Mechanistic Contrasts between Manganese and Rhenium Bipyridine Electrocatalysts for the Reduction of Carbon Dioxide

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Relative reaction rates for dimerization

For Re(bpy)$(CO)_3$Cl (**1-Re**), Fujita and Muckerman investigated dimerization of the singly reduced complex in THF and the corresponding $Re(CO)_5$ complex.[1] The $Re(CO)_5$ complex dimerizes with a reaction rate that is several orders of magnitude faster. The authors showed that the $[Re(bpy)(CO)_3]^0$ complex (**2-Re)** binds THF as a sixth ligand in a pre-equilibrium, whereas $Re(CO)_5$ does not bind THF. Removing THF from this complex is thermodynamically unfavorable ($[Re^{I}(bpy^{\bullet-})(CO)_3(THF)]_{solv} \leftrightarrow [Re(bpy)(CO)_3]_{solv} + [THF]_{liq}$, with ΔG = 2.4 kcal/mol), and in equilibrium (without any competing reactions), the fraction of monomeric Re complexes with a free sixth coordination position (**2-Re**) is 1.6 x 10^{-2}. The initial rate of dimerization is proportional to [**2-Re**]^2, and thus dependent on this pre-equilibrium. Consequently, the dimerization rate for **2-Re** is several orders of magnitude lower compared to $Re(CO)_5$.

In order to compare the dimerization reaction rates for the Mn and Re catalysts, we follow the scheme proposed by Fujita and Muckerman.[1] The singly reduced Mn complex is most stable in its five-coordinate form (**2-Mn**) and can thus directly dimerize. On the other hand, the singly reduced Re complex prevails in its six-coordinate form, binding Cl^- (**2X-Re**) or MeCN (**2S-Re**). Removing the Cl^- ligand from the complex is endergonic by 7.7 kcal/mol at standard concentration and 3.6 kcal/mol when taking the experimental concentration (1 mM) into account (using $G_A = G_A^0 + RT\, ln[A]$, where $[A]$ is the concentration of A, G_A is its chemical potential and G_A^0 is its chemical potential at the standard state of 1 M). Removing the MeCN ligand is endergonic by 6.0 kcal/mol. A prerequisite for dimerization is removal of the sixth ligand. The fraction *f* of all monomeric species in the five-coordinate form (**2-Re**) is

defined as: $f = K_{eq}/(1 + K_{eq})$, where K_{eq} is the equilibrium constant for dissociation of the sixth ligand. For the Re catalyst, f is approximately 4.0 x 10^{-5}, while it is about 1 for the Mn complex.

The initial dimerization rate is approximately (eq. 18 from ref. 1)

$$-d[Re]/dt = 2k_2([Re]_0 \cdot f)^2 \quad \text{(S1)}$$

where the initial Re catalyst concentration is $[Re]_0$. Comparing both fractions, we can readily see that the initial rate for dimerization for the Re complex is approximately 1.6 x 10^9 times slower than for the Mn complex.

Binding affinities to $[Re(CO)_5]^0$ and $[Mn(CO)_5]^0$

We calculated the binding affinities of Br^- and Cl^- to the Re and Mn pentacarbonyl complexes, applying the same methodology as for the species **2** and **2X**.

Table S1. Reaction free energies (kcal/mol) for removing Cl^- or Br^- (X^-) from the one-electron reduced $[Mn(CO)_5Br]^-$ and $[Re(CO)_5Cl]^-$ complexes. Both values are given for standard states at room temperature.

Reaction	ΔG (M = Mn)	ΔG (M = Re)
$[M(CO)_5X]^- \rightarrow [M(CO)_5] + X^-$	– 2.2	– 2.2

3-Mn electronic structures

All singlet intermediates were investigated for singlet diradical solutions. For this purpose, spin-polarized DFT was used. The geometries were optimized in the same fashion as all other intermediates (see Computational Methodology in main text). The only intermediate with a stable singlet diradical structure

was **3-Mn**. This electronic configuration has been previously reported in the literature.[2,3] Qualitative molecular orbital diagrams for closed shell singlet and singlet diradical **3-Mn** are shown in Figure S1. The two singly occupied molecular orbitals (SOMOs) of the singlet diradical have an overlap of 0.91, indicating that they mostly overlap and that the spin polarization is quite small.

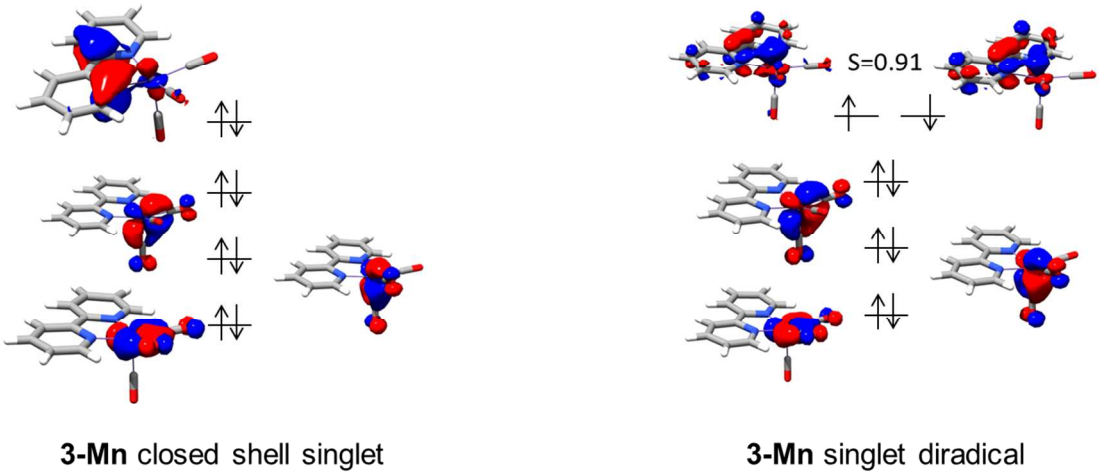


Figure S1. Schematic molecular orbital (MO) diagram for the **3-Mn** closed shell singlet and the singlet diradical structure. The spin-coupled MO pair is represented by unrestricted corresponding orbitals (for their definition, see reference 4). S is their spatial overlap. The doubly occupied MOs of the singlet diradical are localized quasi-restricted orbitals. For the closed shell singlet, localized canonical MOs are shown.

Table S2. Bimolecular reaction rate constants (M^{-1} s^{-1}) obtained using equation (2) in the main text with the standard free energies of activation from Tables 3 and 9 in the main text for the chemical steps of the microkinetics simulation.

	Mn catalyst		Re catalyst	
Reaction	DFT-B3LYP	ULPNO-CCSD	DFT-B3LYP	ULPNO-CCSD
3 → 4	9.35×10^{2}		2.58×10^{3}	
3 → 5	2.37×10^{10}		2.80×10^{10}	
6 → 7	1.18×10^{4}	4	1.18×10^{4}	2.05×10^{2}
8 → 2CO	1.18×10^{4}	4	1.95×10^{4}	1.46×10^{2}

Table S3. Equilibrium constants for the (redox) reactions of the microkinetics simulation at different applied potentials (V vs. SCE). The values are obtained using the relationship K=exp(–$\Delta G^{o}/RT$), where ΔG^{o} is the reaction free energy, at standard temperature (298.15 K) and concentration (1 M), from Tables 1, 3, 4 and 5 in the main text, adjusted to account for the applied potential. The singly reduced species is assumed to be in its five-coordinate state for Mn (**2-Mn**) and in its six-coordinate state for Re (**2X-Re** and **2CO-Re**).

	Mn catalyst			Re catalyst		
	Applied Potential (V vs. SCE)			Applied Potential (V vs. SCE)		
Reaction	–1.4	–1.7	–2.0	–1.4	–1.7	–2.0
1 → 2(X)	1.58E+02	1.86E+07	2.19E+12	7.48E+02	8.81E+07	1.04E+13
2(X) → 3	1.43E-01	1.68E+04	1.98E+09	8.22E-07	9.68E-02	1.14E+04
3 → 4	1.25E-05	1.48E+00	1.74E+05	1.97E-03	2.33E+02	2.74E+07
3 → 5	2.33E+02	2.74E+07	3.23E+12	7.72E+03	9.10E+08	1.07E+14
5 → 6	1.43E-01	1.68E+04	1.98E+09	2.73E-05	3.21E+00	3.79E+05
6 → 8	3.07E+27	3.07E+27	3.07E+27	1.99E+31	1.99E+31	1.99E+31
7 → 2(CO)	2.44E-02	2.44E-02	2.44E-02	3.11E+02	3.11E+02	3.11E+02
2(CO) → 3	3.04E+24	3.04E+24	3.04E+24	8.36E+24	8.36E+24	8.36E+24
6 → 7	2.39E+20	2.39E+20	2.39E+20	1.08E+18	1.08E+18	1.08E+18
8 → 2(CO)	7.97E+26	7.97E+26	7.97E+26	3.59E+24	3.59E+24	3.59E+24

Table S4. Computed pK_a values for phenol and the protonated species **4** and **6**. The values are obtained using a thermochemical cycle as detailed in the SI of reference 5. The pK_a values are computed as $\boldsymbol{pK_a = -log(K_a) = \frac{\Delta G^0}{2.303 \cdot RT}}$, where $\boldsymbol{K_a}$ is the equilibrium constant and $\boldsymbol{\Delta G^0 = G(B^-) + G(H^+) - G(BH)}$ is the reaction free energy for the reaction $\boldsymbol{BH \rightarrow B^- + H^+}$, at standard temperature (298.15 K) and concentration (1 M). The solution phase total Gibbs free energies of the Brønsted base $\boldsymbol{B^-}$ ($\boldsymbol{G(B^-)}$)

and the Brønsted acid $\boldsymbol{BH}$ ($\boldsymbol{G(BH)}$) are calculated as described in the methodology section. The solution phase total Gibbs free energy $\boldsymbol{G(H^+)}$ of the proton is computed as detailed in reference 5, using the free energy of a proton in gas phase (–6.3 kcal/mol), the explicit solvation energy of a proton in acetonitrile (–260.2 kcal/mol) and the energy to bring the proton from 1 atm gas phase standard state to 1 M solution phase standard state (1.89 kcal/mol).

Species	pK_a (Mn catalyst)	pK_a (Re catalyst)
4	27.4	31.3
6	24.5	24.9
Phenol	22.4	

Experimental cyclic voltammetry

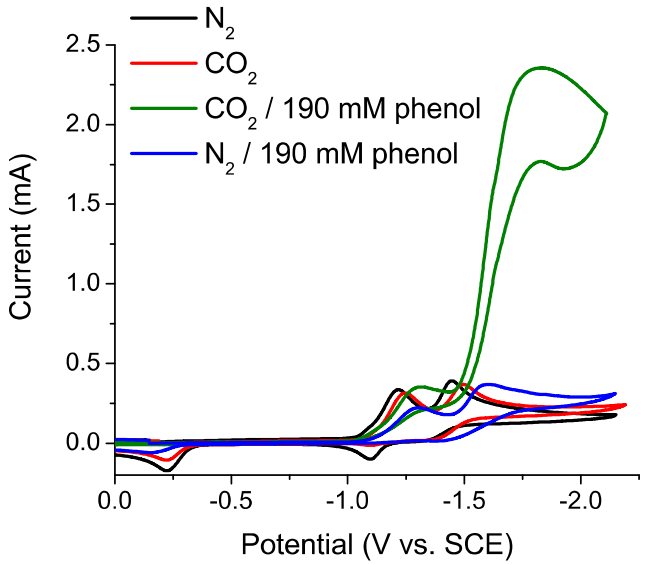


Figure S2. Cyclic voltammograms (CVs) of 1 mM Mn(bpy)$(CO)_3$Br (**1-Mn**) under various experimental conditions. The different conditions are as follows: CV under N_2 with no added phenol (black), CV under "dry" CO_2 with no added phenol (red), CV under CO_2 with 190 mM phenol (green), CV under N_2 with

190 mM phenol (blue). The catalytic current increase in the green CV is due solely to the electrocatalytic reduction of CO_2 to CO, as no current increase is observed in the blue CV. CVs were taken in 0.1 M $TBAPF_6$/MeCN with a scan rate of 100 mV/s, a glassy carbon working electrode (3 mm diameter), a platinum wire counter electrode, and a Ag/AgCl wire pseudo-reference with ferrocene (Fc) added as an internal reference.

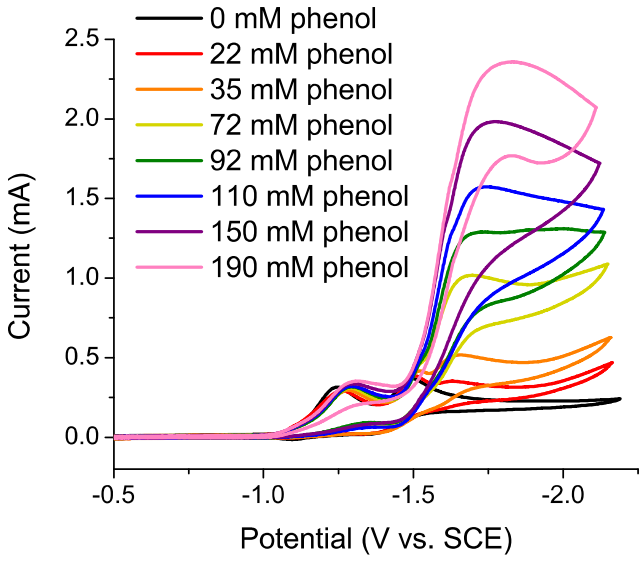


Figure S3. Cyclic voltammograms (CVs) showing the electrocatalytic reduction of CO_2 to CO by 1 mM $Mn(bpy)(CO)_3Br$ (**1-Mn**) with various [phenol]. The solution is under an atmosphere of, and saturated with (ca. 0.28 M), CO_2. CVs were taken in 0.1 M $TBAPF_6$/MeCN with a scan rate of 100 mV/s, a glassy carbon working electrode (3 mm diameter), a platinum wire counter electrode, and a Ag/AgCl wire pseudo-reference with ferrocene (Fc) added as an internal reference.

Calculation of experimental TOF values:

Equations 2–4 were used to calculate experimental i_{cat}/i_p and TOF values from catalytic CVs.

$$i_{cat} = n_{cat} FA[\text{cat}]\left(Dk_{cat}[\text{Q}]^{y}\right)^{1/2} \quad (2)$$

$$i_p = 0.4463 n_p^{3/2} FA[\text{cat}]\left(\frac{F}{RT}\right)^{1/2} \upsilon^{1/2} D^{1/2} \quad (3)$$

$$\text{TOF} = k_{cat}[\text{Q}] = \frac{F\upsilon n_p^3}{RT}\left(\frac{0.4463}{n_{cat}}\right)^2\left(\frac{i_{cat}}{i_p}\right)^2 \quad (4)$$

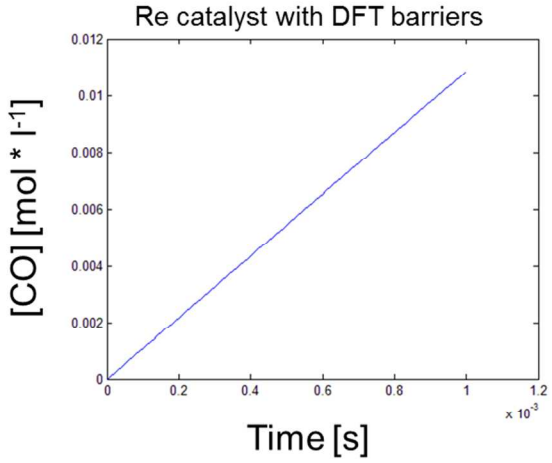
For a reversible electron-transfer reaction followed by a fast catalytic reaction (E_RC_{cat} scheme), the peak catalytic current (i_{cat}) is given by eq 2.[6] The derivation of eq 2 assumes that pseudo-first-order kinetics apply, i.e., the reaction is first order in catalyst and that the concentrations of the substrates, Q, are large in comparison to the concentration of catalyst. In eq 2, n_{cat} is the number of electrons required for the catalytic reaction (n_{cat} = 2 for the reduction of CO_2 to CO), F is Faraday's constant, A is the surface area of the electrode, [cat] is the catalyst concentration, D is the diffusion constant of the catalytically-active species, k_{cat} is the rate constant of the catalytic reaction, and [Q] is the substrate concentration. Previous studies of Mn bipyridine catalysts have shown that, at high [H^+], the electrocatalytic reduction of CO_2 is first order in catalyst, first order in CO_2, independent of acid concentration, and at steady state conditions.[7]

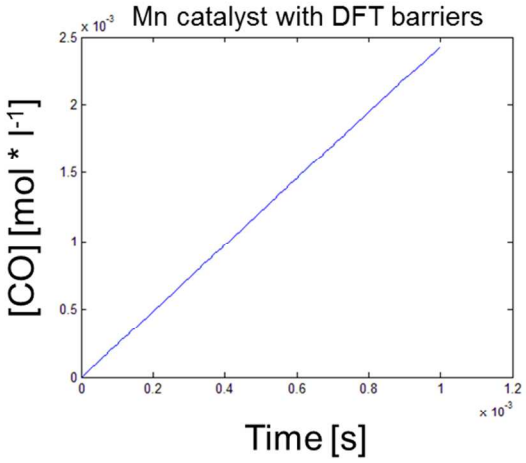
Equation 3 describes the peak current of a reversible electron transfer and with no following reaction.[8] In eq 3, R is the universal gas constant, T is temperature, n_p is the number of electrons in the reversible, non-catalytic reaction, and υ is scan rate (0.1 V/s). Dividing eq 2 by eq 3 allows for determination of i_{cat}/i_p and allows one to further calculate the catalytic rate constant (k_{cat}) and the turnover frequency (TOF), as shown in eq 4. In this equation, A cancels out because the same electrode was used for the experiments under CO_2 and N_2. D also cancels out because we are assuming that the diffusion constant of the catalytically-active species does not change significantly under CO_2 or N_2.

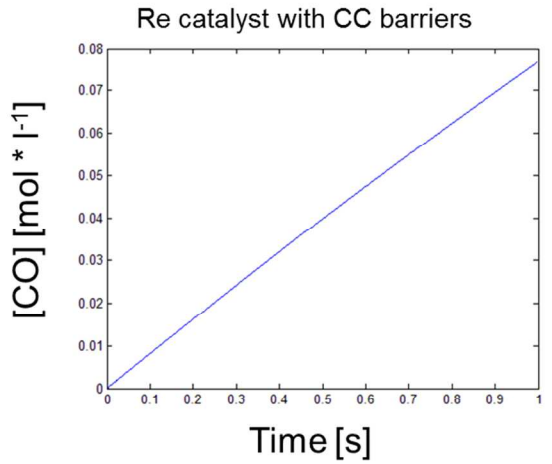
Using eqs 2–4, we can calculate peak i_{cat}/i_p and TOF values for Mn(bpy)$(CO)_3$Br (**1-Mn**) and Re(bpy)$(CO)_3$Cl (**1-Re**) with added phenol. For these calculations, i_p is determined as the peak current under N_2 with an equivalent amount of added phenol corresponding to peak i_{cat} conditions. For **1-Re**, CV data was taken from a previous report.[9] Under CO_2, with 0.20 and 0.57 M phenol (for Mn and Re,

respectively), TOF values of 7.2 s^{-1} and 300 s^{-1} are calculated for the Mn and Re catalysts, respectively (derived from i_{cat}/i_p = 6.1 and 40 for Mn and Re, respectively).

Results from microkinetics simulation







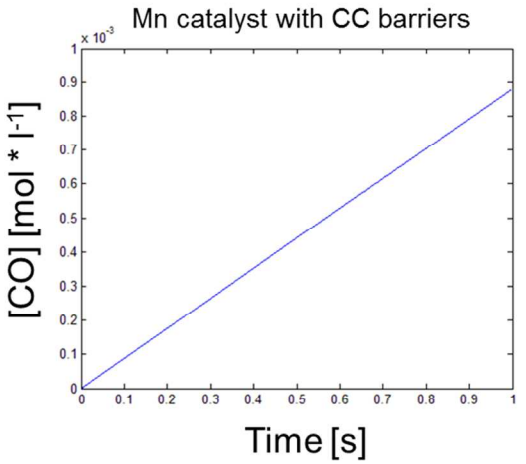


Figure S4. Accumulating CO during the microkinetics simulations. The plots show [CO] vs. time (s) for both catalysts and for barriers obtained with DFT-B3LYP and with Coupled Cluster (CC) calculations. The conditions of the microkinetics analysis are given in the Methods section in the main text.

References

(1) Fujita, E.; Muckerman, J. T. *Inorganic Chemistry* **2004**, *43*, 7636.

(2) Scarborough, C. C.; Wieghardt, K. *Inorganic Chemistry* **2011**, *50*, 9773.

(3) Hartl, F.; Rosa, P.; Ricard, L.; Le Floch, P.; Záliš, S. *Coordination Chemistry Reviews* **2007**, *251*, 557.

(4) Neese, F. *J. Phys. Chem. Solids* **2004**, *65*, 781

(5) Keith, J. A.; Grice, K. A.; Kubiak, C. P.; Carter, E. A. *Journal of the American Chemical Society* **2013**, *135*, 15823.

(6) Savéant, J.-M.; Vianello, E. *Electrochim. Acta* **1962**, *8*, 905.

(7) Sampson, M. D.; Nguyen, A. D.; Grice, K. A.; Moore, C. E.; Rheingold, A. L.; Kubiak, C. P. *Journal of the American Chemical Society* **2014**, *136*, 5460.

(8) Bard, A. J.; Faulkner, L. R. *Electrochemical Methods*; Wiley: New York, 1980.

(9) Wong, K.-Y.; Chung, W.-H.; Lau, C.-P. *Journal of Electroanalytical Chemistry* **1998**, *453*, 161.

Cartesian coordinates (in Å) and energies (in E_h) for the molecular species discussed in the main text. The geometries and single point DFT energies were obtained using the methodology described in the main text. Gas phase absolute energies were obtained for the gas phase geometries, solvent phase absolute energies were calculated for the solvated phase geometries. If only one optimized geometry is available, both energies are calculated for this geometry.

CO_2

gas phase geometry

C	-0.000003	0.000000	0.000000
O	1.163418	0.000000	0.000000
O	-1.163415	0.000000	0.000000

Total gas phase energy = -188.5809148738

solvent phase geometry

C	-0.000001	-0.000002	0.000000
O	1.163288	0.000001	0.000000
O	-1.163286	0.000001	0.000000

Total solvent phase energy = -188.5843458135

CO

gas phase geometry

C	0.134685	0.000000	0.000000
O	1.265315	0.000000	0.000000

Total gas phase energy = -113.3065670003

solvent phase geometry

C	0.134861	0.000000	0.000000
O	1.265139	0.000000	0.000000

Total solvent phase energy = -113.3075332433

Water

gas phase geometry

O	-1.028360	-1.404569	-2.200540
H	-1.028360	-0.647722	-1.598636
H	-1.028360	-2.161416	-1.598636

Total gas phase energy = -76.428996364

solvent phase geometry

O	-1.028360	-1.404569	-2.204210
H	-1.028360	-0.649573	-1.596801
H	-1.028360	-2.159565	-1.596801

Total solvent phase energy = -76.4396597330

Acetonitrile

gas phase geometry

C	-3.938207	0.004263	-9.044697
H	-3.397715	-0.950975	-8.952612
H	-3.209795	0.826165	-8.967175
H	-4.651655	0.087683	-8.210196
C	-4.647540	0.066440	-10.320109
N	-5.214534	0.110939	-11.329259

Total gas phase energy = -132.7283311911

solvent phase geometry

C	-3.936677	0.004166	-9.042113
H	-3.399161	-0.952929	-8.956996
H	-3.210690	0.828318	-8.971506
H	-4.655998	0.088079	-8.213239
C	-4.644263	0.066122	-10.315220
N	-5.212658	0.110759	-11.324973

Total solvent phase energy = -132.7398101487

Phenol

gas phase geometry

H	-0.820400	-2.584850	-1.858625
C	-0.689725	-6.768792	0.066903
C	-1.602960	-5.721902	0.222441
C	0.393128	-6.609573	-0.808622

H	-2.455437	-5.835341	0.898190
H	1.113390	-7.422078	-0.942892
C	-1.439088	-4.524587	-0.483284
C	0.566160	-5.421253	-1.519441
H	-2.154990	-3.705063	-0.352918
H	1.405958	-5.279138	-2.203465
C	-0.351348	-4.370782	-1.357281
H	-0.825146	-7.703026	0.617083
O	-0.132136	-3.231002	-2.065328

Total gas phase energy = -307.4112838442

solvent phase geometry

H	-0.822806	-2.578116	-1.861446
C	-0.689302	-6.770755	0.067099
C	-1.603528	-5.721823	0.222928
C	0.394568	-6.611842	-0.808588
H	-2.456087	-5.835496	0.898937
H	1.115295	-7.424078	-0.943771
C	-1.440761	-4.522898	-0.481972
C	0.567059	-5.421231	-1.519401
H	-2.154164	-3.701772	-0.354127
H	1.409028	-5.282932	-2.202700
C	-0.351725	-4.370080	-1.356881
H	-0.825032	-7.705545	0.616938
O	-0.135139	-3.230818	-2.064253

Total solvent phase energy = -307.4210036807

Deprotonated Phenol

gas phase geometry

C	-1.035531	0.001177	-4.617503
C	-1.035530	1.231939	-3.933223
C	-1.035530	-1.174026	-3.842031
H	-1.035530	2.166021	-4.513414
H	-1.035529	-2.149425	-4.350120
C	-1.035529	1.296510	-2.544073
C	-1.035529	-1.133008	-2.452185
H	-1.035528	2.262462	-2.024027
H	-1.035528	-2.057065	-1.861285
C	-1.035532	0.111835	-1.694613
H	-1.035532	-0.042231	-5.712144
O	-1.035534	0.158576	-0.437600

Total gas phase energy = -306.8440632296

solvent phase geometry

C	-1.035475	0.001279	-4.613174
C	-1.035430	1.233318	-3.934616
C	-1.035604	-1.175714	-3.843346
H	-1.035532	2.165685	-4.512489
H	-1.035638	-2.149254	-4.349155
C	-1.035562	1.294704	-2.542049

C	-1.035443	-1.131086	-2.450356
H	-1.035706	2.261456	-2.024268
H	-1.035572	-2.055965	-1.861392
C	-1.035220	0.111360	-1.708609
H	-1.035542	-0.041734	-5.706459
O	-1.035636	0.158716	-0.436305

Total solvent phase energy = -306.9379035867

KCl

gas phase geometry

K	-0.399864	0.000000	0.000000
Cl	2.399864	0.000000	0.000000

Total gas phase energy = -43.0713790842

solvent phase geometry

K	-0.521103	0.000000	0.000000
Cl	2.521103	0.000000	0.000000

Total solvent phase energy = -43.1290050567

KBr

gas phase geometry

K	-0.500010	0.000000	0.000000
Br	2.500010	0.000000	0.000000

Total gas phase energy = -41.2977669061

solvent phase geometry

K	-0.664245	0.000000	0.000000
Br	2.664245	0.000000	0.000000

Total solvent phase energy = -41.3543747089

1X-Re

gas phase geometry

Re	0.751109	-0.152593	-0.000081
Cl	0.362072	2.360358	0.000005
C	0.836992	-2.071196	-0.000245
O	0.857843	-3.230689	-0.000642
N	-0.996142	-0.117747	1.330177
N	-0.996181	-0.117508	-1.330282
C	-0.910216	-0.089893	2.669890
C	-0.910362	-0.089602	-2.670004
C	-2.029394	-0.000029	3.492264
C	-2.029625	-0.000076	-3.492304
C	-3.291728	0.064413	2.899577
C	-3.291943	0.063935	-2.899537
C	-3.381514	0.048756	1.510007
C	-3.381622	0.048263	-1.509963
C	-2.213544	-0.033907	0.739573
C	-2.213571	-0.033967	-0.739602
H	0.094618	-0.138422	3.091482
H	0.094490	-0.137696	-3.091612

H	-1.900647	0.022463	4.576212
H	-1.900972	0.022496	-4.576263
H	-4.195172	0.133539	3.509168
H	-4.195453	0.132726	-3.509069
H	-4.356335	0.110314	1.027923
H	-4.356434	0.109393	-1.027803
C	2.099799	-0.027944	1.375628
C	2.100246	-0.027843	-1.375385
O	2.856975	0.052080	2.244125
O	2.858155	0.052131	-2.243239

Total gas phase energy = -952.3775210771

solvent phase geometry

Re	0.755180	-0.130934	0.000019
Cl	0.459464	2.427745	0.000617
C	0.798245	-2.040904	-0.000260
O	0.806288	-3.201884	0.000381
N	-0.991871	-0.076385	1.334144
N	-0.991808	-0.075982	-1.334277
C	-0.910378	-0.061834	2.675629
C	-0.910294	-0.061687	-2.675771
C	-2.035030	-0.001172	3.493964
C	-2.034998	-0.001995	-3.494117
C	-3.295509	0.044590	2.896037
C	-3.295509	0.043327	-2.896220
C	-3.381948	0.036975	1.504918
C	-3.381958	0.036134	-1.505110
C	-2.210541	-0.018839	0.739462
C	-2.210523	-0.018954	-0.739624
H	0.090283	-0.103016	3.107468
H	0.090424	-0.102208	-3.107571
H	-1.911400	0.009105	4.578532
H	-1.911352	0.007845	-4.578689
H	-4.202617	0.088679	3.502043
H	-4.202630	0.086471	-3.502270
H	-4.357018	0.077502	1.021515
H	-4.357036	0.076253	-1.021660
C	2.103455	-0.050237	1.375776
C	2.103737	-0.049502	-1.375452
O	2.873165	0.005745	2.239108
O	2.873620	0.006918	-2.238591

Total solvent phase energy = -952.4054643743

1X+K-Re

gas phase geometry

Re	0.655234	0.049650	0.000009
Cl	0.000851	2.555587	-0.004537
C	1.027321	-1.845934	0.001528
O	1.243839	-2.976630	0.000045
N	-1.087199	-0.117644	1.333550

N	-1.087851	-0.120669	-1.332719
C	-1.006573	-0.140340	2.675055
C	-1.008011	-0.145279	-2.674241
C	-2.131415	-0.125895	3.495123
C	-2.133336	-0.131236	-3.493701
C	-3.392633	-0.084425	2.898996
C	-3.394207	-0.088309	-2.896948
C	-3.478556	-0.067135	1.508503
C	-3.479341	-0.069100	-1.506443
C	-2.307540	-0.085100	0.740390
C	-2.307898	-0.086456	-0.738973
H	-0.003191	-0.170560	3.102182
H	-0.004894	-0.176420	-3.101913
H	-2.009411	-0.146299	4.579835
H	-2.012001	-0.153007	-4.578462
H	-4.300076	-0.067595	3.506370
H	-4.301982	-0.071709	-3.503844
H	-4.454977	-0.037191	1.026927
H	-4.455477	-0.037872	-1.024363
C	1.972732	0.406025	1.351690
C	1.972948	0.401730	-1.352377
O	2.745877	0.734853	2.152834
O	2.746713	0.728275	-2.153940
K	2.952499	3.420442	-0.010576

Total gas phase energy = -957.4049074155

solvent phase geometry

Re	0.655338	0.070005	0.038589
Cl	-0.021440	2.577720	-0.002889
C	1.035796	-1.804432	0.088082
O	1.270131	-2.939037	0.115110
N	-1.092587	-0.120769	1.362828
N	-1.074733	-0.091303	-1.305086
C	-1.019740	-0.182290	2.703995
C	-0.986428	-0.053436	-2.646207
C	-2.151472	-0.247095	3.512676
C	-2.107862	-0.004488	-3.469801
C	-3.408610	-0.247438	2.905920
C	-3.372410	0.004684	-2.879002
C	-3.486245	-0.189382	1.515477
C	-3.466938	-0.039539	-1.489090
C	-2.309040	-0.129384	0.759821
C	-2.299238	-0.084988	-0.717990
H	-0.020732	-0.178650	3.142162
H	0.017175	-0.057065	-3.073172
H	-2.036646	-0.299000	4.596940
H	-1.978755	0.031448	-4.553132
H	-4.320469	-0.297905	3.504443
H	-4.276721	0.048532	-3.489266
H	-4.458789	-0.196767	1.025185

H	-4.445476	-0.030312	-1.010944
C	1.970193	0.457978	1.398723
C	1.992605	0.319003	-1.318042
O	2.734272	0.754569	2.215365
O	2.780613	0.500659	-2.150138
K	2.839652	3.780436	-0.780558

Total solvent phase energy = -957.4970799284

2-Re

gas phase geometry

Re	-0.770847	0.116401	-0.000135
N	0.932610	0.077680	-1.311145
N	0.932506	0.077616	1.310912
C	0.862514	0.058095	-2.671977
C	0.862350	0.057916	2.671757
C	1.972874	0.031992	-3.488442
C	1.972667	0.031754	3.488268
C	3.257066	0.022779	-2.896124
C	3.256899	0.022614	2.896021
C	3.349527	0.029623	-1.517707
C	3.349429	0.029569	1.517610
C	2.182222	0.049678	-0.721874
C	2.182172	0.049651	0.721712
H	-0.142700	0.064229	-3.096112
H	-0.142880	0.063995	3.095852
H	1.842508	0.017663	-4.572207
H	1.842242	0.017312	4.572025
H	4.158210	0.006788	-3.512483
H	4.158010	0.006586	3.512426
H	4.327638	0.016680	-1.036760
H	4.327566	0.016680	1.036713
C	-1.341261	-1.686529	0.000051
O	-1.653462	-2.803870	0.002135
C	-2.063933	0.574318	-1.368018
C	-2.063985	0.574003	1.367750
O	-2.798948	0.877253	-2.210236
O	-2.799055	0.876766	2.209987

Total gas phase energy = -939.1993252623

solvent phase geometry

Re	-0.254979	0.311344	-0.006943
N	1.433593	0.083194	1.311504
N	1.431447	0.079239	-1.314035
C	1.360031	0.074696	2.671150
C	1.357727	0.046910	-2.674290
C	2.472672	0.014534	3.486845
C	2.468331	-0.040311	-3.488844
C	3.751553	-0.038435	2.894755
C	3.747591	-0.095317	-2.896950
C	3.843947	-0.039061	1.512704

C	3.840922	-0.071762	-1.515027
C	2.676677	0.017652	0.724539
C	2.675684	0.009098	-0.726711
H	0.358195	0.123485	3.099729
H	0.356503	0.097022	-3.103748
H	2.343116	0.010305	4.570988
H	2.336499	-0.066141	-4.572322
H	4.652615	-0.080330	3.509806
H	4.647465	-0.159439	-3.511565
H	4.820766	-0.083319	1.031568
H	4.817677	-0.118880	-1.034022
C	-0.441481	2.188661	0.058026
O	-0.529772	3.350088	0.093462
C	-1.603606	0.016312	1.344846
C	-1.595686	0.162215	-1.390375
O	-2.388400	-0.203364	2.174574
O	-2.373417	0.066939	-2.249663

Total solvent phase energy = -939.2144946719

2X+K-Re

gas phase geometry

Re	0.850762	-0.161367	-0.106826
Cl	0.861234	2.471787	-0.123533
C	0.793391	-2.065744	-0.068714
O	0.752532	-3.224686	-0.043776
N	-0.799893	0.032031	1.325868
N	-0.960055	-0.033607	-1.335698
C	-0.655088	0.208056	2.650923
C	-0.973510	0.049050	-2.678065
C	-1.718521	0.330955	3.535265
C	-2.134313	0.105643	-3.437092
C	-3.034078	0.233225	3.012810
C	-3.378292	0.043625	-2.757852
C	-3.212301	0.044487	1.658367
C	-3.394637	-0.051112	-1.381898
C	-2.082827	-0.031254	0.783422
C	-2.168842	-0.070621	-0.642598
H	0.374815	0.255158	3.012581
H	0.005489	0.070654	-3.161838
H	-1.528513	0.480328	4.599105
H	-2.071691	0.172486	-4.524128
H	-3.900890	0.291417	3.676249
H	-4.316120	0.051118	-3.319402
H	-4.218696	-0.058522	1.249114
H	-4.345960	-0.129142	-0.853259
C	2.306749	-0.135792	1.165387
C	2.073871	-0.178445	-1.598735
O	3.144350	-0.112507	1.962738
O	2.730955	-0.177122	-2.551254
K	-2.038477	2.941656	-0.047159

Total gas phase energy = -957.5651230005

solvent phase geometry

Re	0.815898	-0.319896	0.028278
Cl	0.893340	2.325092	0.085672
C	0.687443	-2.212700	0.013775
O	0.601923	-3.374110	0.008706
N	-0.877118	-0.073047	1.375788
N	-0.894489	-0.050375	-1.292103
C	-0.795548	-0.048648	2.723078
C	-0.839998	-0.008213	-2.642471
C	-1.886971	0.125700	3.556064
C	-1.946285	0.176925	-3.453017
C	-3.165588	0.286339	2.959723
C	-3.223501	0.299956	-2.831416
C	-3.273157	0.271353	1.585782
C	-3.307786	0.249590	-1.456333
C	-2.116268	0.094978	0.770422
C	-2.131717	0.093218	-0.658919
H	0.202572	-0.182928	3.145242
H	0.150996	-0.128663	-3.085528
H	-1.749078	0.136084	4.638800
H	-1.826183	0.211080	-4.537215
H	-4.054950	0.425668	3.579234
H	-4.125046	0.429669	-3.434823
H	-4.248346	0.401896	1.114856
H	-4.278941	0.340357	-0.967952
C	2.170694	-0.375379	1.402252
C	2.128674	-0.349012	-1.385457
O	2.943109	-0.395893	2.269105
O	2.861163	-0.353167	-2.286710
K	-1.753399	3.355880	-1.224833

Total solvent phase energy = -957.6115538218

2X-Re

gas phase geometry

Re	0.756775	-0.143133	0.000002
Cl	0.539337	2.426443	-0.000672
C	0.773041	-2.051619	0.000180
O	0.773878	-3.217525	-0.000809
N	-0.972664	-0.065564	1.336964
N	-0.972676	-0.065764	-1.336895
C	-0.908661	-0.028867	2.677347
C	-0.908680	-0.028948	-2.677280
C	-2.020128	0.019328	3.505806
C	-2.020139	0.019463	-3.505732
C	-3.302103	0.033025	2.894047
C	-3.302112	0.033256	-2.893969
C	-3.391051	0.011197	1.520818
C	-3.391052	0.011331	-1.520740

C	-2.214695	-0.028183	0.713323
C	-2.214698	-0.028216	-0.713250
H	0.097590	-0.039918	3.103203
H	0.097581	-0.040028	-3.103116
H	-1.891621	0.051284	4.589530
H	-1.891637	0.051555	-4.589453
H	-4.209760	0.066433	3.503447
H	-4.209765	0.066853	-3.503365
H	-4.369189	0.030134	1.038275
H	-4.369184	0.030388	-1.038187
C	2.092831	-0.064481	1.386369
C	2.092978	-0.065193	-1.386264
O	2.848346	-0.015122	2.268177
O	2.848900	-0.016373	-2.267756

Total gas phase energy = -954.2029933881

solvent phase geometry

Re	0.746355	-0.146689	0.000284
Cl	0.531275	2.463023	-0.002588
C	0.776459	-2.045363	0.001264
O	0.779059	-3.211065	-0.001037
N	-0.970275	-0.062606	1.334924
N	-0.970204	-0.064043	-1.334426
C	-0.906574	-0.039186	2.682908
C	-0.906210	-0.039687	-2.682374
C	-2.018107	0.011685	3.505458
C	-2.017526	0.012652	-3.505125
C	-3.302555	0.035332	2.894166
C	-3.302066	0.036682	-2.894060
C	-3.391788	0.020163	1.519993
C	-3.391558	0.020919	-1.519891
C	-2.214733	-0.019413	0.714321
C	-2.214681	-0.019647	-0.714047
H	0.096635	-0.065075	3.114853
H	0.097029	-0.066755	-3.114160
H	-1.892690	0.031133	4.589764
H	-1.891897	0.032682	-4.589397
H	-4.208356	0.066783	3.504757
H	-4.207791	0.069029	-3.504714
H	-4.370075	0.041446	1.038283
H	-4.369963	0.042780	-1.038443
C	2.086710	-0.065046	1.384854
C	2.086209	-0.067370	-1.384846
O	2.854995	-0.008516	2.255717
O	2.853768	-0.012094	-2.256440

Total solvent phase energy = -952.5051228561

2S-Re

gas phase geometry

Re	-0.873638	0.270114	-0.075681

C	2.088559	0.182403	0.658243
N	0.841662	0.246931	1.274692
C	0.773135	0.300645	2.621764
C	1.881383	0.299680	3.447971
C	3.166236	0.232345	2.842753
C	3.260294	0.174569	1.471450
C	-2.233403	0.465161	1.290892
O	-3.013062	0.583173	2.138719
C	2.095246	0.118947	-0.768710
N	0.855167	0.141105	-1.399855
C	0.796218	0.064899	-2.746191
C	1.910041	-0.025700	-3.559343
C	3.188870	-0.050097	-2.939264
C	3.272669	0.021069	-1.567848
C	-1.029863	-1.651935	-0.028283
O	-1.087808	-2.803712	-0.005273
C	-2.199709	0.391944	-1.482422
O	-2.947715	0.468975	-2.362857
H	-0.206397	0.076502	-3.180218
H	-0.233075	0.347338	3.045272
H	1.789848	-0.090571	-4.641920
H	1.753506	0.344802	4.530801
H	4.096008	-0.135965	-3.542172
H	4.069666	0.221016	3.457235
H	4.247528	-0.009950	-1.080473
H	4.239468	0.115633	0.995425
N	-0.451364	2.395253	-0.117220
C	-0.109134	3.499001	-0.104810
C	0.323385	4.887951	-0.085002
H	-0.276621	5.464009	0.635304
H	1.383152	4.945974	0.210615
H	0.204547	5.335251	-1.084519

Total gas phase energy = -1071.9419063306

solvent phase geometry

Re	-0.869602	0.265925	-0.072241
C	2.090609	0.170822	0.661020
N	0.843373	0.241734	1.275792
C	0.773919	0.302955	2.624000
C	1.882536	0.296002	3.449853
C	3.168474	0.216793	2.845622
C	3.263201	0.155550	1.473407
C	-2.225625	0.461797	1.293591
O	-3.009575	0.572818	2.141933
C	2.097097	0.110867	-0.766674
N	0.856139	0.139620	-1.396568
C	0.796844	0.073255	-2.744945
C	1.911136	-0.018325	-3.557578
C	3.191472	-0.051059	-2.937685
C	3.275493	0.013034	-1.564872

C	-1.031675	-1.646102	-0.028919
O	-1.092757	-2.802603	-0.007931
C	-2.194489	0.392310	-1.475292
O	-2.948602	0.464817	-2.354297
H	-0.203704	0.095303	-3.183081
H	-0.230301	0.362456	3.050107
H	1.791252	-0.071789	-4.641175
H	1.754934	0.351458	4.532557
H	4.098386	-0.133623	-3.541480
H	4.071401	0.202659	3.460864
H	4.250990	-0.018827	-1.078654
H	4.242915	0.090718	0.999005
N	-0.443024	2.405831	-0.115799
C	-0.107989	3.511987	-0.109114
C	0.311986	4.901336	-0.097785
H	-0.295490	5.469191	0.622076
H	1.371762	4.965272	0.195187
H	0.183713	5.334578	-1.101847

Total solvent phase energy = -1071.9585055848

2D-Re

gas phase geometry

Re	4.445676	4.634490	-14.288053
O	4.414363	4.810549	-11.215789
O	3.027378	1.905088	-14.188343
O	7.196256	3.231378	-14.285649
N	2.635593	5.742915	-14.680150
N	5.088647	6.682274	-14.642202
C	4.413638	4.773729	-12.375662
C	3.594799	2.921333	-14.218551
C	6.163498	3.763521	-14.278853
C	1.400062	5.181874	-14.711812
H	1.358197	4.107160	-14.534470
C	0.248018	5.909354	-14.950508
H	-0.715630	5.395873	-14.963304
C	0.350261	7.294270	-15.166075
C	1.608152	7.876824	-15.135713
H	1.718692	8.945525	-15.319115
C	2.746826	7.090239	-14.893368
C	4.111509	7.609999	-14.879522
C	4.438472	8.955258	-15.122477
H	3.648200	9.676490	-15.329220
C	5.765286	9.359866	-15.119778
C	6.758196	8.401496	-14.864959
H	7.817269	8.665919	-14.859539
C	6.380535	7.090785	-14.627862
H	7.124008	6.317111	-14.440024
Re	4.833865	4.143944	-17.407056
O	5.154818	3.972201	-20.462074
O	3.370316	6.838582	-17.715725

O	7.553652	5.546247	-16.976338
N	3.039898	2.941225	-17.295978
N	5.516183	2.124846	-16.975554
C	5.045002	4.009650	-19.307438
C	3.950492	5.836210	-17.594957
C	6.526366	5.034764	-17.160632
C	1.786324	3.436535	-17.447780
H	1.716105	4.510386	-17.620813
C	0.651115	2.647900	-17.390262
H	-0.327937	3.112727	-17.522290
C	0.791888	1.266410	-17.175123
C	2.069414	0.749931	-17.021690
H	2.209599	-0.315223	-16.837093
C	3.188184	1.597899	-17.079945
C	4.563776	1.145841	-16.891373
C	4.921626	-0.187254	-16.625391
H	4.148681	-0.951210	-16.542165
C	6.256077	-0.529830	-16.459073
C	7.224921	0.478785	-16.565662
H	8.287667	0.264159	-16.436903
C	6.816846	1.776851	-16.823910
H	7.541392	2.586654	-16.900942
H	-0.081160	0.612864	-17.123057
H	6.544879	-1.560815	-16.242109
H	6.030963	10.399577	-15.323277
H	-0.537119	7.899346	-15.361765

Total gas phase energy = -1878.4219796663

solvent phase geometry

Re	4.470805	4.652739	-14.291505
O	4.423316	4.877636	-11.223906
O	3.085960	1.908351	-14.142263
O	7.222853	3.257127	-14.263013
N	2.640809	5.748341	-14.698820
N	5.094078	6.714518	-14.656122
C	4.420091	4.839594	-12.391009
C	3.637984	2.933887	-14.200748
C	6.187688	3.792917	-14.274653
C	1.412912	5.176415	-14.735970
H	1.375945	4.100631	-14.565337
C	0.253234	5.896773	-14.972648
H	-0.706174	5.376181	-14.994993
C	0.346399	7.281846	-15.176581
C	1.600869	7.876937	-15.138176
H	1.700027	8.949067	-15.308253
C	2.742497	7.094944	-14.900947
C	4.105883	7.630532	-14.879068
C	4.411055	8.984545	-15.094092
H	3.611377	9.701569	-15.278572
C	5.734565	9.407134	-15.084044

C	6.740710	8.458686	-14.851353
H	7.795468	8.740018	-14.836205
C	6.379853	7.137248	-14.637492
H	7.134334	6.372581	-14.455916
Re	4.848476	4.129268	-17.391195
O	5.149533	3.920284	-20.444926
O	3.433551	6.845956	-17.729933
O	7.585666	5.496407	-16.969409
N	3.036879	2.934361	-17.278026
N	5.515831	2.095801	-16.956267
C	5.041636	3.955402	-19.283005
C	3.989416	5.830375	-17.589053
C	6.546655	4.997377	-17.144681
C	1.788948	3.437550	-17.433771
H	1.721616	4.511414	-17.606799
C	0.647756	2.653227	-17.383034
H	-0.329243	3.121868	-17.515217
C	0.782898	1.272672	-17.172241
C	2.059223	0.746879	-17.017546
H	2.191788	-0.321134	-16.843288
C	3.179089	1.591986	-17.068676
C	4.555861	1.126417	-16.887072
C	4.899989	-0.215643	-16.655460
H	4.122443	-0.977074	-16.594217
C	6.234518	-0.574105	-16.505378
C	7.212102	0.426529	-16.591981
H	8.273964	0.197129	-16.481384
C	6.813254	1.735497	-16.817786
H	7.546951	2.537985	-16.886416
H	-0.092945	0.622393	-17.127301
H	6.514111	-1.614023	-16.321933
H	5.984323	10.455596	-15.260848
H	-0.545098	7.881904	-15.368844

Total solvent phase energy = -1878.4462206123

2CO-Re

gas phase geometry

Re	-0.000271	-0.000114	-0.925770
C	2.010070	0.000250	-0.871972
C	-2.010592	0.000222	-0.871640
O	3.152813	0.001495	-0.847070
O	-3.153341	0.001509	-0.846711
N	0.000079	-1.342162	0.802629
N	0.000075	1.341971	0.802635
C	0.000204	-2.692035	0.741534
C	0.000210	2.691858	0.741533
C	0.000152	-3.508328	1.855159
C	0.000172	3.508151	1.855163
C	-0.000036	-2.892161	3.136497
C	-0.000012	2.891983	3.136502

C	-0.000108	-1.519901	3.221979
C	-0.000094	1.519724	3.221985
C	-0.000022	-0.713460	2.045257
C	-0.000019	0.713278	2.045263
H	0.000363	-3.126402	-0.260696
H	0.000365	3.126191	-0.260716
H	0.000269	-4.592650	1.733844
H	0.000296	4.592474	1.733841
H	-0.000128	-3.499841	4.044246
H	-0.000093	3.499665	4.044253
H	-0.000248	-1.036168	4.198794
H	-0.000230	1.035988	4.198798
C	-0.000217	-1.424196	-2.257879
C	-0.000270	1.423627	-2.258271
O	0.000386	-2.319766	-2.985005
O	0.000226	2.318800	-2.985890

Total gas phase energy = -1027.7826924762

solvent phase geometry

Re	-0.000107	-0.000101	-0.924534
C	2.010122	-0.000015	-0.873879
C	-2.010388	0.000404	-0.872890
O	3.153107	0.000855	-0.850179
O	-3.153388	0.001635	-0.850014
N	0.000697	-1.342038	0.804099
N	0.000794	1.341872	0.804094
C	0.000439	-2.692654	0.742142
C	0.000676	2.692494	0.742130
C	-0.000034	-3.508483	1.857261
C	-0.000003	3.508331	1.857249
C	0.000007	-2.892093	3.139850
C	-0.000618	2.891947	3.139839
C	0.000284	-1.518658	3.225939
C	-0.000417	1.518512	3.225935
C	0.000387	-0.713711	2.047342
C	0.000284	0.713553	2.047341
H	0.000878	-3.129041	-0.259047
H	0.001373	3.128855	-0.259074
H	-0.000312	-4.593198	1.736347
H	-0.000089	4.593046	1.736329
H	-0.000096	-3.500264	4.047492
H	-0.001288	3.500118	4.047484
H	0.000629	-1.034845	4.203028
H	-0.001103	1.034706	4.203029
C	-0.000733	-1.415929	-2.261122
C	-0.000436	1.415470	-2.261426
O	-0.000631	-2.301511	-3.002897
O	-0.000032	2.300742	-3.003578

Total solvent phase energy = -1027.7921979038

3-Re

gas phase geometry

Re	-0.221405	0.449981	0.000224
N	1.432500	0.166451	1.291484
N	1.432241	0.166814	-1.291107
C	1.375288	0.142041	2.664404
C	1.375024	0.142310	-2.664120
C	2.463540	0.001832	3.483712
C	2.463193	0.001696	-3.483433
C	3.765556	-0.125834	2.897436
C	3.765258	-0.126362	-2.897291
C	3.862336	-0.107159	1.529917
C	3.862098	-0.107584	-1.529787
C	2.706140	0.032548	0.704127
C	2.706027	0.032570	-0.703921
H	0.374664	0.246714	3.088415
H	0.374444	0.247211	-3.088158
H	2.319794	-0.013040	4.567071
H	2.319376	-0.013241	-4.566786
H	4.654914	-0.241710	3.522487
H	4.654522	-0.242682	-3.522394
H	4.837137	-0.209354	1.048311
H	4.836877	-0.210186	-1.048218
C	-0.633741	2.302133	0.000807
O	-0.871407	3.448182	-0.002579
C	-1.531700	0.054479	1.358974
C	-1.531684	0.056904	-1.359072
O	-2.292619	-0.221630	2.202843
O	-2.292704	-0.217751	-2.203347

Total gas phase energy = -914.5013595099

solvent phase geometry

Re	-0.227772	0.460172	0.033294
N	1.415523	0.095453	1.302885
N	1.436303	0.229526	-1.278601
C	1.362675	-0.002547	2.681654
C	1.372192	0.295515	-2.648512
C	2.456993	-0.178287	3.483554
C	2.468520	0.224730	-3.470131
C	3.756878	-0.271089	2.892974
C	3.764091	0.080092	-2.887482
C	3.848993	-0.185889	1.525215
C	3.860604	0.005192	-1.518829
C	2.689608	-0.009054	0.716520
C	2.696065	0.071721	-0.698090
H	0.366522	0.068734	3.120678
H	0.370549	0.417753	-3.065517
H	2.317777	-0.253105	4.564857
H	2.333457	0.284767	-4.552566
H	4.646002	-0.414610	3.510598

H	4.656957	0.027913	-3.514750
H	4.822547	-0.261070	1.037522
H	4.836185	-0.109612	-1.043838
C	-0.628551	2.272915	-0.341986
O	-0.887667	3.389708	-0.595292
C	-1.501551	0.352738	1.475002
C	-1.505131	-0.185501	-1.250008
O	-2.216759	0.285100	2.401035
O	-2.247526	-0.581459	-2.067403

Total solvent phase energy = -914.5679878057

3+K-Re

gas phase geometry

Re	-0.324306	0.486180	0.033282
N	1.318997	0.103556	1.283624
N	1.324046	0.252009	-1.299498
C	1.283161	0.057140	2.669398
C	1.252597	0.367260	-2.665758
C	2.389167	-0.025482	3.464596
C	2.342650	0.339437	-3.495369
C	3.692689	-0.104088	2.862037
C	3.644287	0.171313	-2.924244
C	3.772459	-0.119919	1.494290
C	3.753957	0.026086	-1.565712
C	2.599561	-0.019825	0.679296
C	2.592885	0.058656	-0.726706
H	0.287066	0.103377	3.112233
H	0.246816	0.499387	-3.069538
H	2.263794	-0.057925	4.549095
H	2.201830	0.439261	-4.573373
H	4.589203	-0.189425	3.479390
H	4.531562	0.138625	-3.560737
H	4.742971	-0.218194	1.003890
H	4.731554	-0.132966	-1.107106
C	-0.642441	2.308402	-0.257296
O	-0.650831	3.480921	-0.405027
C	-1.598316	0.397196	1.493936
C	-1.661421	-0.062070	-1.269600
O	-2.291221	0.345894	2.423681
O	-2.414610	-0.407261	-2.080382
K	2.229626	2.922232	0.418588

Total gas phase energy = -942.5942457217

solvent phase geometry

Re	-0.255110	0.778064	-0.012296
N	1.347280	0.168298	1.251704
N	1.441482	0.644980	-1.286551
C	1.226545	-0.078327	2.599647
C	1.441722	0.917633	-2.640306
C	2.262672	-0.498440	3.393295

C	2.550351	0.814189	-3.439377
C	3.548906	-0.701078	2.812147
C	3.790327	0.393364	-2.871388
C	3.697052	-0.481628	1.462798
C	3.819494	0.090981	-1.530111
C	2.594020	-0.057336	0.668366
C	2.648481	0.205263	-0.729028
H	0.233793	0.087147	3.021501
H	0.485202	1.240574	-3.054698
H	2.083284	-0.677740	4.455471
H	2.468198	1.061386	-4.500197
H	4.392380	-1.031017	3.422129
H	4.688440	0.306255	-3.486818
H	4.664862	-0.640219	0.984921
H	4.745755	-0.247980	-1.063571
C	-1.311558	1.824716	-1.235168
O	-1.922877	2.485942	-1.985336
C	-1.236603	1.531224	1.457113
C	-1.311837	-0.793712	-0.191190
O	-1.771990	2.007061	2.385847
O	-1.982261	-1.751729	-0.288272
K	1.869724	3.561902	0.366354

Total solvent phase energy = -942.6354894173

4-Re

gas phase geometry

H	-0.482757	1.843274	0.000391
Re	-0.793883	0.126838	-0.000098
N	0.952203	0.037694	-1.320647
N	0.952169	0.037517	1.320519
C	0.873699	0.034845	-2.666385
C	0.873632	0.034654	2.666253
C	1.995117	0.050020	-3.487155
C	1.995029	0.049969	3.487052
C	3.263510	0.070404	-2.898245
C	3.263435	0.070496	2.898177
C	3.350882	0.068790	-1.510384
C	3.350842	0.068879	1.510318
C	2.179853	0.050201	-0.736557
C	2.179834	0.050170	0.736463
H	-0.132236	0.025106	-3.088170
H	-0.132311	0.024820	3.088016
H	1.866253	0.048385	-4.571474
H	1.866137	0.048345	4.571368
H	4.168114	0.088370	-3.509634
H	4.168021	0.088588	3.509589
H	4.326964	0.085826	-1.026691
H	4.326934	0.086044	1.026649
C	-1.137080	-1.824819	-0.000014
O	-1.379140	-2.956729	0.000971

C	-2.111935	0.474991	-1.360959
C	-2.111993	0.474638	1.360789
O	-2.867253	0.718595	-2.205342
O	-2.867349	0.718024	2.205200

Total gas phase energy = -915.042028023

solvent phase geometry

H	-0.237357	-1.554344	0.002364
Re	-0.320170	0.193990	-0.000293
N	1.438305	0.073750	1.331307
N	1.438429	0.072379	-1.331484
C	1.361554	0.059251	2.674823
C	1.361941	0.057486	-2.675004
C	2.486905	0.013044	3.491962
C	2.487441	0.012182	-3.491963
C	3.749161	-0.019398	2.894737
C	3.749645	-0.018668	-2.894553
C	3.833021	-0.012034	1.504561
C	3.833268	-0.010973	-1.504350
C	2.659644	0.031712	0.738637
C	2.659717	0.031459	-0.738618
H	0.360709	0.088891	3.107429
H	0.361147	0.086713	-3.107769
H	2.363313	0.003661	4.576669
H	2.364075	0.002851	-4.576695
H	4.656879	-0.052345	3.500568
H	4.657490	-0.050011	-3.500272
H	4.807686	-0.041561	1.019374
H	4.807942	-0.037845	-1.019013
C	-0.275133	2.162420	-0.001301
O	-0.273004	3.321920	0.000708
C	-1.652201	0.118991	1.380192
C	-1.651925	0.117888	-1.381007
O	-2.411643	0.052301	2.259268
O	-2.411173	0.051624	-2.260278

Total solvent phase energy = -915.0676415973

5-Re (gas phase geometry not stable)

solvent phase geometry

Re	-0.869081	0.376830	0.009790
C	-0.623815	-1.959911	0.093644
O	-1.655713	-2.654846	0.236105
O	0.557055	-2.358717	-0.001937
N	0.843972	0.234320	1.325753
N	0.834280	0.222753	-1.328434
C	0.775667	0.240606	2.674554
C	0.759084	0.252991	-2.675324
C	1.876077	0.019288	3.487396
C	1.863843	0.086221	-3.496901
C	3.123061	-0.210736	2.884978

C	3.119267	-0.114203	-2.902629
C	3.202322	-0.216770	1.498735
C	3.203718	-0.151359	-1.516938
C	2.044354	-0.005365	0.727996
C	2.041852	0.005889	-0.738761
H	-0.208123	0.429170	3.105998
H	-0.231970	0.422089	-3.098804
H	1.754668	0.028404	4.572478
H	1.739793	0.119159	-4.581279
H	4.014883	-0.385808	3.490550
H	4.015546	-0.239669	-3.514049
H	4.158869	-0.398795	1.009974
H	4.168514	-0.307078	-1.035343
C	-0.940048	2.316916	-0.058998
O	-1.008291	3.481712	-0.100266
C	-2.198749	0.231662	1.385523
C	-2.203528	0.031596	-1.327426
O	-2.979963	0.118252	2.245047
O	-2.980330	-0.249522	-2.151923

Total gas phase energy = -1103.0660694294

Total solvent phase energy = -1103.1718233792

6-Re

gas phase geometry

Re	-0.898360	0.294598	0.000812
C	-0.681023	-1.896003	0.018032
O	0.389127	-2.477366	0.108545
O	-1.820471	-2.639479	-0.084741
H	-1.532635	-3.574596	-0.065299
N	0.838126	0.174689	1.329292
N	0.834580	0.163794	-1.331426
C	0.759904	0.169752	2.671495
C	0.754841	0.163818	-2.674458
C	1.873201	0.016726	3.489957
C	1.868343	0.023963	-3.494536
C	3.127728	-0.136697	2.893234
C	3.124832	-0.122856	-2.899651
C	3.210019	-0.147764	1.504732
C	3.208669	-0.139009	-1.511304
C	2.045238	-0.004366	0.736218
C	2.044193	-0.005274	-0.739911
H	-0.237010	0.293861	3.096498
H	-0.243614	0.282310	-3.097591
H	1.748754	0.018921	4.574633
H	1.742923	0.032071	-4.579143
H	4.028228	-0.253441	3.500158
H	4.025616	-0.228863	-3.508146
H	4.176114	-0.278978	1.019096
H	4.176700	-0.262460	-1.027532
C	-0.906401	2.267443	-0.006372

O	-0.914388	3.423017	-0.008479
C	-2.241576	0.196201	1.382163
C	-2.244536	0.187915	-1.377448
O	-2.993263	0.115857	2.258512
O	-2.998238	0.104892	-2.251610

Total gas phase energy = -1103.6315892979

solvent phase geometry

Re	-0.903755	0.270500	0.004352
C	-0.726281	-1.918623	0.016092
O	0.322098	-2.540248	0.126721
O	-1.884748	-2.638049	-0.119198
H	-1.633250	-3.585089	-0.102964
N	0.842802	0.144623	1.336242
N	0.838082	0.134637	-1.334070
C	0.767040	0.134212	2.678473
C	0.758330	0.125111	-2.676767
C	1.888403	0.011817	3.493206
C	1.877675	0.008072	-3.494626
C	3.143770	-0.101787	2.891328
C	3.135184	-0.102628	-2.896328
C	3.223929	-0.103473	1.500711
C	3.219529	-0.104463	-1.506003
C	2.053288	0.009760	0.738381
C	2.051154	0.006671	-0.739421
H	-0.228673	0.230701	3.112960
H	-0.239179	0.218230	-3.107930
H	1.768132	0.008339	4.578224
H	1.754291	0.005930	-4.579336
H	4.049545	-0.192744	3.494345
H	4.039411	-0.190385	-3.502126
H	4.193411	-0.198649	1.013627
H	4.190855	-0.196688	-1.022081
C	-0.860025	2.239953	-0.001263
O	-0.850645	3.397412	-0.003188
C	-2.244728	0.205167	1.380622
C	-2.248553	0.201773	-1.368017
O	-3.013209	0.142772	2.249676
O	-3.018263	0.139824	-2.235914

Total solvent phase energy = -1103.6614715616

7-Re

gas phase geometry

Re	-0.000077	-0.000281	-0.927916
C	2.017301	0.000285	-0.907308
C	-2.017463	0.000279	-0.907224
O	3.156679	0.002312	-0.899447
O	-3.156841	0.002343	-0.899398
N	0.000041	-1.339159	0.832172
N	0.000040	1.338830	0.832140

C	0.000065	-2.682724	0.753460
C	0.000065	2.682408	0.753396
C	0.000035	-3.499416	1.880679
C	0.000038	3.499132	1.880604
C	-0.000015	-2.899787	3.140810
C	-0.000004	2.899536	3.140752
C	-0.000020	-1.508360	3.224306
C	-0.000011	1.508113	3.224277
C	0.000010	-0.740517	2.052827
C	0.000013	0.740236	2.052813
H	0.000114	-3.115354	-0.248091
H	0.000111	3.115003	-0.248173
H	0.000052	-4.584510	1.759363
H	0.000053	4.584228	1.759278
H	-0.000049	-3.505213	4.049608
H	-0.000031	3.504982	4.049539
H	-0.000053	-1.025851	4.200677
H	-0.000038	1.025628	4.200659
C	-0.000084	-1.414739	-2.276928
C	-0.000109	1.413887	-2.277270
O	0.000132	-2.302223	-3.003218
O	0.000045	2.300931	-3.004096

Total gas phase energy = -1027.6014335046

solvent phase geometry

Re	0.000767	-0.007118	-0.922976
C	2.014728	0.007853	-0.890521
C	-2.013407	-0.015017	-0.891008
O	3.155259	0.018337	-0.879735
O	-3.153963	-0.018405	-0.881144
N	0.014029	-1.322774	0.846880
N	-0.013917	1.353337	0.814358
C	0.031096	-2.666360	0.782042
C	-0.030980	2.694995	0.718027
C	0.042630	-3.467597	1.919698
C	-0.044258	3.522774	1.836818
C	0.036306	-2.852348	3.172001
C	-0.039802	2.937168	3.103352
C	0.018867	-1.460242	3.240529
C	-0.022321	1.547065	3.204491
C	0.008138	-0.709325	2.059599
C	-0.009725	0.768798	2.041564
H	0.036062	-3.114252	-0.212047
H	-0.034587	3.118783	-0.286723
H	0.057307	-4.553481	1.810687
H	-0.058656	4.605867	1.702620
H	0.045488	-3.446249	4.087928
H	-0.050618	3.551764	4.005502
H	0.013639	-0.964752	4.210139
H	-0.018825	1.074133	4.185310

C	0.008611	-1.437878	-2.244362
C	-0.006001	1.370868	-2.301052
O	0.012363	-2.331664	-2.968956
O	-0.008891	2.225412	-3.071529

Total solvent phase energy = -1027.6761218423

8-Re

gas phase geometry

Re	-0.905120	0.264308	0.006078
C	-0.785201	-1.930755	0.008834
O	0.224315	-2.604268	0.119887
O	-1.980568	-2.615890	-0.141286
H	-1.716707	-3.558077	-0.126210
N	0.830377	0.118163	1.345222
N	0.825843	0.111345	-1.339170
C	0.771452	0.075705	2.684384
C	0.763067	0.065753	-2.678536
C	1.884028	-0.012514	3.509482
C	1.872773	-0.027014	-3.506533
C	3.161951	-0.065313	2.891251
C	3.153019	-0.081096	-2.891630
C	3.244630	-0.043511	1.517890
C	3.239735	-0.054281	-1.518728
C	2.066645	0.035451	0.714325
C	2.064679	0.030963	-0.711171
H	-0.232434	0.120006	3.114567
H	-0.242241	0.110350	-3.105499
H	1.759180	-0.043999	4.593693
H	1.744398	-0.061535	-4.590232
H	4.071370	-0.130209	3.495816
H	4.060353	-0.151082	-3.498670
H	4.219730	-0.095470	1.031670
H	4.216175	-0.107163	-1.035291
C	-0.823092	2.229900	0.004302
O	-0.810905	3.391412	0.003262
C	-2.229967	0.217671	1.398661
C	-2.232751	0.221533	-1.384721
O	-2.973166	0.170737	2.294711
O	-2.975948	0.181558	-2.280631

Total gas phase energy = -1103.6625254903

solvent phase geometry

Re	-0.900116	0.248710	-0.008723
C	-0.840624	-1.963019	0.101757
O	-1.491718	-2.691989	0.835606
O	0.064335	-2.619764	-0.711887
H	0.515122	-1.939222	-1.236465
N	0.839029	0.103010	1.326453
N	0.834513	0.088396	-1.357119
C	0.773107	0.062389	2.671205

C	0.781284	0.093715	-2.711765
C	1.884671	-0.021085	3.494563
C	1.895957	0.032927	-3.525075
C	3.165047	-0.069036	2.881748
C	3.178206	-0.027468	-2.903695
C	3.255355	-0.044590	1.507474
C	3.260356	-0.022763	-1.530178
C	2.078361	0.031944	0.701765
C	2.081949	0.037696	-0.725904
H	-0.229842	0.104938	3.102184
H	-0.220437	0.138226	-3.146244
H	1.759233	-0.047975	4.578611
H	1.778865	0.028524	-4.610303
H	4.070478	-0.129596	3.490851
H	4.086228	-0.079221	-3.509324
H	4.232904	-0.090077	1.026394
H	4.236230	-0.068985	-1.045388
C	-0.816108	2.210380	-0.025622
O	-0.793018	3.371383	-0.036140
C	-2.224030	0.228083	1.382766
C	-2.229302	0.198030	-1.395764
O	-2.976667	0.190423	2.270854
O	-2.988055	0.150642	-2.280192

Total solvent phase energy = -1103.7630803425

Reactant complex 3_4-Re (gas phase TS geometry not converged)

solvent phase geometry

Re	-0.876773	0.677976	-0.055334
C	-0.067639	-2.794203	0.701398
O	-0.665038	-2.820017	1.700560
O	0.539700	-2.830277	-0.290431
N	0.701720	0.165460	1.236236
N	0.789515	0.340722	-1.340799
C	0.614326	0.062789	2.614106
C	0.755695	0.437217	-2.707652
C	1.667367	-0.241318	3.430602
C	1.854621	0.274151	-3.513917
C	2.960781	-0.466743	2.861578
C	3.117859	-0.006476	-2.911769
C	3.088084	-0.369072	1.496685
C	3.180380	-0.118814	-1.543265
C	1.972258	-0.056654	0.670856
C	2.012945	0.046365	-0.741562
H	-0.374817	0.239301	3.037044
H	-0.221283	0.668421	-3.136831
H	1.500500	-0.312078	4.508327
H	1.747299	0.370000	-4.596816
H	3.817285	-0.714335	3.492216
H	4.013422	-0.133833	-3.524735
H	4.057592	-0.540947	1.025476

H	4.130396	-0.340196	-1.054122
C	-1.175904	2.497243	-0.498078
O	-1.366737	3.618155	-0.794168
C	-2.161575	0.669734	1.378674
C	-2.158842	0.038873	-1.331960
O	-2.873461	0.647373	2.309618
O	-2.904417	-0.360718	-2.145424

Total gas phase energy = -1103.09046753
Total solvent phase energy = -1103.1584215117

TS 3_4-Re (gas phase geometry not converged)
solvent phase geometry

Re	-0.838224	0.550707	-0.022641
C	-0.579266	-2.348556	0.382922
O	-1.391482	-2.603885	1.214116
O	0.294700	-2.643302	-0.366489
N	0.791801	0.151327	1.276197
N	0.838483	0.270889	-1.321888
C	0.718138	0.084634	2.648333
C	0.783586	0.338980	-2.683242
C	1.799891	-0.145124	3.460749
C	1.887238	0.214139	-3.496727
C	3.085730	-0.324210	2.879596
C	3.158615	0.007912	-2.900808
C	3.188195	-0.265844	1.506049
C	3.235236	-0.079521	-1.527073
C	2.045899	-0.031872	0.699770
C	2.066198	0.041711	-0.730432
H	-0.273762	0.229243	3.077192
H	-0.206166	0.515337	-3.107942
H	1.653625	-0.187269	4.542764
H	1.768112	0.285049	-4.580094
H	3.964391	-0.506599	3.501645
H	4.057055	-0.082634	-3.515506
H	4.157625	-0.404700	1.025484
H	4.198252	-0.243245	-1.042184
C	-1.027248	2.410271	-0.370496
O	-1.161435	3.547322	-0.627913
C	-2.125426	0.516773	1.404683
C	-2.145303	-0.017751	-1.312617
O	-2.839084	0.469296	2.330630
O	-2.908159	-0.384001	-2.124566

Total gas phase energy = -1103.0812470558
Total solvent phase energy = -1103.15343428

Reactant complex 3_5-Re (gas phase TS geometry not converged)
solvent phase geometry

Re	-1.490594	-0.330225	-0.382994
H	-0.738711	-2.524836	-1.760679
N	-0.453622	-1.657125	0.886334

N	0.539456	-0.289522	-1.066573
C	-1.009555	-2.343834	1.950496
C	0.987535	0.500365	-2.090870
C	-0.343772	-3.289984	2.682504
C	2.277550	0.467077	-2.564580
C	1.002063	-3.618043	2.350795
C	3.201426	-0.439553	-1.973767
C	1.596671	-2.929774	1.318157
C	2.774617	-1.239457	-0.936881
C	0.889448	-1.929604	0.600935
C	1.435682	-1.159336	-0.466240
H	-2.044119	-2.090020	2.183602
H	0.242009	1.170376	-2.524069
H	-0.864712	-3.793300	3.499783
H	2.571313	1.125395	-3.385059
H	1.543322	-4.393596	2.896270
H	4.229236	-0.500697	-2.339436
H	2.623631	-3.158976	1.028678
H	3.466316	-1.940413	-0.467403
C	-1.671302	1.573022	-0.369143
O	-1.757818	2.744294	-0.396698
C	-3.196994	-0.613420	0.465485
C	-2.207033	-0.588802	-2.130034
O	-4.210090	-0.828092	1.016079
O	-2.607211	-0.736250	-3.226387
C	-0.683786	-6.768085	0.074141
C	-1.608542	-5.726328	0.214914
C	0.395560	-6.611346	-0.806916
H	-2.452993	-5.836047	0.901638
H	1.127229	-7.416495	-0.927995
C	-1.462720	-4.538842	-0.508144
C	0.553884	-5.428463	-1.533387
H	-2.167839	-3.712212	-0.386424
H	1.398553	-5.285278	-2.212315
C	-0.373409	-4.382931	-1.382357
H	-0.805274	-7.693420	0.643586
O	-0.174545	-3.253103	-2.103300

Total gas phase energy = -1221.931448962
Total solvent phase energy = -1222.0011206344

TS 3_5-Re (gas phase geometry not converged)
solvent phase geometry

Re	-1.421132	-0.625254	-0.715256
H	-1.153672	-2.221399	-1.820662
N	-0.252604	-1.922452	0.609464
N	0.669686	-0.377337	-1.319322
C	-0.786999	-2.658330	1.612186
C	1.089612	0.456936	-2.304220
C	-0.036966	-3.496631	2.420143
C	2.407472	0.536594	-2.723181

C	1.342809	-3.601879	2.185430
C	3.365045	-0.288684	-2.107486
C	1.903015	-2.852995	1.162053
C	2.951968	-1.140172	-1.093251
C	1.091297	-2.007064	0.381636
C	1.598750	-1.168187	-0.699418
H	-1.863134	-2.557014	1.755985
H	0.319337	1.073213	-2.768782
H	-0.531740	-4.069694	3.205238
H	2.681043	1.227482	-3.523381
H	1.965353	-4.264225	2.790840
H	4.411310	-0.261840	-2.421264
H	2.971637	-2.925915	0.958496
H	3.676782	-1.787675	-0.599906
C	-1.636942	0.821680	0.560950
O	-1.887096	1.664866	1.334105
C	-3.121608	-1.435914	-0.373584
C	-2.153776	0.266001	-2.244677
O	-4.144475	-1.972568	-0.179202
O	-2.552157	0.793050	-3.213483
C	-1.021970	-6.394773	0.677007
C	-2.132907	-5.694744	0.182342
C	0.246188	-6.100844	0.150264
H	-3.127668	-5.907279	0.590458
H	1.126722	-6.624024	0.538389
C	-1.990217	-4.725054	-0.810797
C	0.403049	-5.128381	-0.835966
H	-2.857977	-4.172002	-1.178332
H	1.394151	-4.871588	-1.221683
C	-0.710938	-4.408169	-1.364250
H	-1.142757	-7.148088	1.461063
O	-0.557632	-3.496531	-2.286206

Total gas phase energy = -1221.8969663515

Total solvent phase energy = -1221.9796769198

Reactant complex 5_6-Re (gas phase TS geometry not converged)

solvent phase geometry

Re	-0.808706	-0.285259	-0.010644
C	-0.113718	-2.455610	0.123048
O	1.114932	-2.689831	0.125398
O	-1.020781	-3.351695	0.211233
H	-0.871685	-4.790824	0.542056
N	0.874781	-0.025702	1.354328
N	0.939607	-0.098201	-1.303489
C	0.769988	0.035652	2.696771
C	0.897265	-0.093324	-2.651024
C	1.874269	0.025619	3.539031
C	2.039436	-0.123226	-3.439971
C	3.152567	-0.041959	2.970521
C	3.289744	-0.156414	-2.809902

C	3.266898	-0.094651	1.586419
C	3.339408	-0.154470	-1.420850
C	2.109678	-0.095823	0.790887
C	2.145854	-0.131084	-0.680136
H	-0.242091	0.087284	3.101274
H	-0.094292	-0.068617	-3.105381
H	1.728147	0.071902	4.620041
H	1.943774	-0.119916	-4.527645
H	4.046547	-0.049031	3.597699
H	4.211509	-0.179335	-3.395223
H	4.251912	-0.139452	1.123485
H	4.302548	-0.174341	-0.912352
C	-1.323633	1.601603	-0.077090
O	-1.675233	2.711482	-0.114960
C	-2.113732	-0.759303	1.318503
C	-1.983332	-0.844385	-1.419114
O	-2.862434	-1.092540	2.145783
O	-2.617632	-1.225286	-2.319697
C	2.463986	-8.100609	0.519261
C	2.541154	-6.704165	0.421298
C	1.205159	-8.696809	0.681710
H	3.513654	-6.219435	0.283749
H	1.118976	-9.786154	0.752802
C	1.393551	-5.908481	0.488772
C	0.049768	-7.915522	0.755523
H	1.447986	-4.817706	0.393684
H	-0.934953	-8.374366	0.883493
C	0.125655	-6.507836	0.667649
H	3.366537	-8.714915	0.463827
O	-1.004137	-5.798408	0.754306

Total gas phase energy = -1410.5129563319
Total solvent phase energy = -1410.6093693915

TS 5_6-Re (gas phase geometry not converged)
solvent phase geometry

Re	-0.819418	-0.302046	0.035843
C	-0.156186	-2.445352	0.082467
O	1.050401	-2.737902	0.110001
O	-1.097559	-3.351967	0.092069
H	-0.838328	-4.502436	0.239185
N	0.915719	-0.046856	1.358042
N	0.907662	-0.114992	-1.303375
C	0.847100	0.037476	2.700272
C	0.829943	-0.109164	-2.647892
C	1.975964	0.049128	3.511891
C	1.952429	-0.153918	-3.466344
C	3.236442	-0.025458	2.909486
C	3.216589	-0.204745	-2.869008
C	3.312308	-0.103900	1.522849
C	3.302086	-0.201900	-1.480746

C	2.133228	-0.119162	0.761834
C	2.128573	-0.161957	-0.711914
H	-0.153082	0.093352	3.132654
H	-0.172900	-0.071746	-3.075888
H	1.861364	0.119440	4.595340
H	1.829252	-0.149619	-4.551135
H	4.147936	-0.017609	3.511199
H	4.123315	-0.243362	-3.476500
H	4.284733	-0.154864	1.034554
H	4.277527	-0.234972	-0.997079
C	-1.285553	1.606956	0.015186
O	-1.599994	2.726051	0.008830
C	-2.097740	-0.746929	1.397987
C	-2.096667	-0.784065	-1.314067
O	-2.835630	-1.060765	2.241370
O	-2.829366	-1.115384	-2.155561
C	2.450695	-8.163985	0.734654
C	2.593720	-6.776563	0.579782
C	1.154644	-8.700292	0.784785
H	3.595975	-6.334218	0.541135
H	1.012546	-9.779099	0.914454
C	1.481990	-5.938037	0.472592
C	0.033979	-7.875767	0.680558
H	1.591001	-4.856815	0.344257
H	-0.977753	-8.292096	0.724189
C	0.160321	-6.467509	0.512581
H	3.326936	-8.811996	0.819724
O	-0.915274	-5.726100	0.404813

Total gas phase energy = -1410.5054716929

Total solvent phase energy = -1410.6076841638

Reactant complex 6_7-Re

gas phase geometry

Re	-1.135513	0.389908	-0.108520
C	-1.265194	-1.754219	0.292200
O	-0.938357	-2.649405	-0.459517
O	-1.743435	-2.154076	1.557214
H	-1.880221	-3.121000	1.493621
N	-0.095654	0.645936	1.821537
N	0.961613	-0.175192	-0.478075
C	-0.698857	1.060684	2.950029
C	1.380612	-0.719397	-1.632766
C	-0.005350	1.273008	4.137046
C	2.660622	-1.245708	-1.790480
C	1.376331	1.069883	4.152770
C	3.535352	-1.219313	-0.704230
C	2.001943	0.636995	2.988447
C	3.103248	-0.656008	0.493791
C	1.239638	0.404791	1.836493
C	1.805835	-0.139951	0.586093

H	-1.774715	1.229883	2.887398
H	0.657574	-0.739769	-2.448491
H	-0.546584	1.602009	5.025956
H	2.949931	-1.688426	-2.745207
H	1.958403	1.241071	5.061277
H	4.533338	-1.655273	-0.778660
H	3.075628	0.456938	2.976993
H	3.749126	-0.675993	1.369423
C	-0.887160	2.297240	-0.549675
O	-0.746225	3.411348	-0.818196
C	-2.929552	0.682972	0.537583
C	-1.790844	0.009302	-1.883541
O	-3.986355	0.843089	0.981408
O	-2.123389	-0.251166	-2.959532
C	3.811724	-3.920834	1.811608
C	3.866720	-3.147504	2.978774
C	2.576257	-4.110900	1.183961
H	4.821466	-2.994490	3.490771
H	2.508226	-4.711416	0.272937
C	2.711397	-2.562710	3.501296
C	1.413100	-3.528874	1.694568
H	2.739411	-1.960170	4.411779
H	0.468498	-3.666653	1.168990
C	1.473463	-2.734964	2.853917
H	4.716254	-4.376318	1.400995
O	0.399752	-2.100284	3.376304
H	-0.375673	-2.147845	2.775690

Total gas phase energy = -1411.065010933

solvent phase geometry

Re	-0.905524	0.228553	-0.123946
C	-0.647538	-1.922447	-0.467729
O	-0.372563	-2.460783	-1.526136
O	-0.858030	-2.773141	0.613990
H	-0.761973	-3.694932	0.296350
N	0.772909	0.199954	1.308559
N	0.918342	0.311938	-1.345997
C	0.618098	0.230675	2.643422
C	0.904520	0.336061	-2.689451
C	1.697460	0.222493	3.522148
C	2.069363	0.298568	-3.450045
C	2.989461	0.176413	2.997843
C	3.297853	0.225704	-2.791123
C	3.153385	0.162761	1.613754
C	3.313428	0.185620	-1.398076
C	2.026019	0.186394	0.783703
C	2.104865	0.224694	-0.691493
H	-0.403337	0.241996	3.018426
H	-0.072233	0.395916	-3.169291
H	1.512814	0.241557	4.596718

H	2.002098	0.329374	-4.539130
H	3.861707	0.158235	3.653934
H	4.233674	0.197635	-3.352866
H	4.154075	0.142941	1.184507
H	4.261723	0.119438	-0.866426
C	-1.026079	2.187717	0.035811
O	-1.099648	3.340167	0.101963
C	-2.303429	-0.101383	1.157675
C	-2.144661	0.189550	-1.593860
O	-3.103931	-0.354981	1.958782
O	-2.831130	0.143730	-2.528477
C	2.583139	-3.875634	5.060692
C	1.696353	-3.071812	5.790158
C	2.307352	-4.143787	3.714824
H	1.905867	-2.840355	6.838757
H	2.990568	-4.765989	3.128967
C	0.548102	-2.549566	5.188946
C	1.166042	-3.619331	3.099475
H	-0.149832	-1.921756	5.749426
H	0.960304	-3.822329	2.047201
C	0.274701	-2.817890	3.836098
H	3.477224	-4.287218	5.536027
O	-0.841074	-2.276219	3.293396
H	-0.885714	-2.461450	2.327242

Total solvent phase energy = -1411.0925356654

TS 6_7-Re

gas phase geometry

Re	-1.011629	0.113370	-0.159364
C	-1.382480	-1.942299	0.113302
O	-1.521954	-3.018135	-0.273709
O	-1.969779	-2.024858	2.092525
H	-2.516857	-2.823115	2.126888
N	0.215570	0.193974	1.678480
N	1.061352	-0.343558	-0.794089
C	-0.282179	0.396999	2.905696
C	1.402091	-0.674770	-2.054414
C	0.533155	0.552181	4.027142
C	2.714793	-0.934260	-2.431498
C	1.912385	0.492369	3.866612
C	3.716600	-0.857057	-1.459626
C	2.436028	0.270886	2.588650
C	3.365877	-0.520153	-0.156844
C	1.565779	0.090555	1.516923
C	2.024212	-0.256780	0.157765
H	-1.368027	0.413105	2.993388
H	0.587079	-0.729244	-2.777919
H	0.071849	0.686408	5.005941
H	2.940794	-1.204921	-3.464427
H	2.582355	0.600507	4.720923

H	4.757029	-1.074052	-1.713826
H	3.511744	0.183274	2.449067
H	4.122581	-0.491482	0.625310
C	-0.628568	2.020010	-0.490404
O	-0.382017	3.121377	-0.709895
C	-2.727677	0.502980	0.671977
C	-1.829467	-0.054976	-1.902451
O	-3.723747	0.737803	1.197161
O	-2.258898	-0.182210	-2.967674
C	3.655842	-3.152230	2.558467
C	3.362276	-2.839521	3.894807
C	2.588301	-3.299734	1.659858
H	4.174679	-2.772001	4.626197
H	2.789150	-3.601273	0.626068
C	2.050727	-2.616242	4.310029
C	1.271497	-3.087464	2.062183
H	1.817613	-2.363802	5.348222
H	0.455271	-3.237690	1.357138
C	0.955944	-2.686243	3.396694
H	4.683980	-3.340786	2.236952
O	-0.242164	-2.361701	3.781541
H	-1.153481	-2.210808	2.850911

Total gas phase energy = -1411.0372584112

solvent phase geometry

Re	-0.960690	0.213177	-0.108603
C	-1.054812	-1.885046	-0.247344
O	-0.870665	-2.856931	-0.839977
O	-1.979762	-2.546748	1.475320
H	-2.031042	-3.507767	1.349110
N	0.400903	0.193483	1.633357
N	1.061702	-0.160978	-0.937990
C	0.007568	0.467158	2.889549
C	1.305545	-0.423737	-2.235356
C	0.913218	0.622669	3.935132
C	2.563313	-0.799835	-2.699398
C	2.273465	0.469771	3.673257
C	3.609831	-0.911289	-1.781602
C	2.684582	0.173185	2.375017
C	3.360512	-0.637153	-0.438331
C	1.723791	0.034250	1.369112
C	2.072880	-0.260871	-0.034850
H	-1.062579	0.579198	3.057723
H	0.461318	-0.332414	-2.920206
H	0.542249	0.853392	4.934616
H	2.708850	-1.013332	-3.759781
H	3.011466	0.581795	4.469482
H	4.605716	-1.220177	-2.107268
H	3.742993	0.053380	2.149101
H	4.159680	-0.734611	0.295341

C	-0.759427	2.177882	-0.128943
O	-0.654904	3.322103	-0.158998
C	-2.609150	0.340055	0.900411
C	-1.943958	0.302947	-1.773715
O	-3.569422	0.407431	1.536886
O	-2.507308	0.371061	-2.780626
C	3.445346	-3.282984	3.331533
C	2.837549	-2.911820	4.541381
C	2.647855	-3.373913	2.181209
H	3.438287	-2.852067	5.455577
H	3.099924	-3.682394	1.232353
C	1.477880	-2.608178	4.596201
C	1.283191	-3.085340	2.225890
H	1.006697	-2.296724	5.533300
H	0.675122	-3.175289	1.325096
C	0.649604	-2.661863	3.434458
H	4.511213	-3.523274	3.291581
O	-0.606050	-2.318649	3.498623
H	-1.344857	-2.425119	2.353047

Total solvent phase energy = -1411.0680732116

Reactant complex 8_2CO-Re

gas phase geometry

Re	-0.949937	0.546524	0.037477
C	-1.597518	-1.278614	-1.026398
O	-2.423159	-1.405887	-1.893794
O	-0.858281	-2.470417	-0.732189
H	-0.207514	-2.219225	-0.056033
N	0.796484	-0.595649	0.773977
N	0.477400	0.564547	-1.632877
C	0.941081	-1.104914	2.018072
C	0.193710	1.022909	-2.864435
C	2.123431	-1.629794	2.505579
C	1.058608	0.913552	-3.942355
C	3.270979	-1.599978	1.656718
C	2.297284	0.258046	-3.734421
C	3.149670	-1.084833	0.386649
C	2.603383	-0.228315	-2.481830
C	1.901030	-0.587716	-0.087513
C	1.684431	-0.075769	-1.403366
H	0.040066	-1.082123	2.637439
H	-0.784894	1.491794	-2.982486
H	2.166728	-2.039335	3.515783
H	0.761561	1.306341	-4.916229
H	4.234089	-1.974587	2.014672
H	2.994427	0.106335	-4.562713
H	4.019032	-1.030658	-0.269553
H	3.522103	-0.793969	-2.326665
C	-0.192656	2.145308	0.899005
O	0.266364	3.070885	1.427369

C	-2.152609	0.133860	1.480925
C	-2.290863	1.569008	-0.884179
O	-2.863163	-0.185302	2.346406
O	-3.038803	2.208604	-1.503505
C	4.197941	-3.714165	-3.015009
C	3.510029	-3.696252	-1.796632
C	3.462040	-3.694681	-4.207832
H	4.061425	-3.708830	-0.852528
H	3.983606	-3.706233	-5.170384
C	2.115025	-3.651110	-1.759991
C	2.069086	-3.654902	-4.183877
H	1.591395	-3.627428	-0.802976
H	1.480344	-3.626520	-5.103748
C	1.371396	-3.627966	-2.958040
H	5.290851	-3.749705	-3.037251
O	0.035121	-3.602334	-2.993647
H	-0.345044	-3.297263	-2.129475

Total gas phase energy = -1411.1228180846

solvent phase geometry

Re	-1.082576	0.551626	-0.121353
C	-1.564880	-1.567329	-0.500125
O	-2.522026	-2.058556	-1.064130
O	-0.583151	-2.521364	-0.126414
H	0.112313	-2.028366	0.343830
N	0.821395	-0.172704	0.722436
N	0.243132	0.295944	-1.860778
C	1.083456	-0.356440	2.042251
C	-0.117108	0.509903	-3.141836
C	2.309970	-0.756839	2.533126
C	0.735849	0.335917	-4.219235
C	3.368462	-0.980247	1.601579
C	2.057888	-0.105092	-3.956365
C	3.135028	-0.780952	0.260700
C	2.443561	-0.340779	-2.655795
C	1.853611	-0.363260	-0.206980
C	1.529627	-0.142122	-1.580250
H	0.243116	-0.176946	2.717660
H	-1.142576	0.851216	-3.300131
H	2.451001	-0.903803	3.605389
H	0.381879	0.538187	-5.231894
H	4.349963	-1.311004	1.950726
H	2.762289	-0.270456	-4.774945
H	3.935391	-0.949424	-0.459818
H	3.446995	-0.710246	-2.444745
C	-0.522051	2.422137	0.101758
O	-0.204179	3.529914	0.233854
C	-2.096259	0.521131	1.512463
C	-2.639757	1.050747	-1.126074
O	-2.692273	0.463602	2.512233

O	-3.552455	1.338291	-1.790081
C	4.308751	-4.198171	-2.868866
C	3.713630	-3.997899	-1.617659
C	3.528112	-4.063688	-4.025590
H	4.304284	-4.106960	-0.703693
H	3.979285	-4.230245	-5.008474
C	2.360589	-3.662569	-1.516986
C	2.177188	-3.722763	-3.936829
H	1.904503	-3.499031	-0.538802
H	1.561926	-3.598362	-4.831282
C	1.583949	-3.509971	-2.679505
H	5.363625	-4.474341	-2.943243
O	0.281826	-3.158207	-2.640044
H	-0.012471	-3.026270	-1.710616

Total solvent phase energy = -1411.1965482697

TS 8_2CO-Re

gas phase geometry

Re	-1.024485	0.551831	-0.040786
C	-1.790466	-1.315833	-0.779858
O	-2.614880	-1.881475	-1.345984
O	-0.454867	-2.859860	-0.364738
H	0.273517	-2.457615	0.124034
N	0.742301	-0.389332	0.831175
N	0.399851	0.434874	-1.693015
C	0.883909	-0.748114	2.128060
C	0.156141	0.854758	-2.950164
C	2.002965	-1.381057	2.630994
C	1.075634	0.762550	-3.978332
C	3.061808	-1.694865	1.726390
C	2.336269	0.182751	-3.692855
C	2.950875	-1.318120	0.407412
C	2.594120	-0.277953	-2.422344
C	1.796350	-0.624295	-0.059461
C	1.612598	-0.167392	-1.399473
H	0.033191	-0.520630	2.775377
H	-0.829577	1.291039	-3.125068
H	2.045594	-1.663669	3.684185
H	0.813077	1.121874	-4.974832
H	3.940775	-2.244800	2.072871
H	3.089687	0.068954	-4.475084
H	3.729902	-1.585384	-0.305104
H	3.542085	-0.767379	-2.203946
C	-0.329891	2.306855	0.480689
O	0.061757	3.354950	0.765312
C	-2.127734	0.414266	1.544687
C	-2.451395	1.396238	-1.037433
O	-2.756764	0.301192	2.512890
O	-3.273149	1.913964	-1.671973
C	4.293639	-4.078620	-3.406650

C	3.717493	-4.235549	-2.137173
C	3.502712	-3.523004	-4.426493
H	4.306197	-4.677542	-1.324537
H	3.929776	-3.393244	-5.428831
C	2.402667	-3.846079	-1.882627
C	2.189807	-3.126629	-4.188151
H	1.970881	-3.984931	-0.888340
H	1.581736	-2.674002	-4.976195
C	1.579382	-3.257773	-2.898813
H	5.321312	-4.398181	-3.603219
O	0.373491	-2.846325	-2.683849
H	-0.079075	-2.922931	-1.383542

Total gas phase energy = -1411.1034850001

solvent phase geometry

Re	-1.079959	0.526104	-0.196510
C	-1.734103	-1.485394	-0.571754
O	-2.563162	-2.169017	-0.996802
O	-0.316320	-2.804812	-0.001951
H	0.359724	-2.216352	0.359159
N	0.790117	-0.160306	0.709184
N	0.281123	0.262352	-1.889459
C	1.012263	-0.324197	2.037745
C	-0.035908	0.500669	-3.180205
C	2.206498	-0.773872	2.564471
C	0.848913	0.325139	-4.228590
C	3.270568	-1.076835	1.663002
C	2.153982	-0.145037	-3.928582
C	3.077287	-0.893750	0.313116
C	2.492932	-0.404958	-2.620419
C	1.830936	-0.418841	-0.190746
C	1.550629	-0.199079	-1.573160
H	0.169202	-0.090105	2.692037
H	-1.049928	0.861260	-3.367042
H	2.316374	-0.902653	3.642675
H	0.532314	0.547377	-5.249434
H	4.223489	-1.456173	2.040852
H	2.880849	-0.314721	-4.726005
H	3.876170	-1.130390	-0.388507
H	3.481096	-0.796291	-2.381169
C	-0.497275	2.389425	0.003939
O	-0.167868	3.489969	0.107947
C	-2.101674	0.604661	1.445752
C	-2.628190	1.085230	-1.208182
O	-2.690072	0.644005	2.444505
O	-3.545645	1.415207	-1.837932
C	4.343577	-4.090134	-3.144539
C	3.909100	-3.963093	-1.817180
C	3.393927	-3.964359	-4.170777
H	4.627692	-4.067997	-0.997042

H	3.710264	-4.071575	-5.214744
C	2.570391	-3.707599	-1.515792
C	2.055074	-3.702953	-3.882101
H	2.252740	-3.604943	-0.475492
H	1.320949	-3.581760	-4.684235
C	1.595809	-3.541595	-2.542586
H	5.392088	-4.298298	-3.376294
O	0.343803	-3.255814	-2.294470
H	0.039195	-3.048079	-1.060712

Total solvent phase energy = -1411.1738525162

1X-Mn

gas phase geometry

Mn	0.635940	-0.181255	0.000159
Cl	0.450833	2.238307	-0.001190
C	0.686919	-1.982647	0.000354
O	0.705979	-3.134712	-0.000680
N	-0.957351	-0.123869	1.306221
N	-0.957347	-0.124531	-1.306070
C	-0.857810	-0.082553	2.641746
C	-0.857754	-0.083192	-2.641592
C	-1.966981	0.007459	3.480277
C	-1.966850	0.007473	-3.480152
C	-3.237923	0.054461	2.905296
C	-3.237787	0.055095	-2.905212
C	-3.344640	0.025690	1.516981
C	-3.344557	0.026264	-1.516901
C	-2.182169	-0.055213	0.737822
C	-2.182150	-0.055270	-0.737717
H	0.150234	-0.117962	3.056465
H	0.150276	-0.119067	-3.056299
H	-1.823425	0.042486	4.562087
H	-1.823248	0.042588	-4.561953
H	-4.133599	0.120914	3.526619
H	-4.133405	0.122148	-3.526554
H	-4.324245	0.074738	1.042561
H	-4.324141	0.075923	-1.042502
C	1.913844	-0.029617	1.285664
C	1.913726	-0.030191	-1.285534
O	2.704617	0.089407	2.109515
O	2.704459	0.088884	-2.109411

Total gas phase energy = -952.3775210771

solvent phase geometry

Mn	0.640958	-0.145079	-0.000639
Cl	0.502491	2.318964	-0.002412
C	0.659598	-1.943087	-0.000224
O	0.660013	-3.094800	-0.001884
N	-0.951384	-0.087242	1.310156
N	-0.951827	-0.088324	-1.310179

C	-0.856332	-0.065851	2.647839
C	-0.856881	-0.067329	-2.647887
C	-1.970757	-0.001939	3.482766
C	-1.971406	-0.003440	-3.482665
C	-3.239759	0.037024	2.902451
C	-3.240317	0.035803	-2.902129
C	-3.342741	0.022483	1.512525
C	-3.343117	0.021736	-1.512183
C	-2.176809	-0.035047	0.737718
C	-2.177058	-0.035488	-0.737516
H	0.147550	-0.102163	3.072387
H	0.146986	-0.104175	-3.072442
H	-1.832187	0.014794	4.565578
H	-1.833024	0.013012	-4.565509
H	-4.138961	0.081465	3.520326
H	-4.139655	0.080018	-3.519819
H	-4.322158	0.058673	1.036760
H	-4.322513	0.057984	-1.036359
C	1.917655	-0.044599	1.287543
C	1.918704	-0.045168	-1.288121
O	2.714411	0.036588	2.112762
O	2.719965	0.036941	-2.108842

Total solvent phase energy = -952.4054643743

1X+K-Mn

gas phase geometry

Mn	0.541619	0.030832	-0.000910
Cl	0.042895	2.468409	-0.002022
C	0.808724	-1.771315	-0.000056
O	0.938064	-2.907787	0.002038
N	-1.037530	-0.120940	1.310480
N	-1.038650	-0.122837	-1.310739
C	-0.940713	-0.141767	2.647439
C	-0.942993	-0.146119	-2.647728
C	-2.054393	-0.128758	3.484983
C	-2.057448	-0.135033	-3.484298
C	-3.323995	-0.092870	2.906552
C	-3.326549	-0.098557	-2.904802
C	-3.427991	-0.077196	1.517055
C	-3.429319	-0.080361	-1.515244
C	-2.263787	-0.093157	0.738469
C	-2.264411	-0.094452	-0.737671
H	0.066812	-0.169023	3.065488
H	0.064211	-0.173932	-3.066520
H	-1.916782	-0.146994	4.567948
H	-1.920872	-0.155369	-4.567355
H	-4.222832	-0.079189	3.526635
H	-4.225955	-0.086484	-3.524102
H	-4.408982	-0.051410	1.043908
H	-4.409902	-0.054203	-1.041261

C	1.796818	0.386615	1.249957
C	1.797117	0.385719	-1.251380
O	2.616830	0.740537	1.979918
O	2.618387	0.740116	-1.979777
K	2.883075	3.527282	-0.007005

Total gas phase energy = -980.3804836333

solvent phase geometry

Mn	0.542074	0.056791	0.002383
Cl	-0.027787	2.490425	0.039007
C	0.893895	-1.715092	-0.016512
O	1.095023	-2.846470	-0.026271
N	-1.034379	-0.156457	1.314822
N	-1.041277	-0.124030	-1.307380
C	-0.938130	-0.205201	2.651812
C	-0.952338	-0.140549	-2.645795
C	-2.053448	-0.201344	3.488441
C	-2.072609	-0.120492	-3.475964
C	-3.323203	-0.146149	2.911041
C	-3.339297	-0.081572	-2.890550
C	-3.427747	-0.109477	1.521446
C	-3.436140	-0.076375	-1.499958
C	-2.262363	-0.119401	0.744751
C	-2.266320	-0.102153	-0.730200
H	0.067084	-0.245620	3.073632
H	0.050924	-0.167986	-3.073551
H	-1.915389	-0.239594	4.570669
H	-1.941194	-0.133153	-4.559683
H	-4.222430	-0.133759	3.530495
H	-4.242068	-0.057236	-3.504602
H	-4.408457	-0.070450	1.048408
H	-4.414361	-0.050484	-1.020827
C	1.779551	0.415358	1.283672
C	1.787166	0.449291	-1.255630
O	2.562562	0.712283	2.072310
O	2.590163	0.792768	-2.006851
K	2.911938	3.677882	-0.239116

Total solvent phase energy = -980.470580904

2-Mn

gas phase geometry

Mn	-0.669583	0.092665	0.000177
N	0.887413	0.065416	-1.286569
N	0.887524	0.065750	1.286886
C	0.800178	0.027527	-2.638648
C	0.800422	0.028033	2.638979
C	1.902899	0.005761	-3.474485
C	1.903221	0.006246	3.474713
C	3.190704	0.019687	-2.903690
C	3.190973	0.019997	2.903794

C	3.299292	0.041363	-1.522900
C	3.299432	0.041523	1.522992
C	2.137820	0.057229	-0.725398
C	2.137883	0.057372	0.725601
H	-0.209230	0.017941	-3.052231
H	-0.208943	0.018584	3.052665
H	1.756738	-0.020010	-4.556288
H	1.757163	-0.019432	4.556532
H	4.084234	0.009776	-3.531431
H	4.084561	0.010056	3.531452
H	4.281546	0.044483	-1.049682
H	4.281645	0.044495	1.049688
C	-1.161746	-1.629950	-0.000813
O	-1.456291	-2.745746	-0.002513
C	-1.870157	0.590311	-1.266521
C	-1.870165	0.590286	1.267063
O	-2.622839	0.918974	-2.078172
O	-2.622756	0.918906	2.078800

Total gas phase energy = -939.1993252623

solvent phase geometry

Mn	-0.164493	0.330633	-0.016237
N	1.393442	0.105300	1.289803
N	1.392263	0.079067	-1.304045
C	1.300752	0.134582	2.635695
C	1.305455	0.056643	-2.651873
C	2.408453	0.083835	3.472980
C	2.414063	-0.038309	-3.483279
C	3.684839	0.001078	2.900562
C	3.688685	-0.111913	-2.905600
C	3.792291	-0.031834	1.514233
C	3.792162	-0.093903	-1.518569
C	2.629912	0.019316	0.728220
C	2.629457	-0.002757	-0.737850
H	0.294734	0.207562	3.050657
H	0.302284	0.121263	-3.074420
H	2.266026	0.110797	4.555301
H	2.273238	-0.055868	-4.565930
H	4.579539	-0.038020	3.525367
H	4.584084	-0.186143	-3.526021
H	4.772188	-0.097183	1.041791
H	4.770032	-0.153833	-1.041130
C	-0.275442	2.116525	0.113604
O	-0.327686	3.273637	0.186245
C	-1.408777	-0.137947	1.205138
C	-1.433972	0.228337	-1.285964
O	-2.199671	-0.455499	1.995359
O	-2.258191	0.189969	-2.104037

Total solvent phase energy = -939.2144946719

2X+K-Mn

gas phase geometry

Mn	0.741826	-0.150042	-0.101757
Cl	0.957668	2.385992	-0.128922
C	0.652173	-1.941812	-0.061991
O	0.597213	-3.091760	-0.034011
N	-0.763701	0.036589	1.300465
N	-0.922803	-0.028300	-1.315860
C	-0.610168	0.222150	2.619297
C	-0.927055	0.063816	-2.653900
C	-1.666115	0.334317	3.518758
C	-2.081151	0.106783	-3.428682
C	-2.986221	0.208682	3.014148
C	-3.331445	0.016502	-2.764766
C	-3.176246	0.006735	1.663140
C	-3.359880	-0.089684	-1.389718
C	-2.051741	-0.053542	0.780446
C	-2.138328	-0.092813	-0.642486
H	0.420782	0.293827	2.974296
H	0.052831	0.111492	-3.133382
H	-1.466167	0.497771	4.578747
H	-2.006533	0.186905	-4.514117
H	-3.846113	0.257928	3.687607
H	-4.263113	0.013519	-3.336725
H	-4.184103	-0.114370	1.261697
H	-4.313568	-0.185750	-0.867983
C	2.114186	-0.123511	1.097355
C	1.893386	-0.154528	-1.507895
O	2.966126	-0.103559	1.868449
O	2.577711	-0.145660	-2.431404
K	-1.918004	2.884079	-0.050806

Total gas phase energy = -980.5386167456

solvent phase geometry

Mn	0.719262	-0.318511	0.036150
Cl	1.064475	2.375214	0.126296
C	0.514451	-2.086915	0.002376
O	0.335584	-3.227585	-0.015761
N	-0.856746	-0.082609	1.343370
N	-0.836506	-0.010669	-1.279721
C	-0.783918	-0.085992	2.688527
C	-0.753254	0.068495	-2.624111
C	-1.882823	0.042147	3.524135
C	-1.842980	0.254748	-3.460531
C	-3.164600	0.174540	2.929027
C	-3.138252	0.328468	-2.871794
C	-3.267069	0.183838	1.553910
C	-3.255771	0.235412	-1.501097
C	-2.099440	0.060800	0.744804
C	-2.093489	0.089583	-0.683506

H	0.214129	-0.202085	3.116068
H	0.249265	-0.019493	-3.048796
H	-1.746703	0.035020	4.607272
H	-1.694583	0.327885	-4.539392
H	-4.059436	0.270393	3.549129
H	-4.027415	0.451099	-3.494882
H	-4.243433	0.289477	1.078617
H	-4.239976	0.282971	-1.032112
C	1.978149	-0.365085	1.344615
C	1.995896	-0.320111	-1.255864
O	2.763776	-0.377687	2.188044
O	2.792107	-0.310074	-2.089602
K	-1.679247	3.288482	-0.935175

Total solvent phase energy = -980.5796949106

2X-Mn

gas phase geometry

Mn	0.645155	-0.163198	0.000060
Cl	0.625898	2.316600	-0.000659
C	0.629165	-1.948772	0.000164
O	0.618553	-3.106372	-0.000424
N	-0.933355	-0.074126	1.314669
N	-0.933348	-0.074466	-1.314567
C	-0.857569	-0.029659	2.649333
C	-0.857514	-0.029871	-2.649226
C	-1.960239	0.019872	3.495686
C	-1.960152	0.019965	-3.495599
C	-3.249451	0.020723	2.900375
C	-3.249377	0.020994	-2.900323
C	-3.353819	-0.009514	1.528021
C	-3.353787	-0.009340	-1.527973
C	-2.182555	-0.045094	0.711413
C	-2.182547	-0.045160	-0.711340
H	0.151127	-0.031408	3.070238
H	0.151187	-0.031789	-3.070111
H	-1.817307	0.062851	4.577381
H	-1.817186	0.063070	-4.577284
H	-4.150185	0.051138	3.520647
H	-4.150088	0.051670	-3.520615
H	-4.336163	-0.000674	1.052851
H	-4.336141	-0.000276	-1.052828
C	1.907675	-0.056754	1.290152
C	1.907640	-0.057259	-1.290114
O	2.702901	0.019657	2.123805
O	2.702923	0.018949	-2.123731

Total gas phase energy = -954.2029933881

solvent phase geometry

Mn	0.637131	-0.154784	-0.000206
Cl	0.565758	2.377989	-0.001285

C	0.638029	-1.934673	0.000256
O	0.617445	-3.090570	-0.002859
N	-0.929846	-0.077209	1.311871
N	-0.930099	-0.078201	-1.311737
C	-0.852237	-0.055204	2.653387
C	-0.852537	-0.056306	-2.653262
C	-1.954047	0.001956	3.495710
C	-1.954366	0.001292	-3.495521
C	-3.246027	0.026880	2.901615
C	-3.246301	0.026726	-2.901325
C	-3.352104	0.009485	1.528197
C	-3.352292	0.009614	-1.527897
C	-2.180804	-0.032162	0.712341
C	-2.180939	-0.032374	-0.712155
H	0.154085	-0.084174	3.078337
H	0.153750	-0.085962	-3.078271
H	-1.812829	0.024233	4.578143
H	-1.813232	0.023461	-4.577967
H	-4.144300	0.060661	3.523646
H	-4.144594	0.060745	-3.523319
H	-4.335181	0.030512	1.055224
H	-4.335320	0.031167	-1.054848
C	1.902598	-0.050608	1.288549
C	1.903033	-0.052532	-1.288779
O	2.701834	0.027321	2.117871
O	2.704834	0.024473	-2.115716

Total solvent phase energy = -952.5051228561

2S-Mn

gas phase geometry

Mn	-0.785488	0.279905	-0.079109
C	2.035277	0.195479	0.654166
N	0.782719	0.248710	1.252245
C	0.701562	0.307979	2.593181
C	1.800870	0.323549	3.436408
C	3.092889	0.263809	2.846425
C	3.201935	0.199908	1.476312
C	-2.061417	0.460822	1.206515
O	-2.860880	0.569892	2.026834
C	2.042437	0.130575	-0.769142
N	0.796667	0.141624	-1.382940
C	0.728107	0.068457	-2.723952
C	1.834881	-0.008747	-3.553297
C	3.120230	-0.025545	-2.946923
C	3.216281	0.042253	-1.576023
C	-0.875769	-1.530737	-0.032594
O	-0.882908	-2.676929	-0.009148
C	-2.037818	0.390031	-1.395780
O	-2.817922	0.456468	-2.238856
H	-0.276109	0.072989	-3.155090

H	-0.307004	0.347635	3.012480
H	1.702639	-0.068623	-4.634816
H	1.658783	0.375544	4.517212
H	4.022059	-0.102069	-3.559244
H	3.989619	0.263955	3.471030
H	4.194640	0.017702	-1.094600
H	4.185426	0.147031	1.007810
N	-0.416421	2.301247	-0.124149
C	-0.070158	3.402424	-0.103068
C	0.376632	4.788186	-0.074166
H	-0.216644	5.366264	0.649858
H	1.436829	4.833152	0.221816
H	0.262855	5.243819	-1.070323

Total gas phase energy = -1071.9419063306

solvent phase geometry

Mn	-0.776992	0.282352	-0.073170
C	2.042740	0.177366	0.658834
N	0.790110	0.236639	1.256382
C	0.707826	0.296634	2.597479
C	1.808019	0.302395	3.441656
C	3.100932	0.234503	2.851896
C	3.210815	0.172326	1.480586
C	-2.050929	0.472306	1.209125
O	-2.854132	0.581617	2.027486
C	2.049510	0.118084	-0.764996
N	0.802895	0.135586	-1.378118
C	0.732935	0.070835	-2.719860
C	1.840405	-0.006366	-3.550444
C	3.127418	-0.028523	-2.944391
C	3.224583	0.032095	-1.572091
C	-0.884579	-1.516321	-0.031346
O	-0.897383	-2.666130	-0.012687
C	-2.029838	0.405644	-1.383399
O	-2.815887	0.477134	-2.222342
H	-0.270350	0.082967	-3.152935
H	-0.299533	0.346258	3.018226
H	1.707791	-0.056367	-4.632816
H	1.665908	0.358799	4.522589
H	4.029175	-0.099693	-3.557819
H	3.997507	0.230246	3.477023
H	4.204063	0.008693	-1.092476
H	4.195029	0.116156	1.013482
N	-0.401841	2.313235	-0.118682
C	-0.074715	3.421018	-0.110550
C	0.342277	4.813448	-0.099165
H	-0.267561	5.383342	0.616939
H	1.400609	4.882662	0.197810
H	0.217990	5.247822	-1.103153

Total solvent phase energy = -1071.9585055848

2D-Mn

gas phase geometry

Mn	4.491755	4.784470	-14.355735
O	4.417462	5.029195	-11.433528
O	3.393462	2.052311	-14.193964
O	7.146990	3.490867	-14.222370
N	2.717584	5.684110	-14.721389
N	5.091796	6.688669	-14.734122
C	4.439834	4.959014	-12.586066
C	3.819874	3.125977	-14.288089
C	6.122716	4.024061	-14.305312
C	1.512732	5.070530	-14.715410
H	1.523082	3.996259	-14.533435
C	0.317511	5.740400	-14.927866
H	-0.620302	5.181447	-14.914922
C	0.347936	7.126378	-15.154053
C	1.578362	7.768674	-15.154460
H	1.637420	8.841199	-15.342297
C	2.754382	7.032383	-14.935407
C	4.097818	7.599585	-14.943763
C	4.385215	8.955470	-15.176881
H	3.573291	9.660589	-15.356495
C	5.703768	9.387144	-15.198730
C	6.720210	8.445292	-14.975513
H	7.773878	8.730771	-14.989169
C	6.371225	7.124637	-14.740347
H	7.135649	6.367925	-14.569068
Mn	4.829707	4.001649	-17.310155
O	5.107830	3.768859	-20.219760
O	3.606378	6.664757	-17.660932
O	7.441397	5.360777	-16.969598
N	3.078242	2.995175	-17.239332
N	5.472646	2.124919	-16.864126
C	5.016273	3.838851	-19.070686
C	4.082737	5.622319	-17.485083
C	6.427361	4.816109	-17.087197
C	1.856168	3.537385	-17.443559
H	1.833092	4.612354	-17.619219
C	0.684115	2.797768	-17.434291
H	-0.268013	3.303951	-17.604892
C	0.757010	1.411939	-17.214808
C	2.007151	0.841217	-17.019067
H	2.099956	-0.230284	-16.838331
C	3.157980	1.646729	-17.035639
C	4.513884	1.154637	-16.826189
C	4.844488	-0.192581	-16.598440
H	4.058103	-0.947194	-16.561703
C	6.171285	-0.556505	-16.417508
C	7.152974	0.445370	-16.469221

H	8.210563	0.213546	-16.328050
C	6.762458	1.756249	-16.695399
H	7.499738	2.557409	-16.734718
H	-0.144490	0.795714	-17.198571
H	6.445238	-1.598113	-16.233713
H	5.945238	10.434107	-15.396007
H	-0.571429	7.688049	-15.332793

Total gas phase energy = -1878.4219796663

solvent phase geometry

Mn	4.511303	4.815326	-14.382900
O	4.424309	5.041199	-11.465174
O	3.467930	2.063549	-14.214598
O	7.175865	3.554344	-14.217472
N	2.720915	5.711155	-14.739524
N	5.098095	6.732248	-14.754960
C	4.445235	4.989819	-12.624681
C	3.864298	3.149518	-14.328756
C	6.143450	4.076088	-14.323418
C	1.521003	5.091433	-14.734944
H	1.534031	4.014399	-14.570161
C	0.320131	5.761137	-14.928034
H	-0.616132	5.199742	-14.921767
C	0.345149	7.149491	-15.128306
C	1.574173	7.798810	-15.126497
H	1.625012	8.875911	-15.290011
C	2.752199	7.060029	-14.931893
C	4.095843	7.636816	-14.940177
C	4.367012	9.000226	-15.142949
H	3.548469	9.704228	-15.295338
C	5.683752	9.444120	-15.163282
C	6.710090	8.507375	-14.971203
H	7.760771	8.804447	-14.981667
C	6.373459	7.177161	-14.763133
H	7.146992	6.425847	-14.608772
Mn	4.836903	3.968282	-17.292578
O	5.097685	3.753799	-20.200242
O	3.646076	6.643111	-17.641964
O	7.448518	5.324082	-16.975678
N	3.073196	2.962587	-17.234919
N	5.471339	2.080240	-16.850779
C	5.007794	3.806163	-19.044329
C	4.101928	5.591538	-17.450677
C	6.430578	4.775804	-17.075422
C	1.855688	3.510055	-17.442919
H	1.832532	4.586310	-17.610338
C	0.681177	2.770864	-17.448830
H	-0.270287	3.278399	-17.618447
C	0.752834	1.384582	-17.243358
C	2.002214	0.807965	-17.044847

H	2.090554	-0.266692	-16.880664
C	3.151217	1.615160	-17.043256
C	4.508194	1.116289	-16.828279
C	4.827388	-0.234840	-16.612337
H	4.038140	-0.987188	-16.592001
C	6.152959	-0.607322	-16.424528
C	7.140419	0.388636	-16.458847
H	8.195940	0.147997	-16.315760
C	6.757643	1.705206	-16.675962
H	7.501494	2.500952	-16.707162
H	-0.149156	0.768936	-17.241132
H	6.419307	-1.652697	-16.251551
H	5.913613	10.498607	-15.332335
H	-0.577512	7.711280	-15.288613

Total solvent phase energy = -1878.4462206123

2CO-Mn

gas phase geometry

Mn	0.000090	-0.001492	-1.023121
C	1.870578	-0.002325	-0.905516
C	-1.870405	-0.002307	-0.906770
O	3.005120	-0.004681	-0.798234
O	-3.005006	-0.004685	-0.800072
N	-0.000459	-1.326729	0.573708
N	-0.000472	1.322372	0.574538
C	-0.000502	-2.671518	0.500673
C	-0.000530	2.667183	0.502353
C	-0.000420	-3.503124	1.606545
C	-0.000452	3.498113	1.608732
C	-0.000248	-2.900128	2.894373
C	-0.000257	2.894320	2.896177
C	-0.000216	-1.528942	2.993779
C	-0.000207	1.523066	2.994721
C	-0.000365	-0.713994	1.821459
C	-0.000369	0.708851	1.821896
H	-0.000634	-3.101178	-0.503792
H	-0.000667	3.097450	-0.501850
H	-0.000454	-4.586025	1.473426
H	-0.000501	4.581088	1.476248
H	-0.000115	-3.517339	3.795884
H	-0.000117	3.510975	3.798065
H	-0.000083	-1.051989	3.974250
H	-0.000045	1.045496	3.974891
C	0.000474	-1.317753	-2.286508
C	0.000480	1.315614	-2.285677
O	0.000292	-2.160147	-3.065850
O	0.000300	2.158205	-3.064791

Total gas phase energy = -1052.5269124956

solvent phase geometry

Mn	0.000029	-0.001394	-1.020132
C	1.869296	-0.002423	-0.918488
C	-1.869264	-0.002236	-0.919067
O	3.005649	-0.005399	-0.824701
O	-3.005655	-0.005007	-0.825691
N	-0.000261	-1.326857	0.577054
N	-0.000159	1.322593	0.577916
C	-0.000302	-2.671438	0.503220
C	-0.000123	2.667188	0.504947
C	-0.000260	-3.503559	1.610998
C	-0.000291	3.498617	1.613241
C	-0.000177	-2.900295	2.899848
C	-0.000535	2.894536	2.901695
C	-0.000229	-1.527701	3.000046
C	-0.000513	1.521872	3.001012
C	-0.000318	-0.714309	1.825290
C	-0.000362	0.709230	1.825741
H	-0.000305	-3.102656	-0.500474
H	0.000009	3.099026	-0.498478
H	-0.000256	-4.586856	1.477902
H	-0.000159	4.581989	1.480800
H	-0.000076	-3.517805	3.801516
H	-0.000820	3.511475	3.803749
H	-0.000189	-1.051016	3.981021
H	-0.000884	1.044563	3.981686
C	0.000195	-1.311854	-2.287353
C	0.000351	1.309892	-2.286552
O	0.000069	-2.147763	-3.074102
O	0.000348	2.145966	-3.073108

Total solvent phase energy = -1052.5360014774

3-Mn

gas phase geometry

Mn	-0.128271	0.374594	-0.014193
N	1.371918	0.134989	1.266893
N	1.356919	0.054697	-1.265072
C	1.296629	0.191119	2.627906
C	1.288020	0.004278	-2.632125
C	2.382863	0.151840	3.470510
C	2.372949	-0.106371	-3.466379
C	3.691772	0.058076	2.905876
C	3.685031	-0.167137	-2.900894
C	3.803514	-0.000047	1.537148
C	3.794795	-0.120593	-1.531926
C	2.646500	0.030163	0.706941
C	2.640540	-0.018893	-0.705853
H	0.286737	0.276725	3.034696
H	0.280993	0.057545	-3.050039
H	2.226829	0.198852	4.551505
H	2.213782	-0.150523	-4.547206

H	4.579810	0.036604	3.543484
H	4.571031	-0.250360	-3.535771
H	4.787232	-0.067914	1.067319
H	4.777541	-0.164014	-1.056622
C	-0.282671	2.125146	0.095075
O	-0.347056	3.287385	0.145656
C	-1.356846	-0.111401	1.207251
C	-1.381805	0.211545	-1.286417
O	-2.140590	-0.453034	2.000705
O	-2.195026	0.128517	-2.118281

Total gas phase energy = -939.2532100553

solvent phase geometry

Mn	-0.135272	0.383217	0.018245
N	1.359326	0.060621	1.272683
N	1.368865	0.107837	-1.264185
C	1.291754	0.038246	2.642448
C	1.288706	0.145441	-2.627960
C	2.385591	-0.046920	3.471331
C	2.379559	0.092996	-3.466388
C	3.689730	-0.113288	2.902842
C	3.682764	0.002479	-2.902119
C	3.794422	-0.097553	1.529242
C	3.795484	-0.038308	-1.529444
C	2.633115	-0.017764	0.715729
C	2.635710	0.008911	-0.709251
H	0.287713	0.093314	3.066100
H	0.280710	0.226703	-3.038783
H	2.235077	-0.066138	4.553669
H	2.227472	0.124695	-4.548064
H	4.578141	-0.177103	3.535024
H	4.569764	-0.032882	-3.538898
H	4.774838	-0.146558	1.051779
H	4.778394	-0.105795	-1.059835
C	-0.254311	2.126598	-0.121412
O	-0.341825	3.290783	-0.211651
C	-1.384764	0.245053	1.287534
C	-1.357208	-0.144446	-1.179288
O	-2.206891	0.186599	2.118076
O	-2.151194	-0.491403	-1.967425

Total solvent phase energy = -939.3219694808

3+K-Mn

gas phase geometry

Mn	-0.175903	0.674143	-0.070361
N	1.265151	0.036859	1.163562
N	1.371247	0.621498	-1.292270
C	1.093693	-0.271824	2.482182
C	1.386392	0.960473	-2.632591
C	2.114255	-0.666786	3.315391

C	2.515395	1.020759	-3.404627
C	3.432506	-0.778729	2.783281
C	3.787213	0.700439	-2.830053
C	3.632391	-0.506162	1.450672
C	3.811878	0.299019	-1.516163
C	2.540439	-0.104649	0.624989
C	2.612847	0.240234	-0.747074
H	0.069317	-0.177585	2.850784
H	0.417275	1.209774	-3.065555
H	1.899001	-0.906660	4.358076
H	2.427520	1.314376	-4.453001
H	4.263720	-1.098356	3.415779
H	4.701382	0.750641	-3.425406
H	4.623412	-0.616405	1.006476
H	4.753898	0.011561	-1.044487
C	-1.284638	1.257942	-1.366957
O	-1.968725	1.643630	-2.218654
C	-0.757430	1.900398	1.061117
C	-1.319231	-0.615810	0.427040
O	-1.058075	2.730426	1.831020
O	-2.040916	-1.447412	0.781487
K	2.093716	2.977979	0.482334

Total gas phase energy = -967.3505831706

solvent phase geometry

Mn	-0.149631	0.754112	-0.014731
N	1.308230	0.190108	1.232456
N	1.402044	0.667264	-1.254511
C	1.166407	-0.066742	2.568834
C	1.381155	0.936255	-2.600868
C	2.190979	-0.497557	3.380840
C	2.476657	0.825984	-3.424826
C	3.481662	-0.702918	2.820536
C	3.720782	0.398940	-2.881281
C	3.649541	-0.475289	1.471615
C	3.770507	0.099407	-1.536726
C	2.556912	-0.038568	0.675957
C	2.611500	0.228339	-0.726584
H	0.168163	0.096720	2.978664
H	0.421117	1.264993	-3.001936
H	1.994619	-0.682060	4.439281
H	2.374925	1.074582	-4.483751
H	4.315458	-1.039981	3.440183
H	4.607351	0.304043	-3.512126
H	4.621427	-0.636527	1.002305
H	4.700705	-0.245488	-1.081720
C	-1.155614	1.725041	-1.130043
O	-1.826535	2.372281	-1.836436
C	-1.048581	1.529724	1.313338
C	-1.061240	-0.744195	-0.181119

O	-1.619002	2.056765	2.189620
O	-1.699938	-1.719261	-0.283365
K	1.848135	3.483800	0.403384

Total solvent phase energy = -967.3941677135

4-Mn

gas phase geometry

H	-0.478659	1.637254	0.001467
Mn	-0.688377	0.060227	-0.000759
N	0.903242	0.002944	-1.295177
N	0.902975	0.001879	1.294140
C	0.813217	-0.014244	-2.637549
C	0.812677	-0.015812	2.636491
C	1.923554	0.027433	-3.475040
C	1.922827	0.026202	3.474230
C	3.198737	0.089136	-2.904201
C	3.198101	0.088697	2.903688
C	3.302020	0.096578	-1.517409
C	3.301672	0.096554	1.516917
C	2.137445	0.048445	-0.734698
C	2.137289	0.048121	0.733949
H	-0.194362	-0.056829	-3.053182
H	-0.194963	-0.058972	3.051923
H	1.780651	0.014128	-4.557661
H	1.779713	0.012580	4.556820
H	4.094492	0.131890	-3.527580
H	4.093707	0.131797	3.527262
H	4.281252	0.144696	-1.041322
H	4.280972	0.145387	1.041045
C	-1.039156	-1.737720	0.001219
O	-1.318498	-2.857196	0.008678
C	-1.886778	0.490834	-1.272164
C	-1.886903	0.490249	1.270515
O	-2.619975	0.825255	-2.098561
O	-2.620181	0.824423	2.096960

Total gas phase energy = -939.7928254085

solvent phase geometry

H	-0.221398	-1.330751	0.013906
Mn	-0.195806	0.265368	0.004531
N	1.395454	0.092540	1.303131
N	1.400403	0.131458	-1.306506
C	1.302962	0.037815	2.642633
C	1.313057	0.155494	-2.647388
C	2.412976	-0.072486	3.476256
C	2.428894	0.123314	-3.480484
C	3.684375	-0.125482	2.899003
C	3.699084	0.066655	-2.900728
C	3.788335	-0.075295	1.511346
C	3.797153	0.036148	-1.512002

C	2.624552	0.029548	0.735147
C	2.628292	0.067316	-0.736817
H	0.299234	0.083606	3.066671
H	0.309565	0.205417	-3.072093
H	2.270244	-0.117340	4.557826
H	2.292501	0.146374	-4.563680
H	4.580407	-0.210456	3.517162
H	4.599329	0.045844	-3.518446
H	4.766741	-0.123186	1.034198
H	4.775171	-0.010506	-1.033922
C	-0.170488	2.086242	-0.028859
O	-0.196142	3.241589	-0.048038
C	-1.448737	0.174585	1.280252
C	-1.443455	0.015198	-1.253687
O	-2.250488	0.084079	2.110619
O	-2.231812	-0.241861	-2.061796

Total solvent phase energy = -939.8127811614

5-Mn (gas phase geometry not stable)

solvent phase geometry

Mn	-0.750885	0.364035	0.011791
C	-0.673217	-1.903870	0.096201
O	-1.740091	-2.505407	0.320071
O	0.470805	-2.349059	-0.074412
N	0.796230	0.192624	1.296886
N	0.796229	0.219688	-1.298938
C	0.717664	0.204652	2.643956
C	0.707351	0.272595	-2.641489
C	1.813235	0.017629	3.474077
C	1.801471	0.121454	-3.483023
C	3.075814	-0.183574	2.892635
C	3.066862	-0.084643	-2.910908
C	3.170814	-0.192795	1.507299
C	3.169820	-0.136986	-1.526845
C	2.014500	-0.011814	0.725480
C	2.014107	0.007777	-0.735933
H	-0.273265	0.369168	3.068792
H	-0.287913	0.445926	-3.053508
H	1.675816	0.031625	4.557501
H	1.661244	0.170241	-4.565027
H	3.963620	-0.330881	3.511496
H	3.954261	-0.201607	-3.537065
H	4.136585	-0.347646	1.026041
H	4.139839	-0.295911	-1.055663
C	-0.800808	2.153455	-0.063372
O	-0.866023	3.314397	-0.112413
C	-1.999889	0.248644	1.283916
C	-1.978183	-0.039574	-1.225996
O	-2.812914	0.169112	2.109990
O	-2.765867	-0.354174	-2.022030

Total gas phase energy = -1127.8199235533
Total solvent phase energy = -1127.9188230095

6-Mn

gas phase geometry

Mn	-0.791746	0.265594	0.003642
C	-0.659045	-1.797447	0.004192
O	0.383424	-2.418747	0.094537
O	-1.828464	-2.495031	-0.116871
H	-1.581073	-3.441815	-0.106147
N	0.798236	0.165612	1.311382
N	0.791840	0.150802	-1.305163
C	0.709735	0.169596	2.649586
C	0.698386	0.149867	-2.643973
C	1.816387	0.032425	3.483055
C	1.801963	0.014697	-3.480822
C	3.078770	-0.110635	2.901262
C	3.067231	-0.122948	-2.903358
C	3.174924	-0.125568	1.513436
C	3.168533	-0.132819	-1.515951
C	2.012641	0.001696	0.737848
C	2.009481	-0.004308	-0.735267
H	-0.290484	0.285570	3.069129
H	-0.303956	0.260518	-3.059691
H	1.680183	0.038799	4.566422
H	1.661163	0.018792	-4.563625
H	3.973901	-0.215001	3.518491
H	3.960204	-0.225999	-3.523809
H	4.145909	-0.246119	1.034128
H	4.141904	-0.247551	-1.040113
C	-0.784621	2.096753	0.010138
O	-0.792898	3.247939	0.015139
C	-2.053311	0.141198	1.287889
C	-2.055215	0.165741	-1.283053
O	-2.832987	0.045795	2.130564
O	-2.835395	0.095275	-2.127269

Total gas phase energy = -1128.3808624521

solvent phase geometry

Mn	-0.797068	0.241964	0.006279
C	-0.703135	-1.812633	0.005285
O	0.321886	-2.467959	0.106365
O	-1.886059	-2.492883	-0.132822
H	-1.667974	-3.448290	-0.124771
N	0.802052	0.137944	1.317464
N	0.794888	0.123306	-1.309608
C	0.716507	0.134810	2.656185
C	0.703075	0.113011	-2.648503
C	1.830577	0.024137	3.485525
C	1.813227	0.001164	-3.482251

C	3.093744	-0.081957	2.898378
C	3.079363	-0.100328	-2.900521
C	3.186922	-0.086775	1.508576
C	3.179162	-0.097473	-1.511221
C	2.019074	0.014036	0.738747
C	2.015316	0.007221	-0.735613
H	-0.282431	0.224799	3.084870
H	-0.298074	0.197921	-3.072865
H	1.698295	0.024076	4.569327
H	1.675288	-0.004353	-4.565317
H	3.993827	-0.163544	3.511444
H	3.976538	-0.183990	-3.517446
H	4.160512	-0.174214	1.027426
H	4.155208	-0.181329	-1.034485
C	-0.748717	2.071575	0.010526
O	-0.743244	3.223934	0.016315
C	-2.056027	0.153182	1.285306
C	-2.058248	0.173356	-1.273152
O	-2.855707	0.074876	2.115325
O	-2.853154	0.117096	-2.109042

Total solvent phase energy = -1128.4068907373

7-Mn

gas phase geometry

Mn	0.000026	0.000863	-0.835032
C	1.886370	-0.000015	-0.790511
C	-1.886326	-0.000007	-0.790564
O	3.021979	-0.004150	-0.757294
O	-3.021935	-0.004132	-0.757365
N	0.000000	-1.318847	0.783692
N	0.000000	1.319563	0.783875
C	-0.000017	-2.658908	0.693521
C	-0.000020	2.659619	0.693865
C	-0.000019	-3.489348	1.812520
C	-0.000021	3.489899	1.812966
C	0.000000	-2.903901	3.079284
C	0.000001	2.904273	3.079646
C	0.000015	-1.513460	3.176364
C	0.000020	1.513822	3.176554
C	0.000013	-0.738381	2.009143
C	0.000014	0.738906	2.009235
H	-0.000030	-3.086790	-0.309936
H	-0.000036	3.087545	-0.309567
H	-0.000036	-4.573082	1.679478
H	-0.000040	4.573641	1.680034
H	0.000003	-3.519115	3.981555
H	0.000004	3.519365	3.981994
H	0.000029	-1.037157	4.156072
H	0.000038	1.037374	4.156192
C	0.000033	-1.322169	-2.117936

C	0.000037	1.323583	-2.118352
O	-0.000039	-2.166805	-2.885150
O	-0.000060	2.167815	-2.885992

Total gas phase energy = -1052.3526825129

solvent phase geometry

Mn	-0.000234	-0.006475	-0.827832
C	1.879455	0.010326	-0.777146
C	-1.879793	-0.015964	-0.777723
O	3.016497	0.015456	-0.745242
O	-3.016821	-0.015182	-0.744638
N	0.014630	-1.302643	0.799235
N	-0.015904	1.332065	0.766936
C	0.031695	-2.642875	0.722130
C	-0.032977	2.670028	0.658141
C	0.043403	-3.458614	1.851383
C	-0.044399	3.512135	1.768285
C	0.037207	-2.858337	3.111103
C	-0.038060	2.941797	3.041977
C	0.019534	-1.467094	3.193951
C	-0.020476	1.552900	3.157595
C	0.008662	-0.708067	2.017399
C	-0.009695	0.766658	1.999274
H	0.035962	-3.084702	-0.274607
H	-0.038190	3.087369	-0.349290
H	0.057786	-4.543240	1.729748
H	-0.058780	4.593697	1.621708
H	0.046390	-3.462668	4.020318
H	-0.047251	3.566812	3.937112
H	0.014167	-0.978195	4.167276
H	-0.015205	1.086562	4.141950
C	0.008381	-1.341276	-2.085050
C	-0.007901	1.279309	-2.136802
O	0.012110	-2.189713	-2.851861
O	-0.010853	2.089625	-2.943841

Total solvent phase energy = -1052.4253945917

8-Mn

gas phase geometry

Mn	-0.808914	0.230815	0.007603
C	-0.763031	-1.823467	-0.002885
O	0.223062	-2.526493	0.089747
O	-1.983399	-2.470855	-0.148107
H	-1.751947	-3.421722	-0.145399
N	0.790022	0.108562	1.331076
N	0.783455	0.097435	-1.318615
C	0.724208	0.073617	2.664594
C	0.711166	0.050279	-2.651821
C	1.831951	0.000354	3.505003
C	1.814220	-0.034691	-3.496520

C	3.115010	-0.040912	2.897819
C	3.100451	-0.075222	-2.894826
C	3.208021	-0.020816	1.524717
C	3.200111	-0.041871	-1.522587
C	2.031633	0.043410	0.715027
C	2.028280	0.035252	-0.707229
H	-0.281637	0.107043	3.092541
H	-0.296626	0.082888	-3.074975
H	1.697176	-0.029182	4.588304
H	1.673275	-0.074486	-4.578640
H	4.020565	-0.094208	3.509972
H	4.002650	-0.139260	-3.510720
H	4.186499	-0.061552	1.043317
H	4.180656	-0.082873	-1.045460
C	-0.713971	2.055308	0.015358
O	-0.696667	3.211330	0.022089
C	-2.051185	0.159110	1.297497
C	-2.050400	0.188562	-1.286127
O	-2.832928	0.098309	2.150827
O	-2.826087	0.158015	-2.145853

Total gas phase energy = -1128.4266650474

solvent phase geometry

Mn	-0.806948	0.209674	-0.006154
C	-0.869123	-1.857124	0.123639
O	-1.555381	-2.554928	0.855768
O	0.015876	-2.542824	-0.678841
H	0.487911	-1.861572	-1.186683
N	0.797895	0.053042	1.301751
N	0.800082	0.059530	-1.347315
C	0.722746	0.015413	2.640508
C	0.740495	0.084282	-2.696190
C	1.828559	-0.035917	3.481469
C	1.851172	0.059197	-3.523160
C	3.115795	-0.053574	2.883284
C	3.139266	0.019037	-2.911356
C	3.219014	-0.029652	1.509417
C	3.230684	0.012032	-1.538304
C	2.044770	0.019165	0.695064
C	2.052299	0.037966	-0.729322
H	-0.283735	0.031895	3.065708
H	-0.264132	0.107203	-3.127075
H	1.690901	-0.059642	4.564240
H	1.725909	0.063148	-4.607607
H	4.016485	-0.088195	3.501956
H	4.044228	-0.007083	-3.523808
H	4.201411	-0.048515	1.035552
H	4.209875	-0.016035	-1.057813
C	-0.669982	2.030981	-0.049028
O	-0.617130	3.184844	-0.076990

C	-2.049307	0.236606	1.285402
C	-2.059167	0.135697	-1.281216
O	-2.841110	0.232917	2.129008
O	-2.858047	0.067059	-2.119462

Total solvent phase energy = -1128.5030035199

Reactant complex 3_4-Mn (gas phase TS geometry not converged)

solvent phase geometry

Mn	-0.761524	0.655285	-0.040829
C	-0.186065	-2.761994	0.620855
O	-1.131484	-2.812681	1.299712
O	0.766927	-2.787769	-0.046372
N	0.679807	0.165763	1.221183
N	0.741646	0.312993	-1.306376
C	0.583396	0.057538	2.587526
C	0.675385	0.404295	-2.665054
C	1.640327	-0.215789	3.421808
C	1.763444	0.270465	-3.499268
C	2.941334	-0.394578	2.868504
C	3.043987	0.032148	-2.926848
C	3.075030	-0.295023	1.500352
C	3.137847	-0.070393	-1.555291
C	1.950659	-0.025774	0.679026
C	1.980163	0.063844	-0.742267
H	-0.414902	0.200772	3.002744
H	-0.316618	0.608362	-3.073257
H	1.463521	-0.297342	4.497322
H	1.628731	0.358073	-4.580052
H	3.801610	-0.611700	3.505582
H	3.930539	-0.069880	-3.557444
H	4.051926	-0.434489	1.032856
H	4.103520	-0.257682	-1.082086
C	-0.868058	2.367901	-0.421868
O	-0.959544	3.496164	-0.726940
C	-2.006203	0.663687	1.239344
C	-1.986583	0.035715	-1.171207
O	-2.815097	0.660358	2.083859
O	-2.800719	-0.347915	-1.922526

Total gas phase energy = -1127.843025533

Total solvent phase energy = -1127.9120393534

TS 3_4-Mn (gas phase geometry not converged)

solvent phase geometry

Mn	-0.735706	0.519429	-0.012246
C	-0.506268	-2.267459	0.282026
O	-1.465922	-2.567404	0.919063
O	0.507915	-2.520046	-0.281559
N	0.742706	0.144834	1.254227
N	0.782325	0.265578	-1.295380
C	0.660381	0.105328	2.618351

C	0.703582	0.322984	-2.649470
C	1.742055	-0.081802	3.450575
C	1.789584	0.167268	-3.488221
C	3.033746	-0.239067	2.886649
C	3.066889	-0.052161	-2.917840
C	3.145938	-0.202855	1.510044
C	3.169710	-0.113382	-1.541559
C	2.000589	-0.014543	0.701625
C	2.015195	0.038308	-0.734188
H	-0.338780	0.232594	3.036529
H	-0.290687	0.509377	-3.058637
H	1.585865	-0.107077	4.531845
H	1.647807	0.221056	-4.570107
H	3.912263	-0.385339	3.518760
H	3.950281	-0.174185	-3.549115
H	4.121749	-0.320546	1.035885
H	4.138069	-0.287065	-1.070057
C	-0.806031	2.272448	-0.174029
O	-0.860918	3.435351	-0.286779
C	-1.999098	0.448257	1.246391
C	-1.948558	-0.016703	-1.212739
O	-2.825571	0.399137	2.067869
O	-2.741896	-0.367238	-1.998402

Total gas phase energy = -1127.8356205533

Total solvent phase energy = -1127.9080407828

Reactant complex 3_5-Mn (gas phase TS geometry not converged)

solvent phase geometry

Mn	-1.334276	-0.508106	-0.432677
H	-0.465968	-2.628829	-1.598483
N	-0.314960	-1.633000	0.850426
N	0.551605	-0.248691	-1.083701
C	-0.830399	-2.326919	1.917815
C	0.912720	0.564455	-2.113882
C	-0.095576	-3.161078	2.728664
C	2.213758	0.710118	-2.549781
C	1.286987	-3.344180	2.468965
C	3.235421	-0.036104	-1.909062
C	1.843580	-2.641448	1.418395
C	2.888311	-0.878478	-0.870484
C	1.048589	-1.774050	0.631457
C	1.537003	-0.971884	-0.451399
H	-1.895165	-2.182732	2.105710
H	0.092630	1.108545	-2.586652
H	-0.592610	-3.677948	3.552842
H	2.438672	1.385268	-3.378279
H	1.892706	-4.015400	3.082097
H	4.274598	0.052573	-2.235922
H	2.903899	-2.754277	1.182603
H	3.652316	-1.468388	-0.361705

C	-1.708218	1.223536	-0.413673
O	-1.997376	2.359620	-0.458984
C	-2.917431	-0.871364	0.311010
C	-1.936031	-0.922594	-2.039027
O	-3.952274	-1.110272	0.800677
O	-2.347959	-1.136500	-3.118481
C	-1.257335	-6.934529	-0.106330
C	-1.936827	-5.735093	0.141199
C	-0.149664	-6.925242	-0.966113
H	-2.801039	-5.724609	0.812118
H	0.392891	-7.852426	-1.174100
C	-1.523658	-4.542109	-0.457911
C	0.277979	-5.737204	-1.565233
H	-2.045776	-3.602435	-0.266755
H	1.147331	-5.716402	-2.227745
C	-0.407414	-4.535444	-1.313475
H	-1.588382	-7.862704	0.367298
O	0.038202	-3.410554	-1.919674

Total gas phase energy = -1246.6869411002

Total solvent phase energy = -1246.757763537

TS 3_5-Mn (gas phase geometry not converged)

solvent phase geometry

Mn	-1.262107	-0.750148	-0.596703
H	-1.197647	-2.104510	-1.820252
N	-0.174458	-1.942457	0.658993
N	0.659141	-0.327662	-1.179786
C	-0.685565	-2.773870	1.593713
C	0.990870	0.590529	-2.109281
C	0.082680	-3.669474	2.324376
C	2.305628	0.858132	-2.471133
C	1.459204	-3.741486	2.071985
C	3.333419	0.139197	-1.842288
C	2.001426	-2.893508	1.114321
C	2.997884	-0.816757	-0.888822
C	1.167754	-1.992437	0.430197
C	1.644485	-1.037213	-0.572166
H	-1.761581	-2.715209	1.756077
H	0.154246	1.121081	-2.567119
H	-0.402550	-4.319224	3.053976
H	2.520668	1.616153	-3.227087
H	2.092206	-4.453227	2.606125
H	4.379114	0.329551	-2.096192
H	3.066644	-2.936561	0.882438
H	3.778857	-1.382279	-0.380171
C	-1.538071	0.919420	-0.070155
O	-1.790201	2.043819	0.141316
C	-2.838568	-1.240309	0.079687
C	-1.839136	-0.863045	-2.252028
O	-3.858161	-1.549586	0.550551

O	-2.247941	-0.853067	-3.365507
C	-1.232302	-6.421689	0.571491
C	-2.319415	-5.669224	0.100145
C	0.043940	-6.154538	0.048574
H	-3.321255	-5.862540	0.500964
H	0.907101	-6.718397	0.419112
C	-2.143433	-4.675391	-0.863651
C	0.232767	-5.163729	-0.913290
H	-2.991383	-4.084830	-1.223096
H	1.231648	-4.935557	-1.297822
C	-0.855632	-4.384801	-1.416801
H	-1.377734	-7.194606	1.331988
O	-0.681682	-3.457427	-2.310931

Total gas phase energy = -1246.6487338272

Total solvent phase energy = -1246.7348007945

Reactant complex 5_6-Mn (gas phase TS geometry not converged)

solvent phase geometry

Mn	-0.707732	-0.302429	0.023943
C	-0.125097	-2.394189	0.101501
O	1.092502	-2.648109	0.114955
O	-1.059152	-3.259811	0.144117
H	-0.912490	-4.741352	0.330512
N	0.833084	-0.047875	1.346230
N	0.872955	-0.117616	-1.261716
C	0.727777	0.023606	2.685590
C	0.805659	-0.117174	-2.605538
C	1.829676	0.046332	3.533796
C	1.930636	-0.139289	-3.422168
C	3.112231	0.003413	2.971691
C	3.196346	-0.153700	-2.821944
C	3.230290	-0.054389	1.587970
C	3.275027	-0.138320	-1.434249
C	2.071423	-0.085639	0.794078
C	2.093783	-0.125943	-0.672732
H	-0.284262	0.055292	3.092826
H	-0.193899	-0.107510	-3.043057
H	1.678333	0.099192	4.614003
H	1.809433	-0.145908	-4.507475
H	4.003908	0.020709	3.602320
H	4.105006	-0.172348	-3.427808
H	4.215874	-0.080067	1.123533
H	4.247414	-0.140353	-0.942159
C	-1.195451	1.438467	-0.025682
O	-1.560418	2.539281	-0.058935
C	-1.893373	-0.785285	1.280380
C	-1.825110	-0.853233	-1.261609
O	-2.643319	-1.130184	2.094106
O	-2.519172	-1.242739	-2.104892
C	2.451682	-8.016691	0.631554

C	2.522038	-6.622005	0.510970
C	1.189928	-8.625337	0.690962
H	3.497538	-6.126463	0.459996
H	1.110197	-9.713203	0.787138
C	1.363634	-5.841546	0.449519
C	0.023425	-7.858906	0.634189
H	1.413776	-4.752609	0.337193
H	-0.963094	-8.328931	0.683604
C	0.091367	-6.453509	0.510885
H	3.362107	-8.619951	0.679408
O	-1.050385	-5.758339	0.455991

Total gas phase energy = -1435.2653675017

Total solvent phase energy = -1435.3584734774

TS 5_6-Mn (gas phase geometry not converged)

solvent phase geometry

Mn	-0.712093	-0.357828	0.032738
C	-0.132044	-2.397822	0.087026
O	1.064345	-2.704203	0.119758
O	-1.089601	-3.288677	0.095227
H	-0.829829	-4.423515	0.217490
N	0.842864	-0.081209	1.354673
N	0.875056	-0.152024	-1.260942
C	0.740837	0.004024	2.691973
C	0.805060	-0.146792	-2.603130
C	1.847327	0.049547	3.535539
C	1.931049	-0.156667	-3.421155
C	3.125896	0.012032	2.968309
C	3.195582	-0.166859	-2.822256
C	3.239025	-0.060438	1.583799
C	3.275641	-0.157076	-1.433589
C	2.077263	-0.109612	0.796946
C	2.095296	-0.153037	-0.672992
H	-0.269504	0.030974	3.103631
H	-0.194920	-0.141797	-3.039785
H	1.700855	0.116473	4.615521
H	1.809985	-0.157339	-4.506385
H	4.020503	0.045763	3.594148
H	4.104421	-0.177825	-3.428060
H	4.223231	-0.080330	1.116379
H	4.248656	-0.155392	-0.942902
C	-1.172696	1.402432	-0.001557
O	-1.506840	2.510347	-0.021145
C	-1.901791	-0.817332	1.295869
C	-1.866382	-0.861154	-1.244696
O	-2.652551	-1.147582	2.112633
O	-2.590958	-1.217056	-2.074413
C	2.448870	-8.138448	0.679250
C	2.601026	-6.748909	0.553792
C	1.149152	-8.667981	0.702036

H	3.605967	-6.311206	0.536228
H	0.999578	-9.748651	0.806129
C	1.495079	-5.902709	0.449692
C	0.034297	-7.835359	0.600548
H	1.611546	-4.820252	0.343331
H	-0.979996	-8.247330	0.621496
C	0.168602	-6.423592	0.463539
H	3.320565	-8.792871	0.762325
O	-0.899446	-5.673863	0.358055

Total gas phase energy = -1435.2558499324

Total solvent phase energy = -1435.3536271973

Reactant complex 6_7-Mn

gas phase geometry

Mn	-0.783001	0.078108	0.008556
C	-0.334900	-1.924501	0.104308
O	0.730061	-2.454318	-0.140946
O	-1.365534	-2.768327	0.529455
H	-1.036438	-3.683185	0.416968
N	0.784348	0.285577	1.334087
N	0.831228	0.154189	-1.278620
C	0.669632	0.403792	2.665207
C	0.759996	0.127034	-2.616683
C	1.768885	0.385736	3.520236
C	1.886371	0.058531	-3.432379
C	3.043943	0.238813	2.972410
C	3.145626	0.015232	-2.829081
C	3.168851	0.137616	1.589628
C	3.223749	0.043577	-1.440258
C	2.019158	0.168665	0.789222
C	2.044663	0.108231	-0.683538
H	-0.341039	0.481286	3.062957
H	-0.241426	0.155645	-3.049462
H	1.612378	0.462704	4.596583
H	1.767326	0.036121	-4.517490
H	3.927874	0.198498	3.612184
H	4.054707	-0.041299	-3.432000
H	4.152642	0.024355	1.135377
H	4.193976	0.010105	-0.945723
C	-1.033873	1.890249	-0.118453
O	-1.181500	3.028213	-0.191871
C	-2.071559	-0.053330	1.278708
C	-1.992866	-0.371681	-1.258330
O	-2.894751	-0.099040	2.080073
O	-2.739389	-0.705958	-2.069405
C	2.663576	-3.726164	4.910642
C	1.814187	-2.907090	5.665092
C	2.327387	-4.012464	3.583430
H	2.067336	-2.664957	6.701522
H	2.983720	-4.643748	2.977178

C	0.642748	-2.392941	5.106111
C	1.163729	-3.493966	3.007333
H	-0.038594	-1.765061	5.685967
H	0.935191	-3.693736	1.959229
C	0.307130	-2.684209	3.772449
H	3.573059	-4.139480	5.353716
O	-0.830316	-2.133848	3.285474
H	-1.050666	-2.458542	2.390816

Total gas phase energy = -1435.8110675157

solvent phase geometry

Mn	-0.815763	0.228144	-0.152503
C	-0.611628	-1.791035	-0.468542
O	-0.388375	-2.347256	-1.528610
O	-0.754422	-2.628828	0.636331
H	-0.665324	-3.551985	0.320534
N	0.710105	0.183478	1.255192
N	0.862014	0.328731	-1.349967
C	0.538142	0.212560	2.585324
C	0.838777	0.375736	-2.689682
C	1.603397	0.200954	3.483371
C	1.995991	0.340354	-3.464766
C	2.904079	0.154761	2.980481
C	3.231099	0.247440	-2.820552
C	3.088477	0.145688	1.598899
C	3.258664	0.188922	-1.428239
C	1.969867	0.173304	0.756300
C	2.053403	0.227302	-0.714715
H	-0.487091	0.226268	2.950064
H	-0.139812	0.450688	-3.163347
H	1.401080	0.216203	4.554981
H	1.917129	0.388223	-4.552608
H	3.765467	0.133488	3.650862
H	4.160894	0.218677	-3.392344
H	4.094157	0.128024	1.180405
H	4.209504	0.107931	-0.902571
C	-0.906847	2.053668	-0.006794
O	-0.963487	3.201833	0.054189
C	-2.121216	-0.119595	1.042189
C	-1.990363	0.195265	-1.516268
O	-2.931310	-0.400771	1.814206
O	-2.717152	0.147158	-2.410979
C	2.597898	-3.898359	5.117100
C	1.689057	-3.124475	5.851790
C	2.347181	-4.136852	3.760653
H	1.879632	-2.915077	6.908689
H	3.048585	-4.734269	3.170588
C	0.542453	-2.604241	5.245724
C	1.207371	-3.614388	3.140934
H	-0.172725	-1.999332	5.809755

H	1.021264	-3.792417	2.080219
C	0.293214	-2.844916	3.883075
H	3.490388	-4.308558	5.596662
O	-0.825080	-2.312182	3.337880
H	-0.833942	-2.433184	2.360836

Total solvent phase energy = -1435.8372958775

TS 6_7-Mn

gas phase geometry

Mn	-1.024086	0.123766	-0.126171
C	-1.156973	-1.835620	-0.081683
O	-1.059615	-2.889881	-0.521234
O	-2.020348	-2.167688	1.871957
H	-2.397758	-3.058653	1.838946
N	0.234638	0.147012	1.658777
N	1.027701	-0.271883	-0.873432
C	-0.223251	0.365179	2.895924
C	1.330444	-0.589056	-2.140854
C	0.627904	0.572718	3.983469
C	2.621890	-0.921609	-2.542539
C	2.000012	0.528244	3.772903
C	3.632598	-0.935532	-1.577231
C	2.484003	0.283943	2.482327
C	3.316521	-0.613204	-0.260833
C	1.574439	0.065602	1.448744
C	1.995277	-0.272538	0.071282
H	-1.305400	0.376303	3.023889
H	0.502420	-0.579885	-2.853291
H	0.199604	0.727339	4.974263
H	2.823069	-1.182568	-3.583253
H	2.696967	0.673879	4.599494
H	4.653789	-1.216770	-1.846605
H	3.555671	0.224810	2.302452
H	4.076914	-0.664626	0.516928
C	-0.668419	1.943373	-0.250983
O	-0.388752	3.049109	-0.335299
C	-2.609913	0.366167	0.773454
C	-1.890798	0.079238	-1.719755
O	-3.585519	0.546047	1.341219
O	-2.436467	0.020107	-2.729041
C	3.637357	-3.134446	2.789094
C	3.247767	-2.768432	4.087855
C	2.637335	-3.324890	1.822411
H	4.005790	-2.668205	4.872368
H	2.913123	-3.673895	0.821052
C	1.911247	-2.530472	4.398487
C	1.295783	-3.100278	2.120676
H	1.604317	-2.234659	5.405764
H	0.529092	-3.283092	1.369210
C	0.881537	-2.637519	3.410500

H	4.686332	-3.334608	2.552423
O	-0.335806	-2.293570	3.682891
H	-1.272804	-2.234823	2.644123

Total gas phase energy = -1435.7846017358

solvent phase geometry

Mn	-0.983663	0.209218	-0.102944
C	-1.115716	-1.768244	-0.200096
O	-0.927822	-2.729944	-0.809813
O	-1.996068	-2.437737	1.502784
H	-2.099407	-3.386391	1.324364
N	0.320665	0.170405	1.662141
N	1.028521	-0.214121	-0.904235
C	-0.091550	0.448778	2.906255
C	1.286124	-0.512256	-2.186005
C	0.796386	0.637555	3.963670
C	2.552263	-0.894443	-2.626672
C	2.162567	0.520010	3.714719
C	3.586522	-0.968981	-1.691134
C	2.594535	0.218370	2.423723
C	3.317856	-0.659883	-0.358610
C	1.645538	0.038311	1.411521
C	2.019856	-0.282865	0.015187
H	-1.166804	0.538133	3.061019
H	0.446767	-0.447895	-2.881248
H	0.409191	0.869400	4.956963
H	2.713878	-1.140011	-3.677860
H	2.889552	0.663492	4.516143
H	4.589205	-1.278938	-1.994700
H	3.658014	0.124494	2.209513
H	4.107166	-0.733441	0.388238
C	-0.606475	2.027834	-0.151995
O	-0.319870	3.134263	-0.195555
C	-2.531339	0.399231	0.843232
C	-1.881328	0.302496	-1.678788
O	-3.486228	0.506988	1.469243
O	-2.451044	0.361347	-2.674873
C	3.510981	-3.224214	3.192917
C	2.923461	-2.893555	4.424624
C	2.686097	-3.327363	2.063342
H	3.546066	-2.825120	5.323382
H	3.122964	-3.605277	1.098316
C	1.556364	-2.638393	4.519871
C	1.314278	-3.085197	2.148000
H	1.100491	-2.355674	5.473542
H	0.686414	-3.175775	1.260536
C	0.702350	-2.697412	3.378131
H	4.583752	-3.423092	3.119914
O	-0.561323	-2.389481	3.481496
H	-1.311565	-2.400188	2.372417

Total solvent phase energy = -1435.8130169017

Reactant complex 8_2CO-Mn

gas phase geometry

Mn	-0.871297	0.467187	0.005485
C	-1.638798	-1.194177	-0.938788
O	-2.527391	-1.283211	-1.748365
O	-0.905984	-2.390924	-0.713089
H	-0.220822	-2.132134	-0.070475
N	0.780881	-0.626028	0.722109
N	0.369454	0.464033	-1.658358
C	0.945642	-1.127547	1.962751
C	0.034915	0.876279	-2.888175
C	2.143092	-1.624176	2.449363
C	0.894243	0.836482	-3.980371
C	3.283550	-1.574520	1.591575
C	2.195044	0.316381	-3.778428
C	3.145526	-1.058551	0.323617
C	2.554797	-0.132605	-2.526170
C	1.882101	-0.581213	-0.137442
C	1.626766	-0.074921	-1.445777
H	0.047264	-1.135000	2.586896
H	-0.982165	1.256917	-3.001316
H	2.198971	-2.036722	3.457849
H	0.553041	1.191455	-4.954408
H	4.252990	-1.943564	1.939097
H	2.902993	0.243899	-4.608872
H	4.007241	-1.005170	-0.342936
H	3.533160	-0.586657	-2.367389
C	-0.083200	1.938510	0.770907
O	0.408014	2.847636	1.286474
C	-1.933478	0.049797	1.382995
C	-2.167829	1.441216	-0.767380
O	-2.624066	-0.285010	2.251724
O	-2.983070	2.079117	-1.280183
C	4.179892	-3.976063	-2.812918
C	3.395152	-3.882123	-1.658576
C	3.578067	-3.756137	-4.059924
H	3.842639	-4.048701	-0.674391
H	4.173194	-3.839141	-4.974975
C	2.036985	-3.567872	-1.738026
C	2.224968	-3.432314	-4.150795
H	1.441248	-3.488779	-0.829068
H	1.745340	-3.238563	-5.113060
C	1.434063	-3.321442	-2.988425
H	5.240002	-4.234986	-2.743132
O	0.147167	-2.985489	-3.133319
H	-0.294620	-2.851929	-2.258173

Total gas phase energy = -1435.8648716399

solvent phase geometry

Mn	-1.066151	0.433092	-0.110849
C	-1.474083	-1.523546	-0.573013
O	-2.421379	-2.025720	-1.144811
O	-0.433554	-2.430246	-0.277166
H	0.212019	-1.901902	0.232804
N	0.775917	-0.137609	0.729495
N	0.151947	0.368334	-1.799706
C	1.053986	-0.269895	2.047783
C	-0.241159	0.569729	-3.067885
C	2.329269	-0.429715	2.558271
C	0.612048	0.525582	-4.162603
C	3.423304	-0.450978	1.639995
C	1.978934	0.235039	-3.926095
C	3.171879	-0.306202	0.295164
C	2.405431	0.013592	-2.635100
C	1.837802	-0.127709	-0.182253
C	1.483377	0.078216	-1.547823
H	0.188827	-0.255244	2.716298
H	-1.301407	0.790960	-3.212608
H	2.482343	-0.545032	3.633052
H	0.222595	0.713111	-5.165108
H	4.446983	-0.577237	2.002889
H	2.687247	0.177253	-4.756976
H	3.999556	-0.305211	-0.416039
H	3.449309	-0.237011	-2.439331
C	-0.592959	2.164563	0.255098
O	-0.291108	3.246698	0.518512
C	-2.035358	0.190584	1.374528
C	-2.541560	0.888746	-1.018403
O	-2.694193	-0.014930	2.305357
O	-3.485442	1.164423	-1.628001
C	4.110521	-5.019960	-2.845292
C	3.531738	-4.657448	-1.622990
C	3.510931	-4.587652	-4.036544
H	3.992933	-4.979936	-0.684686
H	3.956253	-4.860927	-4.998044
C	2.365556	-3.886636	-1.583551
C	2.347115	-3.815400	-4.010649
H	1.920389	-3.604126	-0.627343
H	1.870224	-3.470045	-4.931472
C	1.755926	-3.467687	-2.782105
H	5.021971	-5.622588	-2.870583
O	0.614457	-2.749913	-2.804943
H	0.268397	-2.635208	-1.891808

Total solvent phase energy = -1435.9336674851

TS 8_2CO-Mn

gas phase geometry

Mn	-0.895399	0.529359	-0.068191

C	-1.698668	-1.211838	-0.713374
O	-2.579521	-1.726146	-1.242252
O	-0.433228	-2.844605	-0.367959
H	0.331116	-2.483065	0.097210
N	0.729761	-0.363667	0.838792
N	0.392695	0.394740	-1.668336
C	0.843391	-0.722120	2.131773
C	0.146976	0.802060	-2.924386
C	1.937826	-1.386234	2.659012
C	1.067078	0.715472	-3.956061
C	3.003612	-1.726479	1.772567
C	2.335887	0.156101	-3.666801
C	2.922665	-1.349837	0.451193
C	2.598175	-0.295506	-2.393874
C	1.785469	-0.635127	-0.033152
C	1.610603	-0.191666	-1.374956
H	-0.006468	-0.473165	2.772595
H	-0.842281	1.226468	-3.108860
H	1.951820	-1.671262	3.712360
H	0.797566	1.063021	-4.954921
H	3.863776	-2.296858	2.133933
H	3.092057	0.050503	-4.447516
H	3.702863	-1.638846	-0.251964
H	3.552094	-0.770471	-2.167905
C	-0.164430	2.158038	0.339697
O	0.297227	3.186307	0.560527
C	-1.908496	0.442966	1.429956
C	-2.206174	1.342092	-1.011329
O	-2.541959	0.366124	2.390707
O	-3.017438	1.883929	-1.626325
C	4.307858	-3.971369	-3.482389
C	3.755545	-4.137728	-2.203412
C	3.478962	-3.462450	-4.496783
H	4.373494	-4.545644	-1.394538
H	3.886575	-3.325641	-5.506375
C	2.429596	-3.799090	-1.934010
C	2.154766	-3.117177	-4.243579
H	2.020940	-3.942074	-0.930510
H	1.519695	-2.695646	-5.027589
C	1.568066	-3.251778	-2.942577
H	5.345119	-4.250317	-3.690626
O	0.354085	-2.877192	-2.713253
H	-0.089568	-2.924223	-1.390093

Total gas phase energy = -1435.8141752879

solvent phase geometry

Mn	-1.111822	0.497350	-0.193871
C	-1.736762	-1.309576	-0.840550
O	-2.468056	-1.893831	-1.519784
O	-0.511801	-2.706604	-0.119951

H	0.109066	-2.091214	0.298789
N	0.791303	-0.268556	0.668957
N	0.209218	0.356959	-1.902142
C	1.069327	-0.459507	1.977832
C	-0.145309	0.623184	-3.171951
C	2.316780	-0.820446	2.455275
C	0.687080	0.424692	-4.262760
C	3.374351	-0.975293	1.509373
C	1.975601	-0.119830	-4.020446
C	3.118767	-0.763820	0.173886
C	2.355491	-0.407306	-2.728818
C	1.812809	-0.398103	-0.272497
C	1.471138	-0.155022	-1.638613
H	0.228098	-0.329789	2.665035
H	-1.152735	1.022608	-3.314244
H	2.473579	-0.987047	3.522655
H	0.340025	0.675085	-5.267078
H	4.375461	-1.261565	1.843127
H	2.653770	-0.334187	-4.849982
H	3.920947	-0.873849	-0.555916
H	3.320269	-0.877429	-2.536922
C	-0.423100	2.166405	0.183103
O	0.036587	3.198150	0.383363
C	-2.040396	0.331580	1.354744
C	-2.520945	1.234940	-1.050832
O	-2.612986	0.183113	2.343324
O	-3.405062	1.730556	-1.600078
C	4.399393	-4.157806	-2.881749
C	3.888499	-3.971052	-1.588726
C	3.515071	-4.065847	-3.968541
H	4.556214	-4.043744	-0.723503
H	3.892622	-4.217900	-4.986222
C	2.536539	-3.695232	-1.378383
C	2.163485	-3.786470	-3.771126
H	2.159237	-3.537603	-0.365220
H	1.478590	-3.695762	-4.619644
C	1.624838	-3.575942	-2.467581
H	5.457074	-4.386776	-3.041097
O	0.359344	-3.291433	-2.308657
H	-0.042627	-2.995664	-1.120608

Total solvent phase energy = -1435.9116028883