189
C	-2.692548	-2.925567	0.162093
C	-0.821760	1.354968	-1.481763
C	-1.571862	2.497853	-0.764391
O	-1.598520	3.592425	-1.345627
O	-2.083137	-1.388287	-2.042997
O	-2.097640	2.239903	0.371649
H	-0.512980	0.260426	0.356138
H	-2.396037	-3.710865	0.862888
H	-3.682957	-2.546626	0.450292
H	-2.757382	-3.336883	-0.849357
H	0.169036	1.749846	-1.721411
H	-1.320608	1.145743	-2.435148
O	-3.091557	-0.129070	-0.432189
H	-2.778002	0.683690	0.026457
O	-0.537684	1.526383	2.554503
H	-1.128174	0.757974	2.676075
H	-0.924577	1.919164	1.748695
O	-2.333943	-0.626689	2.452984
H	-3.093884	-0.154177	2.090319
H	-2.017540	-1.126039	1.655534

el energy= -2091.61315503
zpe= -2091.341908
th energy= -2091.316820
th enthalpy= -2091.315876
free energy= -2091.396795

TS16

P	2.301234	-0.194734	-0.251587
O	2.411609	-1.159132	1.026899
O	1.806391	1.216170	0.338023
C	1.239019	-1.392313	1.846649
H	0.830278	-0.441034	2.201066
H	0.478413	-1.928636	1.270607
H	1.585556	-1.996438	2.684559
C	2.517452	1.791704	1.447759
H	3.574817	1.907505	1.195585
H	2.063184	2.764302	1.623156
H	2.397130	1.169284	2.335134
S	4.010174	-0.198077	-1.195984
S	0.700955	-0.756976	-1.441863
C	-0.726630	0.128743	-0.660979
C	-1.965906	-0.725767	-0.959951
O	-1.495023	-2.129428	0.347007
C	-2.422842	-3.151541	0.188671
C	-0.889786	1.508299	-1.300693
C	-1.947803	2.396715	-0.607397
O	-2.691880	3.067660	-1.347206
O	-2.102337	-1.264790	-2.056984
O	-1.941207	2.404393	0.657857
H	-0.552624	0.229556	0.412021
H	-1.979491	-4.143194	0.374656
H	-3.286761	-3.052274	0.871488
H	-2.821678	-3.158155	-0.839384
H	0.068062	2.034730	-1.233880
H	-1.143234	1.395955	-2.358463
O	-3.087332	-0.271320	-0.320518
H	-2.844709	-0.031065	0.597567
O	-0.382373	1.388132	2.631826
H	-0.975639	0.616685	2.708925
H	-0.779548	1.829954	1.849387
O	-2.111183	-0.722052	2.256374
H	-2.777858	-1.159237	2.795726
H	-1.806808	-1.408192	1.500632

el energy= -2091.60468867
zpe= -2091.335498
th energy= -2091.310930
th enthalpy= -2091.309986
free energy= -2091.388978

29

P	2.266679	0.024972	-0.277305
O	2.309428	-1.295494	0.640828
O	1.766590	1.184442	0.708626
C	1.127930	-1.689827	1.370357
H	0.719861	-0.844148	1.931492
H	0.376260	-2.085710	0.682765
H	1.445133	-2.481187	2.048441
C	2.422202	1.381312	1.979318
H	3.055093	2.266800	1.910384
H	1.620326	1.508924	2.705334
H	3.028084	0.511453	2.244630
S	4.005382	0.257497	-1.127728
S	0.694414	-0.106203	-1.626606
C	-0.769654	0.507309	-0.656357
C	-2.003573	-0.194878	-1.268731
O	-1.351181	-3.793161	0.662347
C	-1.587282	-3.503416	-0.699217
C	-0.910431	2.021489	-0.812171
C	-2.143205	2.543550	-0.038873
O	-3.075760	3.026731	-0.708607
O	-2.052966	-0.273037	-2.505228
O	-2.100987	2.436088	1.221366
H	-0.633777	0.250921	0.395415

```
H    -1.415494 -4.417458 -1.274471
H    -2.611280 -3.156722 -0.882147
H    -0.907775 -2.727818 -1.086395
H    -0.010068  2.501430 -0.417881
H    -1.015402  2.259742 -1.873217
O    -2.890977 -0.578377 -0.447202
H    -2.418679 -0.992919  0.926798
O    -0.616202  0.839180  2.794950
H    -1.110988  0.024741  2.597985
H    -1.037336  1.487087  2.180125
O    -2.068757 -1.393283  1.804215
H    -2.847746 -1.526377  2.357889
H    -1.602557 -2.991976  1.165443
   el energy= -2091.63889455
         zpe= -2091.368357
   th energy= -2091.342345
 th enthalpy= -2091.341401
 free energy= -2091.424724
```

```
30
P     1.174309  1.187616  0.060690
O     1.806572  0.389468  1.291221
O     0.140018  2.115261  0.876496
C     1.333421 -0.916255  1.695065
H     0.279977 -0.871516  1.982975
H     1.492874 -1.626363  0.880705
H     1.952546 -1.186800  2.548833
C    -0.797764  2.966516  0.190353
H    -1.799518  2.544160  0.323371
H    -0.731848  3.952283  0.651197
H    -0.554302  3.050503 -0.872536
S     2.525957  2.163240 -0.958434
S     0.039799 -0.054145 -1.149691
C    -1.508249 -0.266856 -0.149708
C    -1.649997 -1.750125  0.278287
O    -1.955955 -1.941807  1.473938
C    -2.717305  0.174915 -0.971661
C    -3.925766  0.403608 -0.026479
O    -4.948926 -0.287852 -0.220218
O    -1.484645 -2.604210 -0.628975
O    -3.748806  1.282632  0.857354
H    -1.432543  0.369968  0.732170
H    -2.498636  1.124590 -1.472483
H    -2.944627 -0.578514 -1.730424
O     3.174579 -1.540625 -0.939952
H     2.910318 -0.721181 -1.372499
O     1.357123 -3.327801 -0.752049
H     2.028261 -2.564318 -0.873168
H     0.474974 -2.928061 -0.790508
O     4.403747 -0.898229  1.164414
H     3.898537 -1.161988  0.289139
H     3.901557 -0.128029  1.449921
   el energy= -2051.82769475
         zpe= -2051.600330
   th energy= -2051.576169
 th enthalpy= -2051.575225
 free energy= -2051.655192
```

```
TS17
P    -1.367521 -0.948042  0.088366
O    -1.918572 -0.107800  1.337442
O    -0.398399 -1.927519  0.973371
C    -1.379351  1.186322  1.661543
H    -0.356672  1.082233  2.035756
H    -1.404150  1.833866  0.783395
H    -2.030541  1.586766  2.437787
C     0.286051 -3.006752  0.341202
H     0.867463 -2.655513 -0.518488
H     0.965527 -3.423351  1.085020
H    -0.426260 -3.767483  0.012394
S    -2.707435 -2.061477 -0.832970
S     0.011236  0.072399 -1.105137
C     1.574127  0.069983 -0.120759
C     1.770702  1.466899  0.529378
O     2.111531  1.464322  1.732938
C     2.748678 -0.248941 -1.044625
C     4.027140 -0.482046 -0.194229
O     4.986546  0.301707 -0.379942
O     1.607088  2.464019 -0.219355
O     3.967651 -1.447116  0.606879
H     1.514304 -0.693318  0.653282
H     2.538272 -1.166136 -1.607238
H     2.897384  0.573303 -1.750244
O    -2.664839  1.110641 -1.013370
H    -3.027260  0.690547 -1.801073
O    -1.098435  3.192938 -1.133149
H    -1.694183  2.381847 -1.173686
H    -0.226392  2.835122 -0.896821
O    -4.385232  1.322545  0.838222
H    -3.726905  1.257069  0.047601
H    -4.061384  0.608243  1.397182
   el energy= -2051.82394864
         zpe= -2051.596574
   th energy= -2051.573107
 th enthalpy= -2051.572163
 free energy= -2051.650527
```

```
31
P    -1.613893 -0.736390 -0.031919
O    -2.089419  0.173779  1.259387
O    -0.588386 -1.600691  1.043409
C    -1.182856  1.162558  1.753236
H    -0.235300  0.709468  2.056072
H    -0.995493  1.925085  0.989952
H    -1.666456  1.622604  2.617473
C     0.084352 -2.757079  0.605227
H     0.491220 -2.642691 -0.409480
H     0.924716 -2.934092  1.284713
H    -0.579218 -3.628261  0.612605
S    -2.853172 -2.285768 -0.508210
S     0.053904 -0.028005 -1.196322
C     1.575096 -0.012832 -0.173047
C     1.786880  1.377931  0.485562
O     2.221965  1.362711  1.656880
```

```
C     2.776627 -0.351882 -1.062406
C     4.050239 -0.567759 -0.202677
O     4.998338  0.233836 -0.377337
O     1.553393  2.400261 -0.217416
O     4.009190 -1.540698  0.590803
H     1.490934 -0.764199  0.607679
H     2.568543 -1.282053 -1.604843
H     2.939826  0.449256 -1.790134
O    -2.474812  0.390666 -1.129475
H    -3.274650 -0.069311 -1.420608
O    -1.001144  3.049596 -1.175798
H    -1.448786  2.201283 -1.313183
H    -0.103201  2.770161 -0.898798
O    -3.934217  2.190256  0.526991
H    -3.350447  1.740121 -0.109767
H    -3.866297  1.585501  1.274709
    el energy= -2051.84225217
          zpe= -2051.612692
    th energy= -2051.588542
  th enthalpy= -2051.587598
  free energy= -2051.666190

32
P    -1.641090 -0.477370 -0.189028
O    -3.155431 -0.534340  0.713074
O    -0.955164 -1.419232  0.973246
C    -3.126237 -0.345333  2.118620
H    -2.720741 -1.222723  2.629001
H    -2.526168  0.527305  2.408459
H    -4.155444 -0.182659  2.454381
C    -0.472954 -2.719583  0.667078
H     0.268272 -2.682849 -0.136262
H    -0.011995 -3.101019  1.579688
H    -1.297492 -3.378029  0.374648
S    -2.542176 -1.168809 -1.867545
S     0.386194 -0.313205 -1.275974
C     1.741317 -0.194611 -0.023276
C     1.829697  1.215570  0.595992
O     1.324879  1.392137  1.723477
C     3.036784 -0.579031 -0.726111
C     4.286780 -0.600930  0.184753
O     5.392480 -0.620146 -0.413560
O     2.404961  2.099967 -0.112430
O     4.100031 -0.629602  1.425935
H     1.521445 -0.903717  0.777288
H     2.938222 -1.574970 -1.179485
H     3.227612  0.123256 -1.542340
O    -1.500145  1.118331  0.149853
H    -2.381246  1.508794  0.352796
O     0.110758  3.240243 -1.078167
H    -0.396121  2.443709 -0.857804
H     1.003750  2.974312 -0.773211
O    -4.147490  1.919250  0.223474
H    -4.546054  2.209255  1.052228
H    -4.183317  0.942749  0.250786
    el energy= -2051.84336385
          zpe= -2051.613998
    th energy= -2051.589771
  th enthalpy= -2051.588826
  free energy= -2051.668873

TS18
P    -1.963656 -0.500477 -0.109965
O    -3.437349 -0.540803  0.705393
O    -1.120107 -1.189887  1.081108
C    -3.466157 -0.140434  2.075035
H    -2.956681 -0.873023  2.704168
H    -2.995769  0.838657  2.218576
H    -4.516066 -0.076184  2.367305
C    -0.538494 -2.482863  0.912848
H     0.125512 -2.473106  0.045055
H     0.026466 -2.680242  1.824024
H    -1.319585 -3.238763  0.792465
S    -2.524737 -1.442494 -1.762954
S     0.546457 -0.271257 -1.280401
C     1.936453 -0.182236 -0.052772
C     2.056772  1.226011  0.563076
O     1.558552  1.420347  1.694953
C     3.236645 -0.602864 -0.726741
C     4.486113 -0.659787  0.181504
O     5.589799 -0.741380 -0.419117
O     2.634856  2.108695 -0.146771
O     4.310640 -0.651240  1.425391
H     1.707679 -0.871805  0.765920
H     3.115124 -1.595578 -1.182423
H     3.451994  0.088548 -1.546500
O    -1.778679  1.093214 -0.032176
H    -2.672634  1.533786 -0.005131
O     0.194942  3.130880 -0.957246
H    -0.185578  2.237479 -0.941928
H     1.120073  2.933805 -0.703426
O    -4.303215  1.951809 -0.141089
H    -4.664542  2.465458  0.591478
H    -4.592179  1.038095  0.012305
    el energy= -2051.83877832
          zpe= -2051.609525
    th energy= -2051.586044
  th enthalpy= -2051.585099
  free energy= -2051.662898

33
P     2.648265 -0.541876  0.064677
O     3.968803 -0.640784 -0.851592
O     1.586882 -1.433923 -0.716038
C     3.845505 -0.371673 -2.261915
H     3.165442 -1.090190 -2.722163
H     3.479926  0.645100 -2.423181
H     4.844199 -0.478215 -2.680889
C     0.698916 -2.354455 -0.051097
H     0.049049 -1.809838  0.640896
H     0.112952 -2.815110 -0.845003
H     1.278504 -3.115064  0.475018
S     3.054884 -1.056757  1.891977
S    -1.348142  0.190520  1.847850
```

```
C    -2.391388 -0.204328  0.356009
C    -2.222556  0.893988 -0.712381
O    -1.362082  0.719864 -1.605878
C    -3.855065 -0.401231  0.722973
C    -4.779719 -0.821753 -0.444068
O    -6.013779 -0.662661 -0.250076
O    -2.954453  1.927348 -0.592011
O    -4.244819 -1.313778 -1.470443
H    -2.013930 -1.132139 -0.083825
H    -3.940113 -1.168023  1.506432
H    -4.248199  0.524978  1.150758
O     2.118796  0.932588 -0.180841
H     2.885636  1.581285 -0.143141
O    -0.878204  3.257982  0.655894
H    -0.762912  2.417019  1.136687
H    -1.659273  3.013027  0.119549
O     4.343533  2.274070 -0.165816
H     4.485312  2.909197 -0.879228
H     4.999985  1.576967 -0.302016
   el energy= -2051.85474371
         zpe= -2051.626573
   th energy= -2051.602052
 th enthalpy= -2051.601107
 free energy= -2051.684753

1
P    -2.135421 -0.794709  0.129112
O    -3.467321 -0.933894 -0.746127
O    -2.487672  0.179232  1.349381
C    -4.390958  0.164360 -0.887555
H    -4.753366  0.475491  0.093575
H    -3.916323  1.000830 -1.406993
H    -5.215367 -0.214949 -1.486975
C    -2.375191  1.618678  1.348372
H    -2.896505  2.056219  0.496164
H    -2.842680  1.944191  2.275513
H    -1.323979  1.910260  1.330310
S    -1.465469 -2.502721  0.743316
S    -0.902893  0.269448 -1.200113
C     0.673123  0.228109 -0.238751
C     1.297232  1.606981 -0.385157
O     0.907914  2.427618  0.586556
C     1.410889  3.769165  0.498113
C     1.603499 -0.847077 -0.774624
C     2.886890 -0.854237  0.023544
O     3.713946 -1.814747 -0.381216
C     4.964487 -1.887345  0.317310
O     2.028209  1.917195 -1.294631
O     3.134593 -0.078753  0.921005
H     0.443953  0.060362  0.816337
H     0.995099  4.296354  1.352917
H     2.500652  3.759781  0.542057
H     1.085714  4.229055 -0.436027
H     1.131187 -1.830988 -0.709356
H     1.844232 -0.656990 -1.824518
H     5.508782 -2.712157 -0.136000
H     5.514687 -0.952564  0.200126
H     4.791842 -2.076897  1.377671
   el energy= -1902.63611600
         zpe= -1902.389196
   th energy= -1902.367687
 th enthalpy= -1902.366743
 free energy= -1902.442919

34
P    -2.100933 -1.116381 -0.091596
O    -2.661223 -0.238540  1.127779
O    -1.171454 -2.222093  0.625149
C    -1.737048  0.508877  1.960549
H    -0.958720 -0.156442  2.346231
H    -1.313230  1.337986  1.375909
H    -2.336357  0.880756  2.790856
C    -1.778591 -3.070099  1.620443
H    -2.563768 -3.676163  1.163245
H    -0.983455 -3.709252  1.997927
H    -2.194147 -2.465156  2.429155
S    -3.562073 -1.773472 -1.186093
S    -0.667535 -0.073913 -1.184374
C     0.869435 -0.256273 -0.178068
C     1.413247  1.140807  0.073191
O     1.257856  1.521545  1.327765
C     1.673242  2.864490  1.615810
C     1.869397 -1.094735 -0.965032
C     3.169652 -1.230806 -0.207697
O     4.007109 -2.068189 -0.818367
C     5.277660 -2.244056 -0.177807
O     1.950084  1.793469 -0.797303
O     3.427994 -0.648995  0.822526
H     0.627884 -0.735216  0.769494
H     1.325106  3.066351  2.627019
H     2.763203  2.926123  1.572351
H     1.217384  3.544498  0.896950
H     1.461465 -2.088924 -1.162778
H     2.084153 -0.626919 -1.931188
H     5.827528 -2.947040 -0.798852
H     5.804065 -1.290272 -0.118089
H     5.139746 -2.645397  0.827307
O    -1.045069  2.978454  0.118953
H    -1.263874  3.558640  0.859384
O     0.585102  4.384018 -1.237759
H    -0.122231  3.838024 -0.727994
H     1.283674  3.725563 -1.332698
O    -3.259318  2.024752 -0.712036
H    -2.363510  2.422469 -0.392208
H    -3.517800  1.439656  0.007404
   el energy= -2131.35188369
         zpe= -2131.042721
   th energy= -2131.014454
 th enthalpy= -2131.013510
 free energy= -2131.102864

TS19
P    -1.868320 -0.956621 -0.144852
O    -1.582622 -0.514116  1.375840
```

```
O    -1.632115 -2.575343 -0.026114
C    -0.866314 -1.288336  2.353181
H    -0.504550 -2.229925  1.938781
H    -0.030124 -0.676931  2.693786
H    -1.549521 -1.489634  3.179847
C    -2.624541 -3.364929  0.640082
H    -3.495849 -3.492770 -0.005212
H    -2.163066 -4.330284  0.846969
H    -2.939662 -2.903339  1.581394
S    -3.656553 -0.646735 -0.879856
S    -0.259962 -0.643337 -1.471766
C     1.145645 -0.397787 -0.319831
C     1.233658  1.052153  0.130586
O     0.885345  1.212862  1.399315
C     0.929265  2.566143  1.876374
C     2.407453 -0.766239 -1.097263
C     3.635604 -0.602131 -0.232358
O     4.735910 -0.997577 -0.870588
C     5.956973 -0.871102 -0.129780
O     1.641358  1.936616 -0.590460
O     3.628246 -0.165314  0.896768
H     1.035850 -1.050674  0.547032
H     0.517454  2.535378  2.883091
H     1.963749  2.915402  1.898789
H     0.333305  3.203493  1.219680
H     2.359140 -1.797885 -1.453387
H     2.517390 -0.116920 -1.971752
H     6.742209 -1.231069 -0.790111
H     6.127941  0.172619  0.137946
H     5.910523 -1.475496  0.777315
O    -1.596654  1.625742 -0.071017
H    -1.459575  1.644722  0.883342
O    -0.551876  3.855847 -0.848525
H    -0.982503  2.974579 -0.576880
H     0.363431  3.582399 -0.981674
O    -3.957996  2.694072 -0.228952
H    -4.487686  1.923183 -0.459548
H    -3.032646  2.284686 -0.166748
    el energy= -2131.33907446
          zpe= -2131.029573
    th energy= -2131.002034
  th enthalpy= -2131.001090
  free energy= -2131.087996

35
P    -1.932826 -0.662632 -0.145004
O    -3.291688 -0.512116  0.907144
O    -1.043039 -1.427052  1.004591
C    -3.122460  0.230269  2.110930
H    -2.100239  0.158133  2.496205
H    -3.355947  1.289682  1.953031
H    -3.814828 -0.173810  2.853838
C    -1.641492 -2.472249  1.777207
H    -2.276942 -3.104581  1.151102
H    -0.814179 -3.064043  2.169828
H    -2.232244 -2.072969  2.603761
S    -2.922629 -1.659994 -1.580815
S     0.085937 -0.742520 -1.409798
C     1.459060 -0.409426 -0.230187
C     1.409314  1.048135  0.145894
O     0.679666  1.263517  1.235883
C     0.351808  2.632800  1.495212
C     2.791545 -0.738930 -0.883739
C     3.940151 -0.493913  0.066245
O     5.109933 -0.851864 -0.471444
C     6.258250 -0.642692  0.358394
O     1.925520  1.942463 -0.501068
O     3.833411 -0.027333  1.179157
H     1.295730 -1.013650  0.662729
H    -0.336220  2.617604  2.338307
H     1.251342  3.198549  1.745398
H    -0.125751  3.063366  0.612596
H     2.818451 -1.781620 -1.210701
H     2.947400 -0.115418 -1.769793
H     7.112602 -0.975979 -0.226256
H     6.355028  0.414638  0.610329
H     6.172049 -1.225429  1.277000
O    -1.755364  0.964322 -0.219704
H    -2.645320  1.390440 -0.142120
O    -0.434592  2.880059 -1.870425
H    -0.809100  2.056639 -1.517531
H     0.500849  2.793316 -1.643166
O    -4.379238  1.646123 -0.401967
H    -4.873196  2.229766  0.185515
H    -4.523960  0.746155 -0.062284
    el energy= -2131.38640209
          zpe= -2131.074050
    th energy= -2131.046130
  th enthalpy= -2131.045186
  free energy= -2131.132441

TS20
P    -1.963351 -0.655018 -0.130611
O    -3.351589 -0.529974  0.879970
O    -1.073342 -1.362645  1.050509
C    -3.229530  0.143269  2.128741
H    -2.318156 -0.146120  2.660151
H    -3.221365  1.231716  1.997193
H    -4.098087 -0.130343  2.732060
C    -1.569666 -2.555552  1.661372
H    -1.706988 -3.338759  0.909650
H    -0.808724 -2.868173  2.376531
H    -2.516540 -2.379102  2.175833
S    -2.904252 -1.659818 -1.591206
S     0.093166 -0.743528 -1.400692
C     1.465193 -0.398521 -0.223608
C     1.425652  1.065866  0.124359
O     0.706501  1.305739  1.216438
C     0.390388  2.681125  1.456069
C     2.798726 -0.750886 -0.863375
C     3.947143 -0.493086  0.083255
O     5.114854 -0.876746 -0.441777
C     6.263360 -0.655839  0.384549
O     1.940787  1.945968 -0.543163
```

```
O     3.843110  0.003914  1.183223
H     1.293605 -0.982765  0.681453
H    -0.283132  2.685013  2.310966
H     1.296707  3.246722  1.680852
H    -0.099884  3.098335  0.574006
H     2.819443 -1.800297 -1.168518
H     2.961252 -0.147736 -1.762300
H     7.115382 -1.015800 -0.187603
H     6.371506  0.407386  0.605215
H     6.168540 -1.209887  1.319910
O    -1.768996  0.963680 -0.182263
H    -2.658059  1.400599 -0.118263
O    -0.453086  2.847738 -1.885021
H    -0.818359  2.025821 -1.519328
H     0.487337  2.763287 -1.677996
O    -4.354047  1.715675 -0.342524
H    -4.796527  2.301498  0.282936
H    -4.541444  0.812377 -0.034526
   el energy= -2131.38617074
         zpe= -2131.074714
   th energy= -2131.047150
 th enthalpy= -2131.046206
 free energy= -2131.133486

36
P     3.019916  0.200282  0.031604
O     4.294636 -0.765107 -0.108920
O     2.893188  0.252556  1.630218
C     4.255008 -2.055032  0.535417
H     4.248468 -1.927606  1.618448
H     3.374205 -2.612585  0.210654
H     5.156983 -2.577440  0.221743
C     1.860889  1.065969  2.210914
H     0.906437  0.914153  1.698848
H     1.779526  0.761936  3.253825
H     2.144739  2.119510  2.148601
S     3.314824  1.911231 -0.849826
S    -1.087343  2.310079 -0.110927
C    -2.326057  1.050637  0.420295
C    -1.611434 -0.264278  0.602167
O    -1.139500 -0.425944  1.839294
C    -0.345720 -1.600595  2.051770
C    -3.454172  0.888400 -0.587612
C    -4.471435 -0.132250 -0.134469
O    -5.490882 -0.232061 -0.994208
C    -6.500349 -1.185528 -0.645214
O    -1.439881 -1.090694 -0.277771
O    -4.390640 -0.791635  0.879172
H    -2.736325  1.340959  1.390040
H    -0.049388 -1.569827  3.098637
H    -0.936234 -2.495579  1.848327
H     0.530278 -1.581342  1.398785
H    -3.959061  1.844050 -0.750791
H    -3.058441  0.568562 -1.557087
H    -7.242145 -1.138125 -1.439238
H    -6.070226 -2.186552 -0.582571
H    -6.950259 -0.926513  0.314677
O     1.795339 -0.640421 -0.467853
H     1.094479 -0.178229 -1.175541
O     0.174868  0.297352 -2.015745
H    -0.196705  1.090195 -1.506301
H    -0.540191 -0.355695 -1.911661
O     3.353186 -2.192160 -2.483336
H     2.624344 -1.869825 -1.936016
H     4.098215 -1.664264 -2.171812
   el energy= -2131.42411640
         zpe= -2131.114985
   th energy= -2131.086612
 th enthalpy= -2131.085668
 free energy= -2131.177389

1
P    -2.135421 -0.794709  0.129112
O    -3.467321 -0.933894 -0.746127
O    -2.487672  0.179232  1.349381
C    -4.390958  0.164360 -0.887555
H    -4.753366  0.475491  0.093575
H    -3.916323  1.000830 -1.406993
H    -5.215367 -0.214949 -1.486975
C    -2.375191  1.618678  1.348372
H    -2.896505  2.056219  0.496164
H    -2.842680  1.944191  2.275513
H    -1.323979  1.910260  1.330310
S    -1.465469 -2.502721  0.743316
S    -0.902893  0.269448 -1.200113
C     0.673123  0.228109 -0.238751
C     1.297232  1.606981 -0.385157
O     0.907914  2.427618  0.586556
C     1.410889  3.769165  0.498113
C     1.603499 -0.847077 -0.774624
C     2.886890 -0.854237  0.023544
O     3.713946 -1.814747 -0.381216
C     4.964487 -1.887345  0.317310
O     2.028209  1.917195 -1.294631
O     3.134593 -0.078753  0.921005
H     0.443953  0.060362  0.816337
H     0.995099  4.296354  1.352917
H     2.500652  3.759781  0.542057
H     1.085714  4.229055 -0.436027
H     1.131187 -1.830988 -0.709356
H     1.844232 -0.656990 -1.824518
H     5.508782 -2.712157 -0.136000
H     5.514687 -0.952564  0.200126
H     4.791842 -2.076897  1.377671
   el energy= -1902.63611600
         zpe= -1902.389196
   th energy= -1902.367687
 th enthalpy= -1902.366743
 free energy= -1902.442919

34
P    -2.100933 -1.116381 -0.091596
O    -2.661223 -0.238540  1.127779
O    -1.171454 -2.222093  0.625149
```

```
C    -1.737048  0.508877  1.960549
H    -0.958720 -0.156442  2.346231
H    -1.313230  1.337986  1.375909
H    -2.336357  0.880756  2.790856
C    -1.778591 -3.070099  1.620443
H    -2.563768 -3.676163  1.163245
H    -0.983455 -3.709252  1.997927
H    -2.194147 -2.465156  2.429155
S    -3.562073 -1.773472 -1.186093
S    -0.667535 -0.073913 -1.184374
C     0.869435 -0.256273 -0.178068
C     1.413247  1.140807  0.073191
O     1.257856  1.521545  1.327765
C     1.673242  2.864490  1.615810
C     1.869397 -1.094735 -0.965032
C     3.169652 -1.230806 -0.207697
O     4.007109 -2.068189 -0.818367
C     5.277660 -2.244056 -0.177807
O     1.950084  1.793469 -0.797303
O     3.427994 -0.648995  0.822526
H     0.627884 -0.735216  0.769494
H     1.325106  3.066351  2.627019
H     2.763203  2.926123  1.572351
H     1.217384  3.544498  0.896950
H     1.461465 -2.088924 -1.162778
H     2.084153 -0.626919 -1.931188
H     5.827528 -2.947040 -0.798852
H     5.804065 -1.290272 -0.118089
H     5.139746 -2.645397  0.827307
O    -1.045069  2.978454  0.118953
H    -1.263874  3.558640  0.859384
O     0.585102  4.384018 -1.237759
H    -0.122231  3.838024 -0.727994
H     1.283674  3.725563 -1.332698
O    -3.259318  2.024752 -0.712036
H    -2.363510  2.422469 -0.392208
H    -3.517800  1.439656  0.007404
    el energy= -2131.35188369
          zpe= -2131.042721
    th energy= -2131.014454
  th enthalpy= -2131.013510
  free energy= -2131.102864

TS19
P    -1.868320 -0.956621 -0.144852
O    -1.582622 -0.514116  1.375840
O    -1.632115 -2.575343 -0.026114
C    -0.866314 -1.288336  2.353181
H    -0.504550 -2.229925  1.938781
H    -0.030124 -0.676931  2.693786
H    -1.549521 -1.489634  3.179847
C    -2.624541 -3.364929  0.640082
H    -3.495849 -3.492770 -0.005212
H    -2.163066 -4.330284  0.846969
H    -2.939662 -2.903339  1.581394
S    -3.656553 -0.646735 -0.879856
S    -0.259962 -0.643337 -1.471766
C     1.145645 -0.397787 -0.319831
C     1.233658  1.052153  0.130586
O     0.885345  1.212862  1.399315
C     0.929265  2.566143  1.876374
C     2.407453 -0.766239 -1.097263
C     3.635604 -0.602131 -0.232358
O     4.735910 -0.997577 -0.870588
C     5.956973 -0.871102 -0.129780
O     1.641358  1.936616 -0.590460
O     3.628246 -0.165314  0.896768
H     1.035850 -1.050674  0.547032
H     0.517454  2.535378  2.883091
H     1.963749  2.915402  1.898789
H     0.333305  3.203493  1.219680
H     2.359140 -1.797885 -1.453387
H     2.517390 -0.116920 -1.971752
H     6.742209 -1.231069 -0.790111
H     6.127941  0.172619  0.137946
H     5.910523 -1.475496  0.777315
O    -1.596654  1.625742 -0.071017
H    -1.459575  1.644722  0.883342
O    -0.551876  3.855847 -0.848525
H    -0.982503  2.974579 -0.576880
H     0.363431  3.582399 -0.981674
O    -3.957996  2.694072 -0.228952
H    -4.487686  1.923183 -0.459548
H    -3.032646  2.284686 -0.166748
    el energy= -2131.33907446
          zpe= -2131.029573
    th energy= -2131.002034
  th enthalpy= -2131.001090
  free energy= -2131.087996

35
P    -1.932826 -0.662632 -0.145004
O    -3.291688 -0.512116  0.907144
O    -1.043039 -1.427052  1.004591
C    -3.122460  0.230269  2.110930
H    -2.100239  0.158133  2.496205
H    -3.355947  1.289682  1.953031
H    -3.814828 -0.173810  2.853838
C    -1.641492 -2.472249  1.777207
H    -2.276942 -3.104581  1.151102
H    -0.814179 -3.064043  2.169828
H    -2.232244 -2.072969  2.603761
S    -2.922629 -1.659994 -1.580815
S     0.085937 -0.742520 -1.409798
C     1.459060 -0.409426 -0.230187
C     1.409314  1.048135  0.145894
O     0.679666  1.263517  1.235883
C     0.351808  2.632800  1.495212
C     2.791545 -0.738930 -0.883739
C     3.940151 -0.493913  0.066245
O     5.109933 -0.851864 -0.471444
C     6.258250 -0.642692  0.358394
O     1.925520  1.942463 -0.501068
O     3.833411 -0.027333  1.179157
```

```
H     1.295730 -1.013650  0.662729
H    -0.336220  2.617604  2.338307
H     1.251342  3.198549  1.745398
H    -0.125751  3.063366  0.612596
H     2.818451 -1.781620 -1.210701
H     2.947400 -0.115418 -1.769793
H     7.112602 -0.975979 -0.226256
H     6.355028  0.414638  0.610329
H     6.172049 -1.225429  1.277000
O    -1.755364  0.964322 -0.219704
H    -2.645320  1.390440 -0.142120
O    -0.434592  2.880059 -1.870425
H    -0.809100  2.056639 -1.517531
H     0.500849  2.793316 -1.643166
O    -4.379238  1.646123 -0.401967
H    -4.873196  2.229766  0.185515
H    -4.523960  0.746155 -0.062284
    el energy= -2131.38640209
          zpe= -2131.074050
    th energy= -2131.046130
  th enthalpy= -2131.045186
  free energy= -2131.132441

37
H    -3.741615 -3.074609 -0.345236
C    -3.282495 -2.230167 -0.858813
O    -2.665332 -1.432193  0.155679
P    -1.821331 -0.077340 -0.268622
S    -3.415255  1.046105 -1.043133
O    -1.466362  0.708392  1.114020
C    -2.465929  1.413533  1.877728
H    -2.025897  1.540964  2.866750
S    -0.026538 -1.540165  0.289165
H    -4.042701 -1.652822 -1.389875
H    -2.527219 -2.598297 -1.559993
H    -3.388940  0.835837  1.944846
H    -2.678090  2.384956  1.428657
O    -0.852779  0.205994 -1.563907
H    -1.333641  0.829713 -2.139739
O    -0.897861  3.220849 -0.420496
H    -1.736413  2.822911 -0.711370
H    -0.680738  2.712797  0.370552
O    -5.241091 -0.606168  1.195999
H    -4.476023 -1.176434  1.341148
H    -4.925300 -0.041645  0.467936
C     1.516775 -0.700446 -0.253367
C     2.655808 -1.531946  0.294394
O     2.953037 -2.561569 -0.506141
C     3.986199 -3.427374 -0.027493
C     1.634202  0.729400  0.249715
C     2.954824  1.344364 -0.144679
O     3.104212  2.564639  0.382500
C     4.322992  3.235473  0.045202
O     3.219406 -1.324175  1.346267
O     3.783751  0.824071 -0.858997
H     1.562399 -0.718787 -1.343173
H     4.098372 -4.203693 -0.781177
H     4.918804 -2.873113  0.092519
H     3.702013 -3.863385  0.931930
H     0.839879  1.346012 -0.179942
H     1.535751  0.771120  1.337706
H     4.282337  4.198600  0.548946
H     5.181462  2.657839  0.392120
H     4.394121  3.371350 -1.035289
    el energy= -2131.35616623
          zpe= -2131.045330
    th energy= -2131.016313
  th enthalpy= -2131.015369
  free energy= -2131.107477

TS21
H    -3.622640 -3.019287 -0.739507
C    -2.946581 -2.228402 -1.061792
O    -2.692729 -1.415716  0.090607
P    -1.696699 -0.131585 -0.112387
S    -3.250218  1.212048 -1.135754
O    -1.695515  0.647786  1.319403
C    -2.876453  1.255129  1.878072
H    -2.718889  1.245520  2.956585
S    -0.006345 -1.421611  0.670614
H    -3.419312 -1.631080 -1.846747
H    -2.012779 -2.664616 -1.426995
H    -3.772886  0.686821  1.623877
H    -2.977908  2.279467  1.517319
O    -0.891505  0.165131 -1.420229
H    -1.924313  0.867124 -1.858528
O    -0.830308  3.203624  0.131556
H    -1.573738  2.829147 -0.371533
H    -0.758860  2.603087  0.883593
O    -5.458906 -0.713433  0.427144
H    -4.679812 -1.204464  0.717652
H    -5.077634 -0.136630 -0.254333
C     1.482512 -0.658380 -0.081291
C     2.652002 -1.527495  0.332537
O     2.826374 -2.557459 -0.500077
C     3.886486 -3.452783 -0.149639
C     1.708153  0.773916  0.373980
C     2.974414  1.339279 -0.222898
O     3.209895  2.581546  0.210088
C     4.389790  3.202271 -0.312367
O     3.334249 -1.338344  1.314571
O     3.695475  0.758421 -1.004545
H     1.371773 -0.700168 -1.164285
H     3.889420 -4.225340 -0.915219
H     4.840058 -2.922034 -0.137351
H     3.704482 -3.888607  0.834264
H     0.877014  1.413546  0.060566
H     1.782105  0.828344  1.463897
H     4.428583  4.192374  0.136082
H     5.273834  2.623478 -0.039690
H     4.328832  3.276445 -1.399372
    el energy= -2131.33005117
          zpe= -2131.025166
    th energy= -2130.996404
```

```
  th enthalpy= -2130.995460
  free energy= -2131.086551

38
H    -3.457771 -2.477750 -1.001643
C    -2.487161 -1.986566 -0.964566
O    -2.494192 -1.202366  0.249167
P    -1.350573 -0.113401  0.471422
S    -4.604908  0.893651 -2.023688
O    -1.927854  0.707912  1.706427
C    -3.167702  1.443126  1.516508
H    -3.349675  1.955400  2.458753
S     0.272648 -1.104719  1.319087
H    -2.371192 -1.329804 -1.826937
H    -1.682726 -2.723797 -0.916040
H    -3.981097  0.753458  1.284804
H    -3.042470  2.166765  0.708400
O    -0.987124  0.672432 -0.736832
H    -3.313452  0.941686 -1.646400
O    -0.435685  3.142734  0.639283
H    -0.636081  2.486493 -0.046533
H    -0.661526  2.688383  1.460251
O    -5.380216 -1.060170  0.470307
H    -4.508607 -1.328406  0.783447
H    -5.170165 -0.494862 -0.306441
C     1.589689 -0.503149  0.175391
C     2.663343 -1.580739  0.194704
O     2.457911 -2.493397 -0.748896
C     3.409262 -3.566294 -0.779580
C     2.157836  0.835284  0.615267
C     3.249940  1.261389 -0.337803
O     3.736656  2.460976 -0.025395
C     4.783248  2.942972 -0.878627
O     3.568021 -1.610358  0.995142
O     3.638819  0.597076 -1.273744
H     1.160543 -0.444674 -0.824633
H     3.098178 -4.213863 -1.595485
H     4.410131 -3.171611 -0.960545
H     3.396345 -4.106205  0.168339
H     1.384127  1.609863  0.631698
H     2.582150  0.761787  1.620812
H     5.060157  3.918096 -0.485284
H     5.634781  2.261434 -0.851501
H     4.421689  3.030859 -1.904226
    el energy= -2131.39003642
          zpe= -2131.082654
    th energy= -2131.052639
  th enthalpy= -2131.051695
  free energy= -2131.147437

39
H    -2.554427 -2.735303  0.270112
S    -2.720516 -1.632410 -0.474749
C    -1.080177 -0.884356 -0.069255
C    -1.191206  0.555742 -0.540554
O    -1.835982  1.319789  0.354122
C    -1.957363  2.692287 -0.020732
C     0.066089 -1.618457 -0.763225
C     1.369437 -1.415644 -0.019278
O     2.309745 -0.854829 -0.778406
C     3.507957 -0.505841 -0.081632
O    -0.888576  0.939027 -1.646560
O     1.551438 -1.787382  1.118566
H    -0.954260 -0.883056  1.014492
H    -2.421007  3.196094  0.824809
H    -0.966998  3.107969 -0.222451
H    -2.576783  2.793320 -0.913808
H    -0.133128 -2.693103 -0.745085
H     0.146526 -1.289921 -1.799830
H     4.131659  0.013095 -0.805493
H     3.243960  0.158689  0.742401
H     4.005000 -1.403186  0.293650
O     0.949124  1.129876  0.820974
H     0.595536  2.012805  0.994035
O    -0.424989  0.290051  2.824293
H    -1.235742  0.722032  2.530245
H     0.210367  0.535372  2.062009
O     2.430322  2.152923 -1.043594
H     3.166770  2.465508 -0.508308
H     1.853709  1.660224 -0.367898
    el energy= -1162.22518281
          zpe= -1161.999045
    th energy= -1161.979119
  th enthalpy= -1161.978175
  free energy= -1162.046429

TS22
H    -2.247425 -2.962015  0.180982
S    -2.468549 -1.858679 -0.549334
C    -0.939929 -0.958921 -0.028740
C    -1.201984  0.485445 -0.445964
O    -1.999201  1.103940  0.481282
C    -2.482710  2.378745  0.078663
C     0.298051 -1.532297 -0.714140
C     1.550673 -1.246156  0.081728
O     2.509019 -0.694499 -0.664837
C     3.642206 -0.226805  0.064386
O    -1.169839  0.854321 -1.608730
O     1.694585 -1.539065  1.248057
H    -0.852456 -1.009743  1.056386
H    -3.071356  2.759378  0.912133
H    -1.652186  3.059391 -0.132919
H    -3.102021  2.294538 -0.816794
H     0.210786 -2.620830 -0.776762
H     0.376314 -1.128002 -1.724406
H     4.279202  0.273039 -0.661459
H     3.305243  0.481705  0.824399
H     4.167111 -1.058173  0.539399
O     0.597285  1.142466  0.421157
H     0.280822  2.037230  0.605059
O    -0.346854  0.496101  2.834718
H    -1.226951  0.755736  2.535579
H     0.170804  0.644565  1.997893
O     2.340497  2.200680 -1.287457
```

```
H     2.950991  2.601301 -0.660359
H     1.706146  1.699133 -0.698908
    el energy= -1162.22302794
          zpe= -1161.996912
    th energy= -1161.977517
  th enthalpy= -1161.976573
  free energy= -1162.043642

40
H    -1.336233 -1.472881  2.772488
S    -1.730351 -1.712340  1.510654
C    -0.482446 -0.648386  0.693317
C    -0.971128 -0.438321 -0.773800
O    -2.095874  0.560224 -0.594389
C    -2.770730  0.808825 -1.808867
C     0.878222 -1.346703  0.674467
C     1.974641 -0.421925  0.210599
O     2.743108 -0.966379 -0.731759
C     3.775767 -0.120645 -1.245489
O    -1.302179 -1.496205 -1.395216
O     2.189832  0.686026  0.667881
H    -0.414787  0.294302  1.243587
H    -3.701545  1.333250 -1.578575
H    -2.165867  1.431525 -2.482161
H    -2.991269 -0.137092 -2.310537
H     1.149498 -1.681649  1.681219
H     0.820877 -2.215143  0.016303
H     4.302498 -0.712205 -1.991028
H     3.333427  0.766725 -1.702936
H     4.454518  0.184241 -0.447515
O     0.061424  0.315354 -1.459224
H     0.136364  1.182601 -1.027418
O     0.489660  2.157698  2.478972
H     0.001284  2.540454  1.729716
H     1.161362  1.628916  2.021180
O    -0.717784  2.713060  0.027292
H    -1.041543  3.497567 -0.428064
H    -1.394426  2.001530 -0.116554
    el energy= -1162.24128514
          zpe= -1162.012394
    th energy= -1161.993328
  th enthalpy= -1161.992384
  free energy= -1162.058873

TS23
H    -1.230255 -2.089639  2.363778
S    -1.641410 -2.050010  1.085984
C    -0.418353 -0.809615  0.536710
C    -0.785141 -0.395393 -0.896031
O    -2.281420  0.735058 -0.324048
C    -2.921790  1.161651 -1.484722
C     0.994401 -1.419793  0.530020
C     2.040485 -0.384744  0.192939
O     2.764469 -0.715976 -0.873473
C     3.729389  0.257418 -1.286693
O    -1.209635 -1.226602 -1.694647
O     2.228513  0.635918  0.826685
H    -0.444079  0.045963  1.214259
H    -4.004576  1.287339 -1.329662
H    -2.531049  2.127280 -1.852796
H    -2.785324  0.424156 -2.291693
H     1.230716 -1.801763  1.527865
H     1.041130 -2.245934 -0.181580
H     4.226738 -0.167062 -2.155704
H     3.224143  1.188888 -1.549276
H     4.446707  0.446479 -0.486767
O     0.024538  0.610490 -1.373483
H    -0.003304  1.365237 -0.737735
O     0.340036  1.663383  2.774330
H    -0.114412  2.102381  2.026665
H     1.098378  1.263774  2.323536
O    -0.762878  2.461171  0.411559
H    -0.996599  3.332820  0.076484
H    -1.558580  1.755549  0.148166
    el energy= -1162.23471126
          zpe= -1162.008636
    th energy= -1161.990264
  th enthalpy= -1161.989320
  free energy= -1162.054706

41
H     1.053442  2.591634  1.938089
S     1.329472  2.452287  0.630182
C     0.253566  1.000432  0.360070
C     0.505319  0.443374 -1.060028
O     3.029336 -0.983529  0.152424
C     3.274227 -1.468106 -1.150927
C    -1.231217  1.387248  0.516040
C    -2.127684  0.218002  0.185727
O    -2.690644  0.339416 -1.014337
C    -3.421228 -0.805143 -1.464428
O     1.042139  1.174919 -1.899916
O    -2.329167 -0.731273  0.918135
H     0.495118  0.237397  1.102869
H     4.021461 -0.821317 -1.619140
H     3.674335 -2.492401 -1.144208
H     2.366455 -1.449773 -1.765755
H    -1.425827  1.680508  1.551209
H    -1.464609  2.224515 -0.144459
H    -3.810580 -0.543706 -2.445805
H    -2.747072 -1.660968 -1.532342
H    -4.236252 -1.033639 -0.776166
O     0.058977 -0.734956 -1.245167
H     0.305103 -1.700928 -0.057740
O    -0.368080 -1.023970  2.976273
H     0.070816 -1.596126  2.321267
H    -1.193927 -0.821625  2.511486
O     0.662726 -2.268597  0.704892
H     0.590837 -3.188675  0.428905
H     2.268957 -1.492412  0.491710
    el energy= -1162.27048772
          zpe= -1162.043188
    th energy= -1162.022623
  th enthalpy= -1162.021679
```

```
  free energy= -1162.094312

42
H     1.792377  2.779382  0.345988
S     2.496662  1.814401 -0.267825
C     1.300896  0.441446 -0.002507
C     2.115406 -0.865477 -0.217778
O     2.286558 -1.587042  0.794020
C     0.129221  0.565221 -0.964043
C    -0.892837 -0.522041 -0.746982
O    -2.082848 -0.178507 -1.275364
C    -3.149562 -1.081443 -0.991185
O     2.543000 -1.050950 -1.378769
O    -0.680332 -1.613490 -0.271014
H     0.947043  0.485405  1.025063
H    -0.379487  1.526113 -0.860252
H     0.504720  0.475701 -1.990012
H    -4.030307 -0.674470 -1.485043
H    -2.923972 -2.079077 -1.371984
H    -3.311869 -1.120638  0.087333
O    -1.519192  0.707412  1.557146
H    -0.956850  1.490424  1.609271
O    -3.521488  1.683465  0.358965
H    -2.725259  1.262185  0.875447
H    -3.238820  1.543407 -0.550494
O     0.122018 -0.993326  2.702738
H     0.721081 -1.285497  1.995536
H    -0.545729 -0.400083  2.237541
    el energy= -1122.47064602
          zpe= -1122.285935
    th energy= -1122.267813
  th enthalpy= -1122.266869
  free energy= -1122.332469

TS24
H     1.986124  2.538531  1.232247
S     2.601745  1.800835  0.293699
C     1.359110  0.442691  0.200111
C     2.110104 -0.732470 -0.489743
O     2.314028 -1.756939  0.209856
C     0.131149  0.892748 -0.577710
C    -0.964958 -0.163805 -0.589598
O    -2.111147  0.404925 -1.136632
C    -3.155638 -0.526967 -1.353368
O     2.482216 -0.524055 -1.664309
O    -0.729876 -1.359982 -0.757376
H     1.097323  0.148655  1.215913
H    -0.270082  1.835013 -0.193824
H     0.436334  1.055835 -1.617867
H    -3.987385  0.032067 -1.785486
H    -2.842228 -1.317917 -2.038968
H    -3.474226 -0.972697 -0.406616
O    -1.490036 -0.025215  1.280030
H    -1.022311  0.737365  1.645213
O    -3.782723  1.243970  1.066860
H    -2.955591  0.693959  1.204390
H    -3.606119  1.593619  0.186293
O     0.272897 -1.906604  2.181246
H     0.920295 -1.929058  1.450654
H    -0.431546 -1.310714  1.833314
    el energy= -1122.46440134
          zpe= -1122.278458
    th energy= -1122.261549
  th enthalpy= -1122.260605
  free energy= -1122.322995

43
H     1.556749  2.593531  1.337516
S     2.248112  2.022842  0.337861
C     1.243167  0.477938  0.194242
C     2.143163 -0.462823 -0.660191
O     2.780297 -1.353200 -0.034955
C    -0.120498  0.750428 -0.425687
C    -1.093948 -0.402186 -0.101956
O    -2.298893 -0.025817 -0.935638
C    -3.342251 -0.965542 -0.806195
O     2.211504 -0.209291 -1.880692
O    -0.666335 -1.596340 -0.342642
H     1.136993  0.050305  1.192267
H    -0.537926  1.697364 -0.061775
H     0.007941  0.828925 -1.508957
H    -4.040932 -0.818411 -1.634440
H    -2.934120 -1.980052 -0.843710
H    -3.883516 -0.841094  0.141913
O    -1.540057 -0.270776  1.261202
H    -1.955536  0.603020  1.340354
O    -3.058805  2.110611  0.531047
H    -3.959981  1.919034  0.814053
H    -2.871296  1.445692 -0.170261
O     0.901590 -2.406488  1.713722
H     1.691275 -2.095397  1.230115
H     0.208350 -2.144864  1.059533
    el energy= -1122.47698138
          zpe= -1122.289003
    th energy= -1122.271979
  th enthalpy= -1122.271035
  free energy= -1122.333675

TS25
H     1.656763  2.556059  1.397640
S     2.298412  2.022034  0.345749
C     1.320150  0.463964  0.244186
C     2.162408 -0.464415 -0.678116
O     2.646221 -1.502411 -0.152034
C    -0.081863  0.725203 -0.312696
C    -0.969061 -0.474922 -0.019514
O    -2.506966  0.327329 -1.033269
C    -3.518253 -0.619399 -0.977066
O     2.317627 -0.072825 -1.851879
O    -0.723925 -1.584452 -0.507934
H     1.268346  0.024830  1.242572
H    -0.522393  1.622439  0.130911
H    -0.006083  0.867440 -1.391577
H    -4.143249 -0.618022 -1.886816
```

```
H    -3.103062 -1.637269 -0.870860
H    -4.205774 -0.466410 -0.122243
O    -1.558633 -0.457881  1.216827
H    -1.970293  0.430510  1.341034
O    -2.871776  1.861743  0.856911
H    -3.781495  1.758283  1.156480
H    -2.792487  1.296296 -0.036592
O     0.898489 -2.502345  1.688796
H     1.613652 -2.172559  1.100707
H     0.122902 -2.349985  1.126657
    el energy= -1122.46928716
          zpe= -1122.284207
    th energy= -1122.267469
  th enthalpy= -1122.266525
  free energy= -1122.328704

44
H    -0.830101 -2.017862 -1.221597
S     0.247384 -2.398097 -0.511092
C     0.798791 -0.679962 -0.152284
C     2.256852 -0.774282  0.367808
O     3.115905 -0.053100 -0.208230
C    -0.121843  0.006513  0.874517
C    -0.085452  1.516844  0.620188
O    -3.506610 -0.886776  0.309130
C    -3.886095  0.381557  0.801218
O     2.453302 -1.558597  1.317636
O     0.771406  2.205777  1.211685
H     0.780225 -0.129610 -1.095133
H    -1.145764 -0.358792  0.760786
H     0.235255 -0.236129  1.878809
H    -4.257848  0.261196  1.822868
H    -3.039031  1.079952  0.816215
H    -4.690213  0.834860  0.203014
O    -0.902114  1.956473 -0.251290
H    -1.516929  0.818858 -1.114195
O    -1.893985  0.037409 -1.648177
H    -2.374958  0.427000 -2.386679
H    -2.965166 -0.698243 -0.487983
O     2.191461  2.263326 -1.301088
H     2.548902  1.406261 -0.977141
H     1.689052  2.561964 -0.527491
    el energy= -1122.50798581
          zpe= -1122.321152
    th energy= -1122.302970
  th enthalpy= -1122.302026
  free energy= -1122.369122
```