

Exploring the mechanisms of aqueous methanol dehydrogenation catalyzed by defined PNP Mn and Re pincer complexes under base free as well as strong base conditions

Zhihong Wei^a, Adiran de Aguirre^b, Kathrin Junge^a, Matthias Beller^a, Haijun Jiao^{a,*}

^aLeibniz-Institut für Katalyse e.V. an der Universität Rostock, Albert-Einstein-Straße 29a, 18059 Rostock, Germany.

^bInstitute of Chemical Research of Catalonia, ICIQ, the Barcelona Institute of Science and Technology, Av. Països Catalans, 16, 43007, Tarragona, Spain.

Email: haijun.jiao@catalysis.de

Contents

Table S1. Comparison of reaction Gibbs free energy (ΔG_r , kJ/mol) and reaction enthalpy (ΔH_r , kJ/mol) of $\text{CH}_3\text{OH} + \text{H}_2\text{O} = \text{CO}_2 + 3\text{H}_2$ using different models	3
Table S2. Comparison of reaction Gibbs free energy (ΔG_r , kJ/mol) and enthalpy barrier ($\Delta H^\ddagger$, kJ/mol) for $2\text{Mn} = 1\text{Mn} + \text{H}_2$ using different models	4
Table S3. Comparison of reaction Gibbs free energy (ΔG_r , kJ/mol) and enthalpy (ΔH_r , kJ/mol) for $2\text{Mn}-\text{OH} = 1\text{Mn} + \text{H}_2\text{O}$ using different models	4
Table S4. Testing calculations for effect of basis set and functional.....	6
Table S5. Relative energies [kJ/mol] of M-PNP (1M) and H-M-PN ^H P (2M) isomers in C_s and C_1 symmetrical geometries	6
Table S6a. Computed bond lengths (Å) of M-PNP (1Mn) and H-M-PN ^H P (2Mn) compared with the available experimental data from X-ray crystal structure analysis.....	7
Table S6b. Computed bond lengths (Å) of 2Mn -BH ₄ , 2Mn -OCHO and 2Mn -Br compared with the available experimental data from X-ray crystal structure analysis.....	7
Table S6c. Computed bond lengths (Å) of 1Re (C_1), 1Re (C_s), 2Re (C_1) and 2Re (C_s)	8
Table S6d. Computed bond lengths (Å) of 2Re -3CO ⁺ as well as experimental available data from the X-ray crystal structures	8
Table S7. The calculated the symmetrical and asymmetrical C–O stretching frequencies [cm ⁻¹] as well as experimental available data ($f = 0.9422$)	9
Table S8. Natural charge (δ/e), natural bond orbitals and atomic hybrid contributions for the σ and π bonds of M-PNP(1M) and H-M-PN ^H P(2M).	10
Table S9. Wiberg bonding indexes (WBI) of M-PNP (1M) and H-M-PN ^H P (2M).	11
Table S10. Second Order Perturbation Theory Analysis of Fock Matrix in NBO Basis (Threshold: 10.00 kcal/mol)	12
Table S11. Pipek-Mezey localized (PML) orbital analysis of 1Mn (C_1) and in 2Re (C_1)	14
Table S12. The calculated reaction enthalpy, entropy and Gibbs free energy [kJ/mol, 298.15 K] as well as experimental available data	15
Table S13. The calculated single point energy difference ($\Delta E = E_K - E$) between the fragment of catalyst and substrate in the corresponding transition states with (E_K) and without K ⁺ (E) assistance [kJ/mol]	16
Table S14. Optimized structures and coordinates optimized structures	17
Table S15. Computed energetic data for all optimized structures.....	98
Table S16. Coordinates of optimized structures in methanol.....	107
Table S17. Computed energetic data for all structures optimized in methanol	171

S1. Benchmark calculations

Since our reaction involves polar molecules like methanol and water, we carried out benchmark calculations under the considerations of solvation effect and van der Waals dispersion correction along with the gas phase calculations. In addition, we also tested different methods and basis sets. It shows that B3PW91 gas phase calculations have the best agreement with the available experimental results. As examples, we used computed the thermodynamics of the title reaction $[\text{CH}_3\text{OH} + \text{H}_2\text{O} = \text{CO}_2 + 3\text{H}_2]$ as well as kinetic and thermodynamic parameters of the catalyst conversion $[2\text{Mn} = 1\text{Mn} + \text{H}_2]$ and the reaction with water $[2\text{Mn}-\text{OH} = 1\text{Mn} + \text{H}_2\text{O}]$, where the available experimental results are used as references for comparison.

First, B3PW91 gas phase calculations were carried out by using the TZVP¹ (LANL2DZ² for Mn) basis sets. For comparison, **1Mn** and **2Mn** were also optimized under the consideration of solvation by using the integral equation formalism polarizable continuum model (IEFPCM) with radii and non-electrostatic terms for Truhlar's SMD solvation model at B3PW91-SCRF/TZVP (LANL2DZ for Mn) level of theory.³ In addition, we also tested the dispersion effect at B3PW91-SCRF-GD3BJ/TZVP (LANL2DZ for Mn) and M06-SCRF/TZVP (LANL2DZ for Mn) levels of theory in solvent by using SMD model.

Experimentally (Table S1), the title reaction of methanol aqueous dehydrogenation $[\text{CH}_3\text{OH} + \text{H}_2\text{O} = \text{CO}_2 + 3\text{H}_2]$ is reversible and considered as either H_2 storage or CO_2 capture;⁴ and this reveals that the reaction Gibbs free energy (ΔG) must be very small, slightly exergonic or endergonic. Our B3PW91 gas phase calculation gives Gibbs free energy (ΔG) of only -5 kJ/mol, i.e.; slightly exergonic for CO_2 formation or endergonic for methanol formation, in full agreement with the experiment.⁵ In contrast, the computed Gibbs free energy (ΔG) is highly positive including the effect of solvation (B3PW91-SCRF/ CH_3OH ; 59 kJ/mol); solvation and dispersion at B3PW91 level (B3PW91-SCRF-GD3BJ/ CH_3OH ; 63 kJ/mol) and solvation and dispersion at M06-SCRF level (M06-SCRF/ CH_3OH , 30 kJ/mol). All these results show that the title reaction has positive Gibbs free energy and would be not possible; and this is in disagreement with the well-known experimental results. In addition, the gas phase computed reaction enthalpy (ΔH) has the best agreement with the experimental value (35 vs. 49 kJ/mol), while those values including solvation as well as solvation with dispersion correction at B3PW91 level and M06 level (B3PW91-SCRF/ CH_3OH ; 113 kJ/mol, B3PW91-SCRF-GD3BJ/ CH_3OH ; 117 kJ/mol, M06-SCRF/ CH_3OH ; 85 kJ/mol, respectively) differ very strongly from the experiment. On the basis of these comparisons, one can clearly see that the gas phase computed thermodynamics has the best agreement with the experimental results, while those including solvation and van der Waals dispersion are totally wrong.

Table S1. Comparison of reaction Gibbs free energy (ΔG_r , kJ/mol) and reaction enthalpy (ΔH_r , kJ/mol) of $\text{CH}_3\text{OH} + \text{H}_2\text{O} = \text{CO}_2 + 3\text{H}_2$ using different models

	$\text{CH}_3\text{OH} + \text{H}_2\text{O} = 3\text{H}_2 + \text{CO}_2$	
	ΔG_r (kJ/mol)	ΔH_r (kJ/mol)
Exp.	equilibrium	49 ⁵
B3PW91/gas phase	-5	35
B3PW91-SCRF/ CH_3OH	59	113
B3PW91-SCRF-GD3BJ/ CH_3OH	63	117
M06-SCRF/ CH_3OH	30	85

For the inter-conversion of the catalysts with hydrogen $[2\text{Mn} = 1\text{Mn} + \text{H}_2]$, experimental results are available (Table S2), i.e.; this reaction is reversible and forms equilibrium in C_6D_6 ;⁶ and the Gibbs free energy of this reaction must be very small, slightly exergonic or endergonic. Indeed, our gas phase Gibbs free energy value of -1 kJ/mol predicts equilibrium and reversibility for this reaction, in reasonable agreement with the experimental results obtained in C_6D_6 .⁶ In addition, the computed gas phase enthalpy barrier has the best agreement with the experimental estimated value⁶ (88 vs. 80 kJ/mol). Next, we also computed non-polar solvation correction in benzene.

Although the computed Gibbs free energies with pure solvation and solvation with dispersion are slightly exergonic (B3PW91-SCRF/C₆H₆: -4 kJ/mol, B3PW91-SCRF-GD3BJ/C₆H₆; -4 kJ/mol), the computed enthalpy barriers (B3PW91-SCRF/C₆H₆; 95 kJ/mol, B3PW91-SCRF-GD3BJ/C₆H₆; 95 kJ/mol) are higher than the experimental estimated value (80 kJ/mol). In addition, M06-SCRF/C₆H₆ gives positive Gibbs free energy (12 kJ/mol) and large enthalpy barrier (98 kJ/mol). Therefore, the computed gas phase enthalpy barrier has the best agreement with the experimental estimated value.

Table S2. Comparison of reaction Gibbs free energy (ΔG_r , kJ/mol) and enthalpy barrier ($\Delta H^\ddagger$, kJ/mol) for **2Mn = 1Mn** + H₂ using different models

	2Mn = 1Mn + H₂	
	ΔG_r	$\Delta H^\ddagger$
Exp./C ₆ H ₆	equilibrium	80 ⁶
B3PW91/gas phase	-1	88
B3PW91-SCRF/C ₆ H ₆	-4	95
B3PW91-SCRF-GD3BJ/C ₆ H ₆	-4	95
M06-SCRF/C ₆ H ₆	12	98
B3PW91-SCRF/CH ₃ OH	14	113
B3PW91-SCRF-GD3BJ/CH ₃ OH	10	112
M06-SCRF/CH ₃ OH	29	115

In polar methanol solvent, calculations with pure solvation and solvation with dispersion give positive Gibbs free energy (B3PW91-SCRF/CH₃OH, 14 kJ/mol; B3PW91-SCRF-GD3BJ/CH₃OH, 10 kJ/mol, M06-SCRF/CH₃OH, 29 kJ/mol), these positive Gibbs free energies will shift the equilibrium much towards **2Mn**, in disagreement with the experimentally observed equilibrium. In addition, the computed corresponding enthalpy barriers (B3PW91-SCRF/CH₃OH, 113 kJ/mol; B3PW91-SCRF-GD3BJ/CH₃OH, 112 kJ/mol, M06-SCRF/CH₃OH, 115 kJ/mol) are much higher than the experimental one (80 kJ/mol).

For the inter-conversion of the catalysts with water [**2Mn-OH = 1Mn + H₂O**], experimental results are available (Table S3)⁷, i.e.; this reaction has endergonic reaction Gibbs free energy of 3 kJ/mol, indicating the possible equilibrium and reversibility; and the reaction is endothermic by 33 kJ/mol. In gas phase (B3PW91), the computed reaction Gibbs free energy and reaction enthalpy is 5 and 51 kJ/mol; in close agreement with the experimental values. In THF solution (B3PW91-SCRF/THF), the reaction becomes exergonic (-15 kJ/mol), in disagreement with the experiment, while the reaction enthalpy (36 kJ/mol) is much close to the experiment. Further including dispersion (B3PW91-SCRF-GD3BJ/THF) gives exergonic reaction Gibbs free energy (-3 kJ/mol) and the reaction enthalpy is 45 kJ/mol. M06 in THF solution (M06-SCRF/THF) gives reasonable endergonic Gibbs free energy (7 kJ/mol) and larger reaction enthalpy (58 kJ/mol). All these show that the gas phase results are in best agreement with the experiment. In addition, we also computed the inter-conversion in polar methanol and water, and the results are model depending and it is not possible to get a general conclusion.

Table S3. Comparison of reaction Gibbs free energy (ΔG_r , kJ/mol) and enthalpy (ΔH_r , kJ/mol) for **2Mn-OH = 1Mn + H₂O** using different models

	2Mn-OH = 1Mn + H₂O	
	ΔG_r	ΔH_r
Exp./THF	3.3 ⁷	33 ⁷
B3PW91/gas phase	5	51
B3PW91-SCRF/THF	-15	36
B3PW91-SCRF-GD3BJ/THF	-3	45

M06-SCRF/THF	7	58
B3PW91-SCRF/H ₂ O	-14	35
B3PW91-SCRF-GD3BJ/H ₂ O	-2	45
M06-SCRF/H ₂ O	-3	55
B3PW91-SCRF/CH ₃ OH	-11	38
B3PW91-SCRF-GD3BJ/CH ₃ OH	0	47
M06-SCRF/CH ₃ OH	3	61

On the basis of these three reactions, one can clearly see that only gas phase calculation can give the best agreement with the experimentally observed equilibrium and the enthalpy values, while those including solvation and dispersion differ very strongly from the experiment.

In addition, we also tested the performance of the all-electron TZVP basis set for Mn for optimization as well as the correlation consistent aug-cc-pVDZ basis set for single-point energy calculations on the basis of the available experimental results for the reactions,^{6, 7} $2\text{Mn} = \text{1Mn} + \text{H}_2$ (308-323 K) and $\text{1Mn} + \text{H}_2\text{O} = \text{2Mn-OH}$ (or reverse, 228-318 K). In addition, the performance of M06/TZVP optimization is included for comparison. As given in Table S4, the best agreement between theory and experiment is found for B3PW91 with the mixed (LANL2DZ + TZVP) and all-electron (TZVP) basis sets; while the worst performance is found for B3PW91 using the aug-cc-pVDZ basis set for the $2\text{Mn} = \text{1Mn} + \text{H}_2$ reaction as well as for M06/TZVP for the $\text{1Mn} + \text{H}_2\text{O} = \text{2Mn-OH}$ (or reverse) reaction. Since we studied both Mn and Re catalysts; and therefore we used the LANL2DZ basis set for general comparison.

Table S4. Testing calculations for effect of basis set and functional

Method	$2\text{Mn} = \text{1Mn} + \text{H}_2$	$2\text{Mn-OH} = \text{1Mn} + \text{H}_2\text{O}$
Experiment	Equilibrium	3
B3PW91/TZVP (LANL2DZ for Mn)//Fopt	-1 (best)	5 (best)
B3PW91/TZVP//Fopt	-6	-1
B3PW91/TZVP-dkh2//B3PW91/TZVP(SP)	-7	-3
B3PW91/aug-cc-pVDZ-DK(SP)	36 (worst)	-6
M06/TZVP	4	22 (worst)

Table S5. Relative energies [kJ/mol] of M-PNP (**1M**) and H-M-PN^HP (**2M**) isomers in C_s and C₁ symmetrical geometries

Symmetry	1Mn	1Re
C _s	4	7
C ₁	0	0
	2Mn	2Re
C _s	0	0
C ₁	7	12

Table S6a. Computed bond lengths (Å) of M-PNP (**1Mn**) and H-M-PN^HP (**2Mn**) compared with the available experimental data from X-ray crystal structure analysis

	1Mn (C₁)	1Mn (C_s)	1Mn-X-ray^a
M–N	1.891	1.889	1.882
M–P	2.272/2.276	2.269	2.256
M–L _{trans}	1.761	1.743	1.765
M–L _{anti}	1.748	1.768	1.771
	2Mn (C₁)	2Mn (C_s)	2Mn-X-Ray^b
M–N	2.150	2.149	2.128
M–P	2.254/2.258	2.250	2.238
M–L _{trans}	1.754	1.755	1.756
M–L _{anti}	1.769	1.770	1.779
M–H	1.584	1.604	1.592
N–H	1.016	1.016	0.863

Experimental values from (a) *Organometallics*, **2016**, 35, 2049-2052 (Cambridge Structural Database, CCDC: 1502624); (b) *ACS Catal.*, **2017**, 7, 2022–2032 (CCDC: 1513978).

Table S6b. Computed bond lengths (Å) of **2Mn–BH₄**, **2Mn–OCHO** and **2Mn–Br** compared with the available experimental data from X-ray crystal structure analysis

	2Mn–BH₄		2Mn–OCHO		2Mn–Br	
	DFT	X-Ray ^a	DFT	X-Ray ^b	DFT	X-Ray ^c
M–N	2.124	2.110	2.143	2.107	2.138	2.122/2.119
M–P	2.302	2.282/2.294	2.311	2.300	2.321	2.299,2.301/2.301,2.302
M–L _{trans}	1.769	1.768	1.774	1.781	1.771	1.781/1.777
M–L _{anti}	1.750	1.758	1.747	1.755	1.741	1.751/1.756
M–H/O/Br	1.730	1.774	2.103	2.048	2.595	2.577/2.575
N–H	1.024	0.847	1.039	0.930	1.024	0.836/0.847

Experimental values from (a) *ACS Catal.*, **2017**, 7, 2022–2032 (CCDC: 1507334_2Mn–BH₄); (b) *Organometallics*, **2016**, 35, 2049-2052 (CCDC: 1502626); (c) *J. Am. Chem. Soc.* **2016**, 138, 8809–8814 (CCDC: 1436386).

Table S6c. Computed bond lengths (Å) of **1Re** (C_1), **1Re** (C_s), **2Re** (C_1) and **2Re** (C_s)

	1Re (C_1)	1Re (C_s)
M–N	2.026	2.025
M–P	2.391/2.395	2.398
M–L _{trans}	1.901	1.888
M–L _{anti}	1.888	1.901
	2Re (C_1)	2Re (C_s)
M–N	2.273	2.271
M–P	2.388/2.388	2.382
M–L _{trans}	1.898	1.898
M–L _{anti}	1.927	1.927
M–H(O)	1.749	1.765
N–H	1.017	1.017

Table S6d. Computed bond lengths (Å) of **2Re–3CO⁺** as well as experimental available data from the X-ray crystal structures

	2Re–3CO⁺-DFT	2Re–3CO⁺-X-Ray^a
Re–N	2.282	2.229
Re–P	2.511/2.518	2.480/2.495
Re–CO	1.943	1.933
Re–CO	1.925	1.918
Re–CO	1.943	1.944
N–H	1.015	0.899

Experimental values from (a) *Chem. Commun.*, **2017**, 53, 3265-3268 (CCDC: 1522448)

Table S7. The calculated the symmetrical and asymmetrical C–O stretching frequencies [cm^{-1}] as well as experimental available data ($f = 0.9422$)

symmetrical	Calculated		Scaled		Exp.	
	symm	asymm	symm	asymm		
1Mn	1996	1943	1881	1831	1888.8 ^a /1894 ^b	1816.3 ^a /1817 ^b
2Mn	1997	1933	1882	1821	1889 ^c /1872.7 ^a	1815 ^c /1786.4 ^a
2Mn–BH₄	2024	1953	1907	1840	1913 ^a	1836 ^a
2Mn–OCHO	2028	1948	1911	1835	1916 ^b	1828 ^b
2Mn–OH	2003	1934	1887	1822	1888 ^c	1800 ^c
2Mn–Br	2028	1946	1911	1834	1921 ^d	1832 ^d

Experimental values from (a) *ACS Catal.*, **2017**, 7, 2022–2032; (b) *Organometallics*, **2016**, 35, 2049–2052; (c) *Organometallics* **2017**, DOI: 10.1021/acs.organomet.7b00618.; (d) *J. Am. Chem. Soc.* **2016**, 138, 8809–8814.

Table S8. Natural charge (δ/e), natural bond orbitals and atomic hybrid contributions for the σ and π bonds of M-PNP(**1M**) and H-M-PN^HP(**2M**).

		1Mn (C ₁)	1Mn (C _s)	1Re (C ₁)	1Re (C _s)
Natural charge	M	-1.430	-1.440	-1.233	-1.225
	N	-0.450	-0.443	-0.508	-0.505
N–M	σ	----	17.69%Mn[sp ^{2.52} d ^{1.74}] 82.31%N[sp ^{1.32}]	20.67%Re[sp ^{2.69} d ^{2.93}] 79.33%N[sp ^{1.23}]	20.56%Re[sp ^{2.72} d ^{2.87}] 79.44%N[sp ^{1.23}]
	π	17.76%Mn[sp ^{7.94} d ^{9.38}] 82.24%N[sp ^{9.51}]	16.00%Mn[sp ^{21.58} d ^{27.40}] 84.00%N[sp ^{69.60}]	15.30%Re[pd] 84.70%N[p]	15.76%Re[pd] 84.24%N[p]
M–CO	σ	32.31%Mn[sp ^{2.94} d ^{1.54}] 67.69%C[sp ^{0.51}]	33.64%Mn[sp ^{2.63} d ^{1.56}] 66.36%C[sp ^{0.52}]	34.76%Re[sp ^{1.98} d ^{1.58}] 65.24%C[sp ^{0.54}]	36.00%Re[sp ^{1.76} d ^{1.67}] 64.00%C[sp ^{0.56}]
	σ	35.76%Mn[sp ^{0.96} d ^{1.56}] 64.24%C[sp ^{0.51}]	32.27%Mn[sp ^{2.94} d ^{1.58}] 67.73%C[sp ^{0.51}]	38.33%Re[sp ^{1.69} d ^{1.80}] 61.67%C[sp ^{0.62} d ^{0.05}]	36.69%Re[sp ^{1.90} d ^{1.74}] 63.31%C[sp ^{0.61} d ^{0.05}]
M–CO _{anti}	π	----	----	84.80%Re[sp ^{33.37} d ^{83.84}] 15.20%C[sp ^{8.99} d ^{4.81}]	85.16%Re[sp ^{33.23} d ^{80.02}] 14.84%C[sp ¹⁰ d ^{5.51}]
N		1LP	----	----	----
M		3LP	3LP	2LP	2LP
		2Mn (C ₁)	2Mn (C _s)	2Re (C ₁)	2Mn (C _s)
Natural charge	M	-2.000	-2.021	-1.842	-1.868
	H _M	0.031	0.031	-0.034	-0.024
	N	-0.471	-0.472	-0.484	-0.484
	H _N	0.397	0.398	0.404	0.402
M–H	σ	46.35%Mn[sp ^{3.16} d ^{2.26}] 53.65%H[s]	46.73%Mn[sp ^{3.17} d ^{2.29}] 53.27%H[s]	45.31%Re[sp ^{4.32} d ^{2.84}] 54.69%H[s]	45.49%Re[sp ^{4.07} d ^{2.45}] 54.51%H[s]
N–H	σ	70.37%N[sp ^{4.38}] 29.63%H[s]	70.43%N[sp ^{4.35}] 29.57%H[s]	70.62%N[sp ^{2.61}] 29.38%H[s]	70.74%N[sp ^{4.57}] 29.26%H[s]
N–M	σ	14.98%Mn[sp ^{3.63} d ^{4.78}] 85.02%N[sp ^{2.59}]	14.92%Mn[sp ^{3.81} d ^{4.89}] 85.08%N[sp ^{2.62}]	----	15.86%Re[sp ^{6.67} d ^{6.08}] 84.14%N[sp ^{2.38}]
M–CO	σ	36.66%Mn[sp ^{2.81} d ^{2.10}] 63.34%C[sp ^{0.51}]	36.50%Mn[sp ^{2.83} d ^{2.01}] 63.50%C[sp ^{0.50}]	40.19%Re[sp ^{0.72} d ^{2.09}] 59.81%C[sp ^{0.56} d ^{0.03}]	36.19%Re[sp ^{2.37} d ^{1.97}] 63.81%C[sp ^{0.52}]
	π	----	----	90.49%Re[pd ^{23.62}] 9.51%C[sp ^{25.85} d ^{8.97}]	80.23%Re[pd ^{11.47}] 19.77%C[p]
M–CO _{anti}	σ	33.79%Mn[sp ^{2.04} d ^{1.51}] 66.21%C[sp ^{0.54}]	36.76%Mn[sp ^{2.02} d ^{1.71}] 63.24%C[sp ^{0.49} d ^{0.09}]	34.25%Re[sp ^{2.45} d ^{1.94}] 65.75%C[sp ^{0.49}]	34.89%Re[sp ^{2.09} d ^{1.73}] 65.11%C[sp ^{0.52}]
	π	81.75%Mn[pd ^{4.61}] 18.25%C[sp ^{31.26} d ^{0.04}]	90.30%Mn[pd ^{4.34}] 9.70%C[sp ^{10.43} d ^{7.86}]	----	80.00%Re[pd ^{12.73}] 20.00%C[p]
	π	----	----	----	80.02%Re[pd ^{11.28}] 19.98%C[p]
N		----	----	1LP	----
M		2LP	2LP	2LP	----
orbital		107 occupied orbital	107 occupied orbital	107 occupied orbital	107 occupied orbital

Table S9. Wiberg bonding indexes (WBI) of M-PNP (**1M**) and H-M-PN^HP (**2M**).

	1Mn (<i>C</i> ₁)	1Mn (<i>C</i> _S)	2Mn (<i>C</i> ₁)	2Mn (<i>C</i> _S)	1Re (<i>C</i> ₁)	1Re (<i>C</i> _S)	2Re (<i>C</i> ₁)	2Re (<i>C</i> _S)
M–N	0.865	0.876	0.399	0.399	0.918	0.926	0.445	0.443
M–P	0.696/0.696	0.700	0.753/0.755	0.758	0.780/0.782	0.781	0.831/0.832	0.834
M–L ₁	1.243	1.287	1.238	1.245	1.423	1.458	1.401	1.407
M–L ₂	1.279	1.244	1.264	1.267	1.460	1.434	1.410	1.415
M–H	--	--	0.671	0.694	--	--	0.745	0.758
N–H	--	--	0.794	0.794	--	--	0.788	0.790

Table S10. Second Order Perturbation Theory Analysis of Fock Matrix in NBO Basis (Threshold: 10.00 kcal/mol)

Donor NBO (i)	Acceptor NBO (j)	$E(2)$ kcal/mol	$E(j) - E(i)$ a.u.	$F(i,j)$ a.u.
1Mn (C_1)				
BD(1)N1-C12	LP*(4)Mn2	13.55	0.91	0.105
BD(1)N1-C15	LP*(4)Mn2	14.14	0.91	0.107
BD(1)Mn2-C5	BD*(1)N1-Mn2	15.15	0.66	0.089
BD(1)Mn2-C7	RY*(1)N1	17.68	5.89	0.295
BD(1)Mn2-C7	RY*(2)N1	15.41	3.00	0.196
BD(1)Mn2-C7	RY*(1)Mn2	22.01	5.99	0.332
BD(1)Mn2-C7	RY*(2)C5	10.67	3.9	0.186
BD(1)Mn2-C7	RY*(4)C5	12.23	3.6	0.192
BD(1)Mn2-C7	RY*(6)C5	15.03	3.82	0.219
BD(1)Mn2-C7	RY*(7)C5	11.2	3.81	0.189
BD(1)Mn2-C7	RY*(1)O6	13.81	3.65	0.205
BD(1)Mn2-C7	RY*(1)C7	10.07	1.8	0.123
BD(1)Mn2-C7	RY*(4)C7	12.82	3.24	0.186
BD(1)Mn2-C7	RY*(6)C7	17.35	4.47	0.255
BD(1)Mn2-C7	RY*(1)O8	22.54	3.31	0.25
BD(1)Mn2-C7	BD*(1)N1-Mn2	13.48	0.66	0.085
BD(1)Mn2-C7	BD*(1)Mn2-P3	20.34	0.96	0.126
BD(1)Mn2-C7	BD*(1)Mn2-P4	19.58	0.96	0.123
BD(1)Mn2-C7	BD*(1)Mn2-C5	15.97	0.95	0.11
BD(1)Mn2-C7	BD*(1)Mn2-C7	11.52	0.99	0.096
CR(1)N1	LP*(4)Mn2	11.24	14.33	0.382
LP(1)N1	LP*(4)Mn2	96.69	0.57	0.218
LP(1)N1	BD*(1)N1-Mn2	10.08	0.47	0.065
LP(1)N1	BD*(1)Mn2-C7	11.31	0.81	0.092
LP(1)Mn2	BD*(1)C5-O6	10.62	0.28	0.049
LP(2)Mn2	BD*(1)C7-O8	12.84	0.29	0.055
LP(3)Mn2	BD*(2)C5-O6	11.06	0.32	0.056
LP(3)Mn2	BD*(2)C7-O8	12.14	0.34	0.06
LP*(4)Mn2	RY*(1)Mn2	10.17	5.24	0.59
LP*(4)Mn2	BD*(1)Mn2-P3	26.43	0.21	0.155
LP*(4)Mn2	BD*(1)Mn2-P4	28.54	0.21	0.16
LP(1)O6	RY*(1)C5	22.57	2.06	0.193
LP(1)O6	BD*(1)Mn2-C5	10.88	1.1	0.099
LP(1)O8	RY*(1)C7	22.36	1.95	0.187
LP(1)O8	BD*(1)Mn2-C7	11.07	1.14	0.102
2Re (C_1)				
BD(1)N1-C12	LP*(3)Re2	13.11	0.96	0.107
BD(1)N1-C13	LP*(3)Re2	13.09	0.96	0.107
BD(1)N1-H18	LP*(3)Re2	24.23	0.87	0.137
BD(1)Re2-P3	BD*(1)Re2-H5	10.28	0.99	0.091
BD(1)Re2-H5	BD*(1)Re2-C59	13.61	0.59	0.081
BD(1)Re2-H5	BD*(1)Re2-C60	15.65	0.60	0.089
BD(1)Re2-C59	RY*(2)Re2	14.51	3.15	0.196
BD(1)Re2-C59	RY*(3)Re2	13.56	3.06	0.186
BD(1)Re2-C59	RY*(6)Re2	10.88	2.44	0.149
BD(1)Re2-C59	RY*(7)Re2	10.01	2.08	0.132
BD(1)Re2-C59	RY*(8)Re2	18.77	9.93	0.395
BD(1)Re2-C59	RY*(9)Re2	18.78	9.94	0.395
BD(1)Re2-C59	RY*(1)O61	14.74	2.25	0.167
BD(1)Re2-C59	BD*(1)Re2-P3	14.14	0.83	0.097
BD(1)Re2-C59	BD*(1)Re2-P4	13.81	0.83	0.096
BD(1)Re2-C59	BD*(1)Re2-H5	25.09	1.04	0.144
BD(1)Re2-C59	BD*(2)Re2-C59	37.35	1.20	0.196
BD(1)Re2-C59	BD*(3)C59-O61	19.52	1.15	0.134
BD(2)Re2-C59	BD*(1)Re2-C59	14.94	0.47	0.079
BD(2)Re2-C59	BD*(2)Re2-C59	23.94	0.80	0.129
BD(2)Re2-C59	BD*(2)C59-O61	15.13	0.75	0.104
BD(2)Re2-C59	BD*(3)C59-O61	51.01	0.75	0.187
BD(2)Re2-C59	BD*(2)C60-O62	22.87	0.23	0.066
BD(2)Re2-C59	BD*(3)C60-O62	30.27	0.21	0.073
BD(2)C59-O61	BD*(2)Re2-C59	42.96	1.57	0.241

BD(2)C59-O61	BD*(3)C59-O61	43.30	1.51	0.230
BD(3)C59-O61	BD*(2)Re2-C59	107.89	1.14	0.319
BD(3)C59-O61	BD*(2)C59-O61	35.29	1.10	0.180
BD(3)C59-O61	BD*(3)C59-O61	12.06	1.09	0.104
CR(1)N1	LP*(3)Re2	11.07	14.40	0.380
LP(1)N1	LP*(3)Re2	84.24	0.55	0.197
LP(1)N1	BD*(1)Re2-C59	15.35	0.67	0.096
LP(1)Re2	BD*(1)C59-O61	32.83	0.25	0.082
LP(2)Re2	BD*(1)C59-O61	14.36	0.25	0.055
LP(2)Re2	BD*(2)C60-O62	18.20	0.26	0.063
LP(2)Re2	BD*(3)C60-O62	18.05	0.24	0.060
LP*(3)Re2	BD*(1)Re2-P3	34.52	0.09	0.120
LP*(3)Re2	BD*(1)Re2-P4	34.61	0.09	0.117
LP*(3)Re2	BD*(1)Re2-H5	22.33	0.30	0.177
LP(1)O61	RY*(1)C59	19.32	1.80	0.167
LP(1)O62	RY*(1)C60	19.07	1.61	0.157

Table S11. Pipek-Mezey localized (PML) orbital analysis of **1Mn** (C_1) and in **2Re** (C_1)

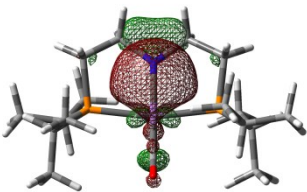
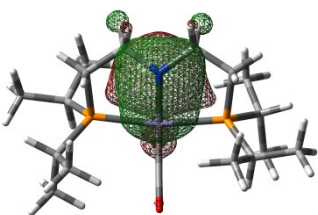
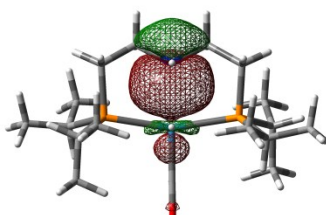
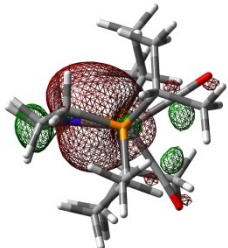
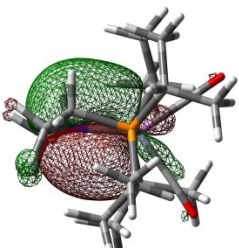
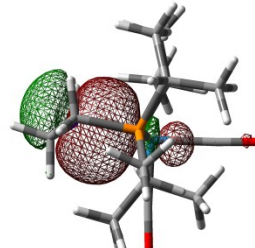
1Mn (C_1)		2Re (C_1)
σ bond (HOMO-68)	π bond (HOMO-3)	σ bond (HOMO-46)
Top 		
Side 		

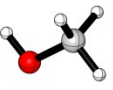
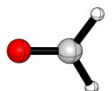
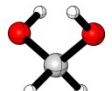
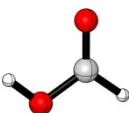
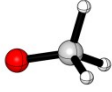
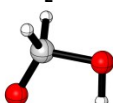
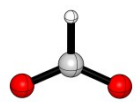
Table S12. The calculated reaction enthalpy, entropy and Gibbs free energy [kJ/mol, 298.15 K] as well as experimental available data

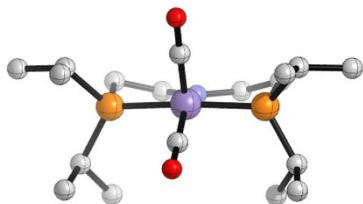
Energy	Expt.	B3PW91	Martin's approximation	1/2 entropy approximation
2Mn = 1Mn + H₂				
ΔH_r		35	35	35
$T\Delta S_r$		36	18	18
ΔG_r	equilibrium	-1 (best agreement)	17	17
2Mn–OH = 1Mn + H₂O				
ΔH_r	33	51	51	51
$T\Delta S_r$	30	46	28	23
ΔG_r	3	5 (best agreement)	23	28

Table S13. The calculated single point energy difference ($\Delta E = E_K - E$) between the fragment of catalyst and substrate in the corresponding transition states with (E_K) and without K^+ (E) assistance [kJ/mol]

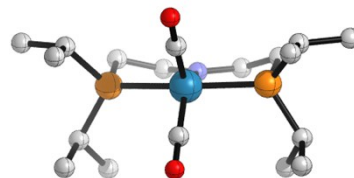
	$\Delta E_{\text{catalyst}}$	$\Delta E_{\text{substrate}}$	$\Delta E_{\text{catalyst}} + \Delta E_{\text{substrate}}$
$2\mathbf{M}^- + \text{H}_2\text{O} = \mathbf{1M-OH}^- + \text{H}_2$			
	$E_K(\mathbf{2M}^-) - E(\mathbf{2M}^-)$	$E_K(\text{H}_2\text{O}) - E(\text{H}_2\text{O})$	$\Delta E_{\mathbf{2M}^-} + \Delta E_{\text{H}_2\text{O}}$
Mn	-1	-21	-22
Re	14	-19	-5
$\mathbf{1M} + \text{CH}_3\text{O}^- = \mathbf{2M}^- + \text{CH}_2\text{O}$			
	$E_K(\mathbf{1M}) - E(\mathbf{1M})$	$E_K(\text{CH}_3\text{O}^-) - E(\text{CH}_3\text{O}^-)$	$\Delta E_{\mathbf{1M}} + \Delta E_{\text{CH}_3\text{O}^-}$
Mn	17	9	26
Re	21	6	27
$\mathbf{1M} + \text{HOCH}_2\text{O}^- = \mathbf{2M}^- + \text{HCOOH}$			
	$E_K(\mathbf{1M}) - E(\mathbf{1M})$	$E_K(\text{HOCH}_2\text{O}^-) - E(\text{HOCH}_2\text{O}^-)$	$\Delta E_{\mathbf{1M}} + \Delta E_{\text{HOCH}_2\text{O}^-}$
Mn	20	29	49
Re	27	42	69
$\mathbf{1M} + \text{HCOO}^- = \mathbf{2M}^- + \text{CO}_2$			
	$E_K(\mathbf{1M}) - E(\mathbf{1M})$	$E_K(\text{HCOO}^-) - E(\text{HCOO}^-)$	$\Delta E_{\mathbf{1M}} + \Delta E_{\text{HCOO}^-}$
Mn	9	6	15
Re	17	10	27

Table S14. Optimized structures and coordinates optimized structures

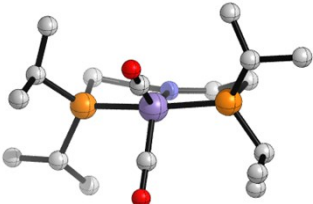
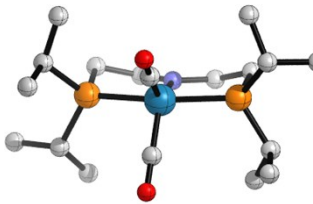
H₂  H 0.00000000 0.00000000 0.37255500 H 0.00000000 0.00000000 -0.37255500	CH₃OH  C 0.04654400 0.66052600 0.00000000 H 1.08924600 0.97928300 0.00000000 H -0.43789100 1.07871700 0.89168600 H -0.43789100 1.07871700 -0.89168600 O 0.04654400 -0.75521600 0.00000000 H -0.86508600 -1.05814400 0.00000000
CH₂O  C 0.00000000 0.00000000 -0.52590900 H 0.00000000 0.93988700 -1.11405200 H 0.00000000 -0.93988700 -1.11405200 O 0.00000000 0.00000000 0.67294400	H₂O  H 0.00000000 0.76127500 -0.46843600 O 0.00000000 0.00000000 0.11710900 H 0.00000000 -0.76127500 -0.46843600
HOCH₂OH  C 0.00000000 0.00000000 0.52787200 H -0.89131100 -0.07550500 1.15828700 H 0.89131100 0.07550500 1.15828700 O 0.00000000 1.16956500 -0.24619000 H -0.80690500 1.17764500 -0.77238700 O 0.00000000 -1.16956500 -0.24619000 H 0.80690500 -1.17764500 -0.77238700	HCOOH  C 0.00000000 0.41956600 0.00000000 H -0.38102000 1.44953600 0.00000000 O 1.15729400 0.11335100 0.00000000 O -1.02731900 -0.44182100 0.00000000 H -0.65878100 -1.33917900 0.00000000
CO₂  C 0.00000000 -0.00012600 0.00000000 O -0.66403700 -0.94978500 0.00000000 O 0.66403700 0.94988000 0.00000000	OH⁻  H 0.00000000 0.00000000 -0.86054000 O 0.00000000 0.00000000 0.10756700
CH₃O⁻  O 0.00000000 0.00000000 0.78890400 C 0.00000000 0.00000000 -0.52882100 H 0.00000000 1.02466600 -1.04610400 H 0.88738700 -0.51233300 -1.04610400 H -0.88738700 -0.51233300 -1.04610400	HOCH₂O⁻  C 0.17622800 0.49748100 -0.00015000 H 0.10800900 1.17688700 0.90254800 H 0.10853000 1.17706000 -0.90290900 O -1.19365400 -0.16796700 0.00021500 H -0.87941200 -1.08062400 -0.00160500 O 1.14434200 -0.36430900 0.00014300
HCOO⁻  C 0.00000000 0.00000000 0.31261300 H 0.00000000 0.00000000 1.45551600 O 0.00000000 -1.13450000 -0.20820000 O 0.00000000 1.13450000 -0.20820000	K⁺ 
1Mn(Cs)	1Re(Cs)

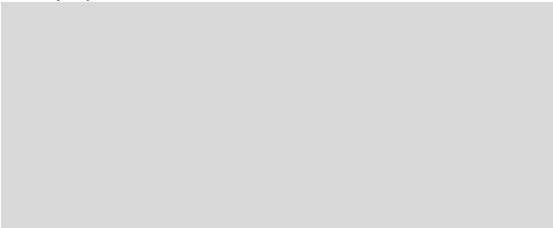
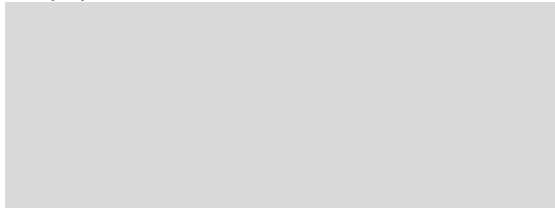


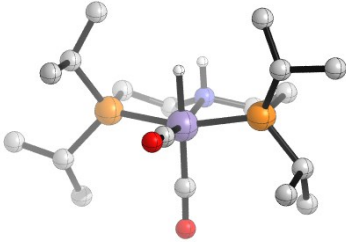
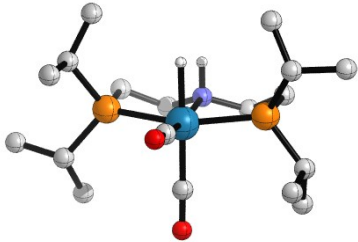
P	-2.25485800	-0.12111000	-0.21873100
P	2.25488100	-0.12097400	-0.21876800
C	-2.44527000	-1.17377100	-1.73006500
C	2.44531600	-1.17313500	-1.73043900
H	-2.54242600	-0.47696200	-2.56712300
H	2.54222400	-0.47603200	-2.56728300
H	-3.34336800	-1.79657300	-1.70615500
H	3.34353400	-1.79577700	-1.70686400
C	-1.18080400	-2.00224000	-1.90135200
C	1.18098300	-2.00179000	-1.90180900
H	-1.03501000	-2.20795700	-2.97335300
H	1.03502200	-2.20713500	-2.97386100
H	-1.30691600	-2.99099700	-1.43257900
H	1.30738200	-2.99069900	-1.43343400
N	0.00006700	-1.33504600	-1.35909300
C	3.36228900	1.34385000	-0.61424100
C	-3.36225200	1.34358400	-0.61471500
H	2.95172200	1.65388900	-1.58265400
H	-2.95158300	1.65337600	-1.58316500
C	3.14882600	-1.11165800	1.10786500
C	-3.14886600	-1.11142600	1.10814200
C	2.41380600	-2.42651600	1.36215300
C	-2.41352700	-2.42597000	1.36314200
H	-4.13338000	-1.34141400	0.68486500
H	4.13351600	-1.34118800	0.68475400
C	-3.34565900	-0.34786100	2.41563800
C	3.34502900	-0.34853900	2.41571200
H	-3.98788900	0.52487000	2.29634400
H	3.98688500	0.52453300	2.29690600
H	-2.39620600	-0.01291700	2.83640700
H	2.39533600	-0.01417900	2.83640600
H	-3.82096600	-1.00335200	3.15196500
H	3.82047600	-1.00411400	3.15187400
C	3.19186200	2.52325600	0.34175500
C	-3.19194800	2.52323400	0.34100300
H	3.66085700	2.33831000	1.30929500
H	-3.66099200	2.33850200	1.30855800
H	2.14179500	2.75644900	0.51601300
H	-2.14190500	2.75652300	0.51526600
H	3.66491000	3.41248800	-0.08498000
H	-3.66501400	3.41233500	-0.08598500
C	4.83247100	0.98188800	-0.81078900
C	-4.83240200	0.98153100	-0.81132600
H	4.96958200	0.17052000	-1.52921400
H	-4.96941500	0.17001600	-1.52960200
H	5.30301600	0.68415600	0.12954100
H	-5.30302700	0.68396400	0.12901600
H	5.38330400	1.84945300	-1.18670300
H	-5.38323400	1.84900000	-1.18746300
H	2.94195400	-3.00479500	2.12628200
H	1.39814300	-2.24365900	1.71972400
H	2.34691500	-3.04638800	0.46711500
H	-2.94190200	-3.00426700	2.12710100

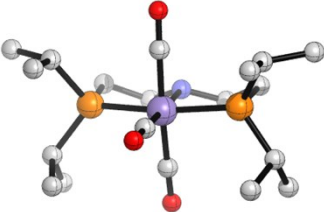
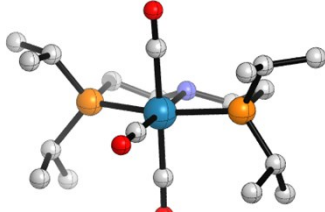


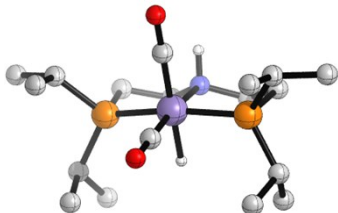
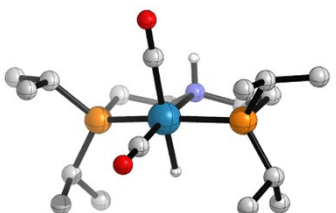
P	-2.37062400	-0.16542300	-0.24294300
P	2.37060500	-0.16550500	-0.24303300
C	-2.45434400	-1.33658200	-1.68304900
C	2.45426800	-1.33674100	-1.68308300
H	-2.51104300	-0.70159500	-2.57172000
H	2.51108100	-0.70180500	-2.57178300
H	-3.35063500	-1.96202700	-1.66219400
H	3.35049900	-1.96226700	-1.66214400
C	-1.18876600	-2.17920900	-1.74879200
C	1.18861900	-2.17926100	-1.74885500
H	-1.04006700	-2.50093700	-2.79028400
H	1.03987700	-2.50091800	-2.79036400
H	-1.31712200	-3.10620800	-1.17044600
H	1.31691400	-3.10631000	-1.17057200
N	-0.00004400	-1.46034300	-1.28876800
C	3.45267800	1.24958800	-0.83940500
C	-3.45260400	1.24977200	-0.83924500
H	2.92927400	1.52285000	-1.76347600
H	-2.92904300	1.52319500	-1.76317900
C	3.33575600	-1.05196100	1.10343900
C	-3.33582300	-1.05184600	1.10351700
C	2.67822300	-2.39163900	1.43084600
C	-2.67883300	-2.39192800	1.43036500
H	-4.32556100	-1.24595300	0.67455600
H	4.32528500	-1.24665500	0.67426100
C	-3.49970000	-0.21462200	2.36964100
C	3.50038700	-0.21444500	2.36927300
H	-4.06724800	0.69924300	2.19645600
H	4.06859200	0.69894000	2.19570600
H	-2.53394600	0.06399900	2.79386000
H	2.53489200	0.06501300	2.79353300
H	-4.03843400	-0.79642300	3.12378300
H	4.03879800	-0.79638800	3.12353800
C	3.43361600	2.47518200	0.07203000
C	-3.43370300	2.47519800	0.07241800
H	4.07988500	2.34232900	0.94130400
H	-4.08022300	2.34221200	0.94148700
H	2.42981200	2.70817300	0.42521600
H	-2.42998000	2.70807100	0.42591600
H	3.80467700	3.34534500	-0.47680000
H	-3.80457100	3.34548600	-0.47634300
C	4.87961700	0.83703600	-1.19252800
C	-4.87949100	0.83730500	-1.19267300
H	4.91444300	-0.00538300	-1.88669300
H	-4.91422800	-0.00500400	-1.88697500
H	5.45037900	0.56585100	-0.30073300
H	-5.45040900	0.56599900	-0.30101300
H	5.40161300	1.67390600	-1.66618200
H	-5.40138900	1.67426300	-1.66628100
H	3.23462600	-2.89014800	2.23009000
H	1.65107100	-2.25005000	1.77573700
H	2.65877900	-3.06700500	0.57420000
H	-3.23506600	-2.89025500	2.22983900
H	-2.66023200	-3.06717700	0.57360900

H -2.34588600 -3.04602200 0.46828300 H -1.39814100 -2.24265900 1.72126200 Mn 0.00001700 0.12226000 -0.15671500 C 0.00000400 0.74337400 1.49886000 C 0.00002300 1.72738100 -0.83660800 O 0.00006000 2.75039600 -1.38792300 O -0.00003800 1.13930900 2.59165900	H -1.65141400 -2.25095100 1.77471900 C 0.00013000 0.62226200 1.78883000 C -0.00006900 1.98670400 -0.44725600 O -0.00014200 3.09449300 -0.81385100 O 0.00022400 0.84080800 2.93485900 Re 0.00000400 0.14138100 -0.04987400
1Mn(C₁)  C -2.46173700 -0.64027700 1.90985400 H -2.65684800 0.24940800 2.51158100 H -3.30929900 -1.31874500 2.03358000 C -1.14937200 -1.27172400 2.34588300 H -1.05401200 -1.17631300 3.43814400 H -1.16511100 -2.35448800 2.14421800 C 1.19290000 -1.00173100 2.46662400 H 1.39741500 -2.08152000 2.39234900 H 1.00503300 -0.81075700 3.53435400 C 2.41524700 -0.21056400 2.02923100 H 3.34930400 -0.71252400 2.29385200 H 2.41333200 0.76678800 2.51560200 C -3.28852000 1.49692000 0.05641900 H -3.12448700 1.84709000 -0.96816600 C -4.78621600 1.30022600 0.27988700 H -4.99142500 0.87546800 1.26684600 H -5.24450800 0.65249100 -0.46886300 H -5.29802600 2.26630500 0.23138500 C -2.73808000 2.56366500 1.00315400 H -3.18604600 3.53350800 0.76981900 H -1.65561400 2.66451100 0.92556900 H -2.98105400 2.33684800 2.04464100 C -3.27017700 -1.31034300 -0.83486900 H -4.26633400 -1.30697100 -0.37897700 C -3.39703400 -0.89245400 -2.29817600 H -2.42291900 -0.85769500 -2.78855900 H -3.86726700 0.08658200 -2.41225300 H -4.01288300 -1.61712100 -2.83929200 C -2.69456300 -2.71871100 -0.70451800 H -3.32844100 -3.42918000 -1.24372700 H -2.64347000 -3.04813800 0.33540800 H -1.69160700 -2.78010200 -1.12890200 C 3.31332400 1.61240900 -0.10597900 H 4.30316500 1.37427100 0.29869400 C 3.44338700 1.87891100 -1.60567100 H 2.47369700 2.10657900 -2.05190000 H 3.87209400 1.03308800 -2.14661400 H 4.09498600 2.74124900 -1.77472900 C 2.78565200 2.84781600 0.62070700 H 3.45175200 3.69491700 0.43121000 H 2.73587600 2.70999000 1.70224800 H 1.79107900 3.12418300 0.26893000 C 3.22747100 -1.28767600 -0.60520800 H 3.02593000 -1.14935500 -1.67259900 C 2.66279300 -2.64931100 -0.19927200	1Re(C₁)  C -2.48274500 -0.65367900 1.96489000 H -2.63199200 0.25430000 2.55318400 H -3.34137500 -1.30685500 2.13948500 C -1.17991800 -1.31839600 2.38911600 H -1.07403800 -1.21466000 3.47916300 H -1.22979600 -2.40122400 2.19794300 C 1.19072500 -1.17925800 2.46146500 H 1.34917000 -2.25912000 2.31966900 H 1.02476800 -1.04280600 3.54043600 C 2.44619600 -0.41387900 2.06369500 H 3.35199900 -0.97185300 2.31388200 H 2.48199900 0.53212800 2.60754200 C -3.47456900 1.40368400 0.09469300 H -3.36953700 1.72386000 -0.94723500 C -4.94796400 1.12779100 0.38622700 H -5.09002300 0.73788800 1.39822300 H -5.39276700 0.41994800 -0.31475300 H -5.51955400 2.05813500 0.31568900 C -2.94636800 2.53106500 0.98019100 H -3.48148700 3.45779400 0.75523400 H -1.88303900 2.71145400 0.82384500 H -3.10367400 2.31652200 2.04068600 C -3.31292700 -1.41506500 -0.76490400 H -4.29573400 -1.48378500 -0.28571200 C -3.49796600 -1.00861400 -2.22501600 H -2.53709500 -0.89658800 -2.72995300 H -4.04651500 -0.07030900 -2.33063100 H -4.06346300 -1.78051900 -2.75539600 C -2.62515800 -2.77307000 -0.64991800 H -3.19108700 -3.52471600 -1.20821500 H -2.55667400 -3.11447000 0.38508500 H -1.61532900 -2.73756800 -1.06290700 C 3.45043800 1.53790700 0.08664500 H 4.42482400 1.26099400 0.50426500 C 3.62119700 1.89885800 -1.38849000 H 2.65884600 2.13621000 -1.84613200 H 4.08029200 1.09510100 -1.96728500 H 4.26184600 2.78024500 -1.48347100 C 2.90525200 2.72680500 0.87436200 H 3.57894100 3.58087300 0.75787000 H 2.82197600 2.52266400 1.94344300 H 1.92216400 3.02597100 0.50849800 C 3.31439600 -1.32276600 -0.63159800 H 3.16325600 -1.07963000 -1.68856900 C 2.67936300 -2.68867100 -0.37378400

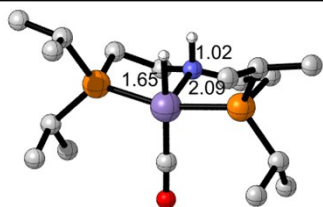
H 3.06620000 -3.43003900 -0.85006900	H 3.10508600 -3.43220300 -1.05331400
H 1.57486800 -2.67726700 -0.27055100	H 1.59934900 -2.66919500 -0.52797600
H 2.94435900 -2.90154000 0.82632400	H 2.87402600 -3.02981200 0.64643400
C 4.73641100 -1.24243100 -0.37858800	C 4.81176700 -1.35400900 -0.33778600
H 4.98710300 -1.30384000 0.68439600	H 5.01171600 -1.53064100 0.72298800
H 5.19965000 -0.34138300 -0.78275900	H 5.31949900 -0.43311700 -0.62792200
H 5.20829700 -2.09911200 -0.86959700	H 5.27956200 -2.17245600 -0.89335300
N 0.00438100 -0.65790700 1.68808600	N -0.00252300 -0.75104000 1.72835300
P -2.26358900 -0.07718600 0.15632100	P -2.36751400 -0.11105300 0.19237500
P 2.25313300 0.09806500 0.21357900	P 2.35920800 0.02494000 0.26346000
Mn -0.00296600 0.07400800 -0.05535700	Re -0.00142300 0.11291500 -0.10416100
C -0.10467900 1.59286400 -0.93996100	C -0.07441100 1.82215200 -0.93285200
C 0.11280100 -0.76504800 -1.58457600	C 0.10271000 -0.57560600 -1.85885000
O 0.22271700 -1.35688100 -2.57946700	O 0.19245800 -1.08460400 -2.90547900
O -0.19673300 2.60182000 -1.50958500	O -0.13211300 2.90288900 -1.36741600
2Mn(Cs)	2Re(Cs)
	
P -2.21525100 0.08123500 -0.29325700	P -2.33720100 0.05190600 -0.34266400
P 2.21527800 0.08091500 -0.29346600	P 2.33716900 0.05229100 -0.34253200
C -2.42373900 -0.94789700 -1.84975100	C -2.44707100 -1.04447100 -1.86879800
C 2.42363300 -0.94854300 -1.84976500	C 2.44708300 -1.04341100 -1.86910300
H -2.43921000 -0.25676000 -2.69880800	H -2.46419300 -0.38256300 -2.74086000
H 2.43949900 -0.25760600 -2.69897400	H 2.46351200 -0.38103700 -2.74083000
H -3.36416000 -1.50091500 -1.87031600	H -3.37014100 -1.62670800 -1.89336300
H 3.36388400 -1.50187500 -1.87001000	H 3.37043000 -1.62517000 -1.89435300
C -1.23286500 -1.88284400 -1.97347600	C -1.23600000 -1.96162600 -1.94698500
C 1.23249100 -1.88315500 -1.97346200	C 1.23641400 -1.96108400 -1.94729100
H -1.22361100 -2.37491100 -2.95691800	H -1.22234400 -2.49734900 -2.90666100
H 1.22310600 -2.37525700 -2.95688500	H 1.22285600 -2.49663200 -2.90706500
H -1.26909100 -2.66214200 -1.20893600	H -1.25732500 -2.70409600 -1.14668400
H 1.26850000 -2.66243000 -1.20888800	H 1.25817200 -2.70370500 -1.14714100
N -0.00009200 -1.11284400 -1.76072900	N 0.00005700 -1.17462300 -1.78096200
C 2.95955100 1.70959000 -0.88627700	C 3.12347100 1.62871400 -1.00790100
C -2.95954400 1.71002200 -0.88572900	C -3.12342200 1.62812300 -1.00870300
H 2.34159200 1.89023000 -1.77378800	H 2.49826200 1.79750900 -1.89247600
H -2.34078000 1.89145600 -1.77250500	H -2.49897900 1.79590100 -1.89401500
C 3.50683000 -0.62882900 0.88102700	C 3.61160000 -0.68322000 0.82880900
C -3.50642800 -0.62844800 0.88171700	C -3.61192700 -0.68332000 0.82849600
C 3.45724800 -2.15383900 0.95621500	C 3.45327200 -2.19474400 0.97790600
C -3.45853200 -2.15359700 0.95521400	C -3.45225800 -2.19450800 0.97948400
H -4.48185400 -0.33732600 0.47825800	H -4.59048400 -0.48280100 0.37942600
H 4.48212600 -0.33928700 0.47610300	H 4.59038300 -0.48122400 0.38089100
C -3.34713500 -0.02891500 2.27833700	C -3.53730400 -0.00214800 2.19381500
C 3.34985800 -0.02755800 2.27713200	C 3.53508300 -0.00379600 2.19490400
H -3.42364500 1.05895900 2.28230300	H -3.72492800 1.07077500 2.13948600
H 3.42857200 1.06016600 2.27987600	H 3.72071200 1.06953800 2.14199500
H -2.37757000 -0.29302400 2.70483800	H -2.55187400 -0.14404400 2.64197800
H 2.38012900 -0.28930900 2.70473500	H 2.54969500 -0.14804500 2.64239100
H -4.12412800 -0.41903800 2.94293800	H -4.28252900 -0.43580000 2.86745500
H 4.12663400 -0.41851200 2.94149800	H 4.28078200 -0.43692300 2.86836100
C 2.71655300 2.87532700 0.06656600	C 2.92334900 2.82973200 -0.08929700
C -2.71796900 2.87518900 0.06818100	C -2.92189600 2.82987700 -0.09137700
H 3.30896400 2.78824500 0.98000700	H 3.53594700 2.76279800 0.81233200
H -3.31163700 2.78734100 0.98073800	H -3.53314000 2.76379100 0.81122400
	H 1.87972100 2.92534100 0.20971500

H 1.66585300 2.94725800 0.34482500	H -1.87781400 2.92554500 0.20601300
H -1.66766700 2.94721900 0.34793100	H 3.21523700 3.74617400 -0.61139500
H 3.00561000 3.81382000 -0.41686100	H -3.21441600 3.74590800 -0.61384700
H -3.00659400 3.81395500 -0.41497100	C 4.57801100 1.48853400 -1.44827100
C 4.42292400 1.63506500 -1.31464700	C -4.57840300 1.48813000 -1.44767000
C -4.42249600 1.63531300 -1.31553800	H 4.74117400 0.63159000 -2.10673700
H 4.62432700 0.80177800 -1.99231400	H -4.74246300 0.63062600 -2.10519500
H -4.62302400 0.80245900 -1.99398000	H 5.25018800 1.38855500 -0.59241600
H 5.09035400 1.53828600 -0.45469300	H -5.24986300 1.38920100 -0.59113100
H -5.09069600 1.53772300 -0.45627600	H 4.88870000 2.38428900 -1.99474900
H 4.70529500 2.55569800 -1.83481800	H -4.88921800 2.38349400 -1.99471700
H -4.70468300 2.55623100 -1.83530600	H -0.00003800 1.39384700 -1.06119700
H 0.00007400 1.27651100 -0.86338400	H -0.00017800 -0.44184500 -2.48648500
H 0.00000000 -0.33275200 -2.41241700	H 4.21635200 -2.57347700 1.66462500
H 4.23353500 -2.50872100 1.64117400	H 2.47969200 -2.45532900 1.39472200
H 2.49882600 -2.50618700 1.33932500	H 3.57973900 -2.72789900 0.03309500
H 3.63958700 -2.63100200 -0.00900400	H -4.21581100 -2.57324500 1.66567000
H -4.23396800 -2.50827200 1.64123900	H -3.57702400 -2.72883600 0.03510200
H -3.64320900 -2.62951600 -0.01017000	H -2.47891300 -2.45366900 1.39771100
H -2.49983500 -2.50746800 1.33625800	Re -0.00002900 0.07698100 0.11440700
Mn 0.00001600 -0.01612700 0.08687800	C -0.00019200 1.31710400 1.55171200
C 0.00018000 1.09435300 1.44576400	C 0.00031300 -1.40961900 1.33995000
C -0.00029600 -1.43593000 1.14443800	O -0.00025800 2.09454000 2.41798800
O 0.00029600 1.84362900 2.33250500	O 0.00046400 -2.29307800 2.10390900
O -0.00065200 -2.32937800 1.89330800	
2Mn(C₁)	2Re(C₁)
	
H 0.00015600 1.46456400 0.20005700	H 0.00839000 1.68493300 0.33558300
P 2.22585300 0.15712700 0.12507400	P 2.34337700 0.16747500 0.20827500
P -2.22128100 0.10402500 0.14038600	P -2.35005200 0.10838000 0.19484000
C 2.45445600 -0.24606200 1.94373800	C 2.45240500 -0.18236100 2.05162400
C -2.41455500 -0.19983100 1.97856600	C -2.45735900 -0.21993200 2.04060000
H 2.52349700 0.69120700 2.50150300	H 2.47994500 0.77597500 2.57645300
H -2.42886400 0.76886100 2.48553400	H -2.49293700 0.74727200 2.55028200
H 3.37980900 -0.79490300 2.12847800	H 3.37273000 -0.71133200 2.30827400
H -3.35011000 -0.70686600 2.22304400	H -3.37086500 -0.75629900 2.30625800
C 1.24709600 -1.04145500 2.41472400	C 1.23810300 -0.98212500 2.50379900
C -1.21397200 -1.00734300 2.44849300	C -1.23192700 -0.99832000 2.50113000
H 1.24319600 -1.12866200 3.51107500	H 1.22034600 -1.06189800 3.59998900
H -1.19323400 -1.07016400 3.54625700	H -1.21733900 -1.07375300 3.59764200
H 1.26347100 -2.05099600 1.99846900	H 1.26478900 -1.99325000 2.09324200
H -1.25507200 -2.02570500 2.05579600	H -1.24068200 -2.01114600 2.09368100
N 0.01851700 -0.39080800 1.93676200	N -0.00067400 -0.34667200 2.01663600
H 0.03490500 0.57770800 2.24493000	H -0.00721800 0.61567000 2.34617800
C -3.07064100 1.77066300 -0.15403700	C -3.30638500 1.72283700 -0.03979200
C 3.04751200 1.84495700 -0.03779200	C 3.25273300 1.80255000 0.01235700
H -2.80834000 1.98579800 -1.19565800	H -3.18303100 1.91257800 -1.11161700
H 4.07296200 1.71389600 0.32193100	H 4.26319100 1.63518400 0.39832300
C -3.46416400 -1.09160800 -0.61468200	C -3.53810100 -1.15120500 -0.53848500
C 3.49971200 -0.96414200 -0.71810100	C 3.57172700 -1.06227700 -0.53793900
C -3.28590900 -2.53118100 -0.13870300	C -3.24970600 -2.57968100 -0.08618800
C 4.96152800 -0.56161300 -0.52778500	C 5.04640000 -0.73435400 -0.31059300
H 3.24546800 -0.87991400 -1.78018200	H 3.35522100 -1.00753900 -1.60976200

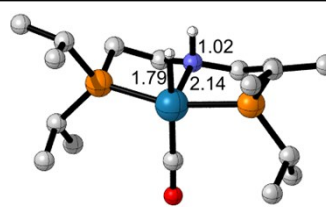
H -4.44781700 -0.75399100 -0.27496000	H -4.52978200 -0.88001300 -0.16448900
C 3.31332900 -2.42502700 -0.30942400	C 3.28064600 -2.48878700 -0.07496900
C -3.41018300 -1.00566600 -2.13859900	C -3.53287300 -1.04039000 -2.06135200
H 2.29110500 -2.77221700 -0.43945000	H 2.23929900 -2.77023500 -0.21548400
H -3.59065900 0.00718500 -2.50642700	H -3.81092300 -0.04207900 -2.40730200
H 3.60699000 -2.58732400 0.73200300	H 3.54385100 -2.62670600 0.97812300
H -2.43536400 -1.32497800 -2.51226200	H -2.54350600 -1.26810200 -2.46294300
H 3.95732400 -3.06158200 -0.92329100	H 3.89037100 -3.19177600 -0.64973500
H -4.16928400 -1.65816000 -2.58058900	H -4.24540900 -1.74979500 -2.49260600
C -4.59292000 1.77640600 -0.02088200	C -4.79936300 1.64905500 0.27886000
C 2.38622300 2.92907900 0.80576900	C 2.62413500 2.94855000 0.79682700
H -4.91420200 1.44361000 0.97092600	H -4.97867600 1.33153600 1.31055700
H 1.34742300 3.07286500 0.50524400	H 1.58975900 3.10602300 0.48831000
H -5.08856200 1.15230400 -0.76517100	H -5.34517500 0.97608100 -0.38320400
H 2.40099900 2.70394600 1.87491500	H 2.63391100 2.77862800 1.87622000
H -4.96779100 2.79582300 -0.15457000	H -5.24596700 2.64158700 0.16663900
H 2.92031300 3.87450900 0.66866400	H 3.18851700 3.86748400 0.61078300
C -2.46578800 2.87773500 0.70630200	C -2.66027400 2.88680100 0.70631000
C 3.08345100 2.27020200 -1.50555600	C 3.33331900 2.15781500 -1.47243100
H -1.37600600 2.83944500 0.69265200	H -1.58482500 2.92066600 0.53263100
H 3.56421700 1.53093500 -2.14958500	H 3.80469900 1.37501800 -2.07049800
H -2.80723200 2.80974500 1.74380700	H -2.83627800 2.81945600 1.78471800
H 2.07389700 2.43274800 -1.88655200	H 2.33643100 2.33165600 -1.88166700
H -2.78176100 3.85470000 0.32959400	H -3.10108100 3.82945600 0.36946300
H 3.63660200 3.20843300 -1.61059100	H 3.91800700 3.07267300 -1.60665700
H -4.06534200 -3.15741600 -0.58416900	H -3.98742900 -3.25488100 -0.53070700
H 5.60916600 -1.29768900 -1.01410600	H 5.66631000 -1.52584000 -0.74264800
H -2.32348400 -2.94502300 -0.43687900	H -2.26381800 -2.91691300 -0.40352700
H 5.24100700 -0.54038600 0.53033100	H 5.29114000 -0.68313000 0.75506200
H -3.38253100 -2.62562200 0.94549800	H -3.32455400 -2.69510300 0.99780300
H 5.19802900 0.41159500 -0.95827000	H 5.35213900 0.20455600 -0.77261200
Mn 0.00151800 -0.07064600 -0.18895300	C -0.02308000 0.68008000 -2.00750000
C -0.04168000 0.55206200 -1.82792900	C 0.01828100 -1.78922200 -0.86517100
C 0.00570000 -1.75400100 -0.73216600	O -0.04554800 1.11702200 -3.08571900
O -0.09092800 1.00939900 -2.89381300	O 0.03877600 -2.86493700 -1.32001200
O 0.00390300 -2.82599700 -1.19181300	Re -0.00083500 0.02868500 -0.22494100
1Mn-3CO	1Re-3CO
	
P 0.05098900 0.21716900 2.27789600	P 0.00942400 0.30746200 2.38762700
P 0.05098900 0.21716900 -2.27789600	P 0.00942400 0.30746200 -2.38762700
C -0.51344800 1.97840700 2.41744200	C -0.50538700 2.09001000 2.43159400
C -0.51344800 1.97840700 -2.41744200	C -0.50538700 2.09001000 -2.43159400
H 0.39543400 2.58677200 2.39560400	H 0.42085700 2.67124400 2.39975700
H 0.39543400 2.58677200 -2.39560400	H 0.42085700 2.67124400 -2.39975700
H -1.03918800 2.18358700 3.35169600	H -1.03758900 2.34633000 3.35005600
H -1.03918800 2.18358700 -3.35169600	H -1.03758900 2.34633000 -3.35005600
C -1.34868400 2.29798100 1.18665900	C -1.31931100 2.39511900 1.18178000
C -1.34868400 2.29798100 -1.18665900	C -1.31931100 2.39511900 -1.18178000
H -1.54409100 3.38444100 1.17037400	H -1.49392300 3.48446100 1.14465700
H -1.54409100 3.38444100 -1.17037400	H -1.49392300 3.48446100 -1.14465700
H -2.34777300 1.82241500 1.28778100	H -2.32741300 1.93802900 1.28365400
H -2.34777300 1.82241500 -1.28778100	H -2.32741300 1.93802900 -1.28365400
N -0.63569300 1.90717400 0.00000000	N -0.61760500 1.96480900 0.00000000
C 1.68667500 0.24585800 -3.20905600	

C 1.68667500 0.24585800 3.20905600 H 2.28898800 0.92086400 -2.59298900 H 2.28898800 0.92086400 2.59298900 C -1.05564000 -0.82397800 -3.39716700 C -1.05564000 -0.82397800 3.39716700 C -2.49666300 -0.32477700 -3.48926800 C -2.49666300 -0.32477700 3.48926800 H -0.60683100 -0.72641500 4.39093400 H -0.60683100 -0.72641500 -4.39093400 C -1.02085500 -2.29970800 3.00065500 C -1.02085500 -2.29970800 -3.00065500 H -0.00745200 -2.69397800 2.92183900 H -0.00745200 -2.69397800 -2.92183900 H -1.51201400 -2.46203100 2.04017400 H -1.51201400 -2.46203100 -2.04017400 H -1.55360100 -2.89435200 3.74902100 H -1.55360100 -2.89435200 -3.74902100 C 2.38544900 -1.11088300 -3.23880000 C 2.38544900 -1.11088300 3.23880000 H 1.86507100 -1.81565600 -3.89209400 H 1.86507100 -1.81565600 3.89209400 H 2.46064200 -1.55892900 -2.24732300 H 2.46064200 -1.55892900 2.24732300 H 3.39991700 -0.99660800 -3.63172600 H 3.39991700 -0.99660800 3.63172600 C 1.59841900 0.85050900 -4.60933700 C 1.59841900 0.85050900 4.60933700 H 1.13577600 1.83887700 -4.61047300 H 1.13577600 1.83887700 4.61047300 H 1.03845000 0.21252100 -5.29776500 H 1.03845000 0.21252100 5.29776500 H 2.60512600 0.95906600 -5.02414900 H 2.60512600 0.95906600 5.02414900 H -3.05163700 -0.96019400 -4.18638200 H -3.00859700 -0.37285400 -2.52778700 H -2.56321000 0.69933900 -3.85841000 H -3.05163700 -0.96019400 4.18638200 H -2.56321000 0.69933900 3.85841000 H -3.00859700 -0.37285400 2.52778700 Mn 0.09834300 -0.07267100 0.00000000 C 0.73743200 -1.72435500 0.00000000 C -1.63800300 -0.57331000 0.00000000 O 1.13954200 -2.80966700 0.00000000 O -2.75851700 -0.83616800 0.00000000 C 1.71968900 0.74223100 0.00000000 O 2.72070400 1.30451500 0.00000000	C 1.64819000 0.34471400 -3.30748000 C 1.64819000 0.34471400 3.30748000 H 2.23474900 1.01535900 -2.67034300 H 2.23474900 1.01535900 2.67034300 C -1.15027300 -0.63085700 -3.53238700 C -1.15027300 -0.63085700 3.53238700 C -2.59949400 -0.15597300 -3.44786800 C -2.59949400 -0.15597300 3.44786800 H -0.78329000 -0.40898300 4.53995100 H -0.78329000 -0.40898300 -4.53995100 C -1.06171400 -2.13910200 3.30269600 C -1.06171400 -2.13910200 -3.30269600 H -0.04210800 -2.51870000 3.36852500 H -0.04210800 -2.51870000 -3.36852500 H -1.44897600 -2.41061700 2.31964300 H -1.44897600 -2.41061700 -2.31964300 H -1.66224600 -2.66138200 4.05352700 H -1.66224600 -2.66138200 -4.05352700 C 2.35983400 -1.00487100 -3.34608100 C 2.35983400 -1.00487100 3.34608100 H 1.88436400 -1.68734400 -4.05431900 H 1.88436400 -1.68734400 4.05431900 H 2.37913700 -1.48815300 -2.36838000 H 2.37913700 -1.48815300 2.36838000 H 3.39406500 -0.86862100 -3.67483300 H 3.39406500 -0.86862100 3.67483300 C 1.56944000 0.97035600 -4.69853800 C 1.56944000 0.97035600 4.69853800 H 1.08791800 1.94991900 -4.69151700 H 1.08791800 1.94991900 4.69151700 H 1.03122400 0.33102700 -5.40274500 H 1.03122400 0.33102700 5.40274500 H 2.57927600 1.10390100 -5.09776800 H 2.57927600 1.10390100 5.09776800 H -3.20448100 -0.72039300 -4.16393000 H -3.02627900 -0.32523400 -2.45878700 H -2.70959100 0.90218400 -3.68822900 H -3.20448100 -0.72039300 4.16393000 H -2.70959100 0.90218400 3.68822900 H -3.02627900 -0.32523400 2.45878700 Re 0.08205200 -0.12145800 0.00000000 C 0.71607500 -1.94034300 0.00000000 C -1.76371600 -0.82433800 0.00000000 O 1.07487700 -3.04438600 0.00000000 O -2.80934800 -1.30644200 0.00000000 C 1.95740200 0.50903200 0.00000000 O 3.05713100 0.84169600 0.00000000
2Mn'  P -2.21741400 -0.12950300 -0.13165900 P 2.21740100 -0.12939900 -0.13162500 C -2.45991900 -1.26225500 -1.59896400 C 2.46002800 -1.26180400 -1.59916900 H -2.60049700 -0.62323200 -2.47690300	2Re'  P -2.34271100 -0.19398600 -0.12894400 P 2.34271700 -0.19398100 -0.12894400 C -2.47786000 -1.38878400 -1.56759600 C 2.47786700 -1.38880400 -1.56757700 H -2.59066400 -0.78189400 -2.47216900

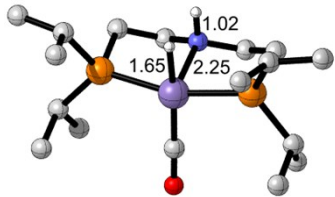
H	2.60044200	-0.62256000	-2.47697200	H	2.59068900	-0.78193000	-2.47215800
H	-3.34638200	-1.89510500	-1.51441400	H	-3.35787700	-2.03284100	-1.50176400
H	3.34660100	-1.89452800	-1.51480000	H	3.35787300	-2.03287400	-1.50172600
C	-1.21161500	-2.10757500	-1.75796400	C	-1.21833700	-2.23259600	-1.65816000
C	1.21186000	-2.10731800	-1.75825500	C	1.21833600	-2.23260300	-1.65814700
H	-1.24923900	-2.69280400	-2.68794000	H	-1.24227900	-2.86698800	-2.55492300
H	1.24951200	-2.69233800	-2.68835900	H	1.24228300	-2.86699900	-2.55490900
H	-1.12721900	-2.80960100	-0.92710700	H	-1.13927600	-2.88429400	-0.78708700
H	1.12767000	-2.80955800	-0.92755800	H	1.13926100	-2.88429800	-0.78707400
N	0.00003400	-1.26860300	-1.72182800	N	0.00000200	-1.39329700	-1.66276600
C	3.36210200	1.28844200	-0.61542800	C	3.47357900	1.18755100	-0.72259500
C	-3.36213300	1.28818800	-0.61585700	C	-3.47358700	1.18754900	-0.72255900
H	2.91320400	1.59320200	-1.56850700	H	2.96964700	1.47560200	-1.65287600
H	-2.91322900	1.59270800	-1.56901200	H	-2.96961300	1.47568800	-1.65279100
C	3.11412100	-1.00439300	1.27507800	C	3.27377800	-1.02645300	1.27786000
C	-3.11420300	-1.00421700	1.27519900	C	-3.27375600	-1.02648900	1.27785300
C	2.76918400	-2.48914600	1.35257600	C	2.91865700	-2.50430900	1.41598100
C	-2.76892000	-2.48885900	1.35329300	C	-2.91858300	-2.50433100	1.41598300
H	-4.18344800	-0.90942200	1.05850800	H	-4.33761300	-0.94384300	1.03144400
H	4.18338700	-0.90928100	1.05865000	H	4.33763500	-0.94376900	1.03146500
C	-2.81132200	-0.33448900	2.61416000	C	-2.99940900	-0.30186100	2.59456800
C	2.81076300	-0.33519200	2.61420400	C	2.99938500	-0.30184200	2.59457400
H	-3.04704500	0.72986600	2.62284500	H	-3.25301200	0.75785600	2.55858700
H	3.04611200	0.72924200	2.62329800	H	3.25295700	0.75788300	2.55860600
H	-1.75326800	-0.43991100	2.85965000	H	-1.94173700	-0.37960500	2.85289800
H	1.75268000	-0.44104200	2.85941000	H	1.94171000	-0.37961900	2.85288400
H	-3.39393900	-0.81183500	3.40826500	H	-3.58461000	-0.75879000	3.39858600
H	3.39337100	-0.81260500	3.40827200	H	3.58458300	-0.75875800	3.39860300
C	3.26678500	2.48494400	0.32812400	C	3.45003800	2.40360000	0.19970500
C	-3.26681500	2.48491500	0.32740600	C	-3.45014100	2.40352600	0.19984000
H	3.76398100	2.28838900	1.28077400	H	4.01586400	2.22362800	1.11678100
H	-3.76410900	2.28860900	1.28005800	H	-4.01601300	2.22345800	1.11686900
H	2.23170400	2.75833000	0.53368800	H	2.43139400	2.68107900	0.47306100
H	-2.23173200	2.75828300	0.53300000	H	-2.43152400	2.68102100	0.47327600
H	3.76051700	3.35198400	-0.12084000	H	3.91103500	3.25914900	-0.30244300
H	-3.76044900	3.35188200	-0.12180300	H	-3.91114100	3.25909900	-0.30226500
C	4.81636500	0.90043800	-0.87169700	C	4.90233300	0.76387800	-1.05318200
C	-4.81640300	0.90012100	-0.87200700	C	-4.90230600	0.76385200	-1.05326100
H	4.91411800	0.05687400	-1.55890200	H	4.94402300	-0.09084900	-1.73221100
H	-4.91417300	0.05645800	-1.55908400	H	-4.94392600	-0.09081800	-1.73236600
H	5.33498900	0.64246000	0.05513300	H	5.46632200	0.50770200	-0.15275300
H	-5.33499000	0.64227200	0.05488000	H	-5.46633700	0.50758000	-0.15288600
H	5.35446300	1.74520400	-1.31305700	H	5.43195200	1.59061900	-1.53646900
H	-5.35453300	1.74481400	-1.31346900	H	-5.43192800	1.59061500	-1.53650800
H	-0.00012800	-0.68430600	-2.55348200	H	0.00000800	-0.84958000	-2.52211100
H	3.27399200	-2.93858600	2.21319900	H	3.44250300	-2.92782200	2.27815700
H	1.69315700	-2.62546800	1.48611100	H	1.84539800	-2.62340400	1.58344100
H	3.08534900	-3.04410900	0.46656600	H	3.20664500	-3.09274500	0.54184300
H	-3.27385000	-2.93813000	2.21393200	H	-3.44244200	-2.92786400	2.27814200
H	-3.08471300	-3.04421200	0.46739600	H	-3.20651500	-3.09278000	0.54183600
H	-1.69289500	-2.62488300	1.48714400	H	-1.84532500	-2.62338600	1.58348200
Mn	-0.00000400	0.18816500	-0.10813100	Re	0.00000400	0.18334600	-0.00144700
C	-0.00002500	1.18205100	1.33600100	C	-0.00000800	1.34720500	1.49523000
O	-0.00000900	1.83106200	2.29922500	O	0.00000500	2.05165100	2.42267900
H	-0.00006200	-1.10106100	0.84168700	H	0.00000500	-1.24419700	1.03050800
C	0.00006200	1.58387700	-1.19666600	C	0.00001300	1.66405700	-1.23523400
O	0.00016100	2.51734400	-1.89361800	O	-0.00005500	2.54981500	-1.99474100
2Mn-CO_{dis}-singlet				2Re-CO_{dis}-singlet			

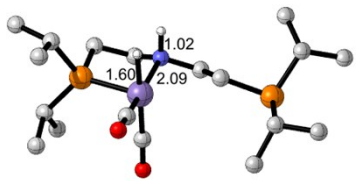
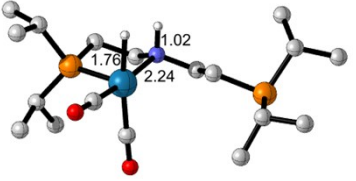


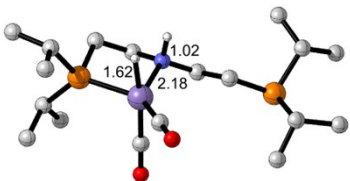
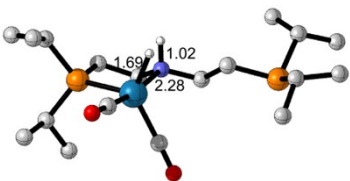
P	2.22993300	0.21769300	0.11609200
P	-2.22995600	0.21768800	0.11611600
C	2.42491100	-0.32846700	1.90195200
C	-2.42491600	-0.32849000	1.90197400
H	2.43175000	0.57484700	2.52070400
H	-2.43175800	0.57481700	2.52073600
H	3.36650300	-0.85021600	2.08328900
H	-3.36650100	-0.85024800	2.08331100
C	1.23487300	-1.19902300	2.27892700
C	-1.23486800	-1.19903800	2.27893400
H	1.22318900	-1.39302400	3.36160800
H	-1.22317200	-1.39304400	3.36161400
H	1.27821800	-2.16154300	1.76433800
H	-1.27820900	-2.16155600	1.76433900
N	-0.00000300	-0.52755000	1.85235400
C	-2.98885000	1.94315200	0.18769300
C	2.98883200	1.94315300	0.18762700
H	-2.41609900	2.36977100	1.01917300
H	2.41596000	2.36986600	1.01897400
C	-3.52115700	-0.81859800	-0.78929400
C	3.52114200	-0.81858000	-0.78931100
C	-3.41715200	-2.30414400	-0.44893700
C	3.41725800	-2.30411000	-0.44884500
H	4.50164600	-0.46003100	-0.45887700
H	-4.50166800	-0.46013400	-0.45879000
C	3.40057600	-0.61334500	-2.29894400
C	-3.40067500	-0.61327900	-2.29892300
H	3.55656700	0.42550000	-2.59401900
H	-3.55678100	0.42556300	-2.59394100
H	2.41294600	-0.91930800	-2.65257400
H	-2.41303000	-0.91912800	-2.65261000
H	4.14521100	-1.22006100	-2.82359100
H	-4.14527200	-1.22004200	-2.82356800
C	-2.64192900	2.76772200	-1.04863500
C	2.64213100	2.76759100	-1.04885000
H	-3.19487200	2.43841700	-1.93147800
H	3.19520700	2.43816700	-1.93156800
H	-1.57295000	2.70406700	-1.26235200
H	1.57318500	2.70393900	-1.26272800
H	-2.89183100	3.82051200	-0.88411700
H	2.89203500	3.82039300	-0.88441300
C	-4.47484500	2.01242700	0.52305900
C	4.47477700	2.01243000	0.52321400
H	-4.73168600	1.42264000	1.40688500
H	4.73146800	1.42273400	1.40714500
H	-5.09409700	1.66127600	-0.30639600
H	5.09414500	1.66116900	-0.30610800
H	-4.76768400	3.04799000	0.72399900
H	4.76761000	3.04800800	0.72408300
H	-0.00000700	1.59206700	0.39851000
H	-0.00000700	0.41052600	2.24701400
H	-4.18722800	-2.85850700	-0.99477800
H	-2.44917300	-2.71514700	-0.73806300
H	-3.57244500	-2.50275600	0.61367400

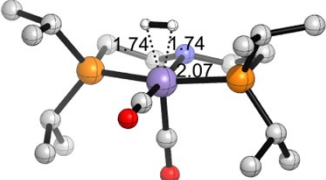
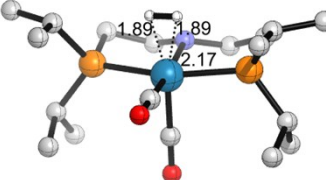


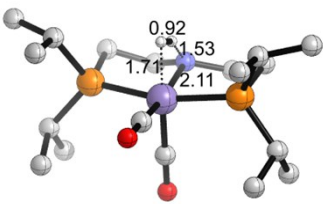
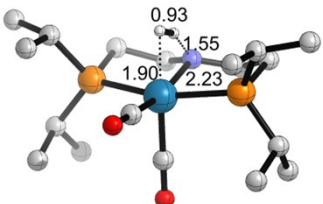
P	2.32855000	0.21885000	0.14355500
P	-2.32855000	0.21885200	0.14355800
C	2.45538100	-0.17851800	1.98047700
C	-2.45537900	-0.17852000	1.98048000
H	2.48122900	0.77271600	2.52233700
H	-2.48122600	0.77271400	2.52234000
H	3.36853000	-0.71972900	2.23534300
H	-3.36852700	-0.71973100	2.23534600
C	1.23049900	-0.97652900	2.39480500
C	-1.23049600	-0.97653000	2.39480500
H	1.17668400	-1.07227700	3.48768200
H	-1.17668100	-1.07228000	3.48768200
H	1.24878700	-1.97724000	1.95995500
H	-1.24878400	-1.97724100	1.95995300
N	0.00000100	-0.31703900	1.89486500
C	-3.16323900	1.91072800	0.10817500
C	3.16323800	1.91072600	0.10816600
H	-2.56914200	2.43381200	0.86660900
H	2.56913100	2.43381900	0.86658500
C	-3.57985100	-0.94964700	-0.64505000
C	3.57985200	-0.94964800	-0.64505000
C	-3.40846400	-2.38995700	-0.16654100
C	3.40847300	-2.38995700	-0.16653300
H	4.57090500	-0.59941900	-0.33764100
H	-4.57090500	-0.59942400	-0.33763600
C	3.47531500	-0.88269200	-2.16789800
C	-3.47531900	-0.88268400	-2.16789800
H	3.66970500	0.11763900	-2.55788900
H	-3.66971600	0.11764800	-2.55788400
H	2.47796000	-1.18446100	-2.49628200
H	-2.47796200	-1.18444400	-2.49628600
H	4.20055300	-1.56275700	-2.62534700
H	-4.20055200	-1.56275100	-2.62534900
C	-2.92870400	2.63922300	-1.21154000
C	2.92872300	2.63920500	-1.21156100
H	-3.51137600	2.20671300	-2.02831400
H	3.51140500	2.20668200	-2.02832200
H	-1.87159800	2.61138600	-1.48404300
H	1.87162100	2.61136800	-1.48407800
H	-3.22677700	3.68843900	-1.12106300
H	3.22679800	3.68842100	-1.12109300
C	-4.63094200	1.93708900	0.52213600
C	4.63093500	1.93709200	0.52214900
H	-4.81044700	1.41098100	1.46328700
H	4.81042700	1.41099400	1.46330800
H	-5.27379500	1.48969500	-0.24028900
H	5.27380000	1.48969000	-0.24026200
H	-4.96627300	2.97050000	0.65606700
H	4.96626400	2.97050500	0.65607400
H	0.00000400	1.83289100	0.24326500
H	0.00000000	0.63553500	2.25937400
H	-4.15115500	-3.02780000	-0.65603000
H	-2.42187000	-2.77995400	-0.42001200
H	-3.55696900	-2.49489100	0.91044400

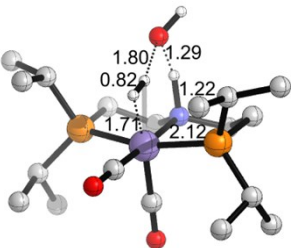
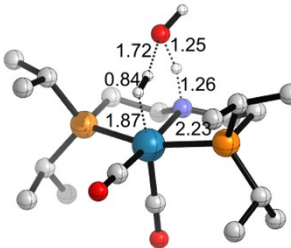
H 4.18735400 -2.85845300 -0.99468000	H 4.15117000 -3.02779700 -0.65601600
H 3.57261100 -2.50263500 0.61377400	H 3.55697600 -2.49488300 0.91045300
H 2.44930000 -2.71520700 -0.73790300	H 2.42188300 -2.77996100 -0.42000400
Mn -0.00001500 0.04384800 -0.15791300	Re 0.00000000 0.10434300 -0.20286900
C -0.00002300 -1.55879100 -0.88004800	C 0.00000200 -1.69684700 -0.81759700
O -0.00002700 -2.60862200 -1.40399200	O -0.00002300 -2.79278700 -1.24962200
2Mn-CO_{dis}-triplet	
	
P 2.30219600 0.21546100 0.11640100	P 2.36664600 0.19719100 0.18675200
P -2.30218700 0.21546900 0.11639300	P -2.36662800 0.19719500 0.18677800
C 2.42521000 -0.25473200 1.93145300	C 2.44941200 -0.07270800 2.04278000
C -2.42521800 -0.25474000 1.93143800	C -2.44937400 -0.07269400 2.04280900
H 2.43195000 0.68223600 2.49772800	H 2.48433000 0.91896100 2.50494900
H -2.43196600 0.68222500 2.49772000	H -2.48427000 0.91898000 2.50497400
H 3.36872100 -0.76238000 2.14478400	H 3.36722900 -0.59190600 2.32798000
H -3.36872900 -0.76239400 2.14475800	H -3.36719300 -0.59187700 2.32802700
C 1.24452600 -1.11027200 2.38467700	C 1.23240400 -0.83356700 2.55142100
C -1.24453400 -1.11027900 2.38466500	C -1.23236600 -0.83356200 2.55143600
H 1.31179300 -1.28538200 3.47051100	H 1.25407700 -0.88061100 3.65084700
H -1.31180900 -1.28539400 3.47049800	H -1.25402800 -0.88060500 3.65086300
H 1.26091800 -2.08364200 1.88850700	H 1.22874000 -1.85632000 2.16905600
H -1.26092000 -2.08364700 1.88849100	H -1.22871000 -1.85631400 2.16907100
N -0.00000400 -0.44774300 2.01381800	N 0.00001700 -0.19332800 2.08023000
C -3.07525000 1.93143900 0.12421000	C -3.19400700 1.87779300 0.01820300
C 3.07525900 1.93143500 0.12421300	C 3.19403900 1.87778400 0.01816900
H -2.51158300 2.39611200 0.94124100	H -2.63026300 2.44815200 0.76524700
H 2.51161500 2.39609800 0.94126500	H 2.63031000 2.44814700 0.76521900
C -3.58048700 -0.90161400 -0.69534600	C -3.59109100 -1.05575800 -0.49134900
C 3.58049400 -0.90164400 -0.69532400	C 3.59108100 -1.05578400 -0.49138700
C -3.34993700 -2.36995000 -0.34335700	C -3.27154900 -2.46597700 -0.00029600
C 3.34989000 -2.36998400 -0.34338700	C 3.27156200 -2.46597800 -0.00024700
H 4.55611600 -0.60017700 -0.29837300	H 4.57419700 -0.76586400 -0.10397800
H -4.55611300 -0.60010300 -0.29843500	H -4.57418300 -0.76585300 -0.10386900
C 3.57672800 -0.70875100 -2.21096300	C 3.61796700 -1.01008700 -2.01795300
C -3.57665800 -0.70875300 -2.21098900	C -3.61807600 -1.00998400 -2.01791200
H 3.84158000 0.30879300 -2.50263200	H 3.95969000 -0.04672300 -2.39920700
H -3.84146500 0.30879500 -2.50269000	H -3.95979600 -0.04659100 -2.39909400
H 2.59281800 -0.93572700 -2.62794000	H 2.62463600 -1.20358500 -2.42878800
H -2.59273900 -0.93577100 -2.62792600	H -2.62477800 -1.20349000 -2.42881900
H 4.30166400 -1.38357700 -2.67633600	H 4.29775800 -1.77695300 -2.40132000
H -4.30159900 -1.38356400 -2.67637400	H -4.29791500 -1.77681200 -2.40127500
C -2.73127100 2.71015700 -1.14287600	C -2.91199300 2.52683200 -1.33427500
C 2.73123700 2.71018000 -1.14284600	C 2.91201900 2.52683400 -1.33430200
H -3.26889300 2.33411100 -2.01614700	H -3.45691300 2.04007100 -2.14586700
H 3.26883700 2.33415700 -2.01613900	H 3.45692100 2.04006900 -2.14590300
H -1.65983500 2.65446200 -1.34469000	H -1.84504400 2.48809600 -1.56255100
H 1.65979600 2.65448200 -1.34463300	H 1.84506600 2.48811200 -1.56256400
H -3.00302500 3.76331900 -1.02166300	H -3.22414200 3.57566800 -1.31379300
H 3.00298600 3.76334100 -1.02161900	H 3.22418400 3.57566500 -1.31382000
C -4.56407900 1.98781300 0.44985600	C -4.67629300 1.90778900 0.37697700
C 4.56409500 1.98781900 0.44982500	C 4.67632800 1.90776600 0.37693300
H -4.81351200 1.44234500 1.36374200	H -4.88296600 1.45799600 1.35170900
H 4.81355700 1.44233100 1.36369100	H 4.88300600 1.45796400 1.35166000
H -5.17107900 1.57930600 -0.36205000	H -5.28219400 1.38795200 -0.36932000

H 5.17108000 1.57934400 -0.36210700	H 5.28222000 1.38793200 -0.36937200
H -4.87725000 3.02684900 0.59256700	H -5.02977600 2.94285200 0.41273600
H 4.87725700 3.02685600 0.59255600	H 5.02981900 2.94282700 0.41269900
H 0.00002900 1.63514900 0.34417800	H 0.00003700 1.84043800 0.22032700
H -0.00000700 0.50227800 2.37334800	H 0.00002200 0.78163600 2.36926100
H -4.10954700 -2.98597500 -0.83452400	H -3.99291200 -3.17127100 -0.42386500
H -2.37273700 -2.71337300 -0.68577400	H -2.27549500 -2.77931100 -0.31670500
H -3.42653900 -2.55987300 0.72950800	H -3.33491500 -2.55487700 1.08671000
H 4.10949200 -2.98601900 -0.83455400	H 3.99289300 -3.17129500 -0.42383100
H 3.42646000 -2.55994400 0.72947300	H 3.33499600 -2.55482600 1.08675900
H 2.37268800 -2.71336600 -0.68584100	H 2.27548400 -2.77931800 -0.31657800
Mn 0.00000600 0.06652700 -0.18124800	Re 0.00000700 0.12258300 -0.23924000
C 0.00001500 -1.46088100 -1.07414500	C -0.00004600 -1.57429800 -1.09654500
O -0.00004600 -2.44108300 -1.72727200	O -0.00014400 -2.58622000 -1.69823900
2Mn-P_{dis}-singlet	
	
N -0.07521200 -1.56065800 0.36046000	N -0.17700200 1.58123500 0.34931400
H -0.04223300 -2.07248300 -0.51589300	H -0.22200500 2.11286600 -0.51589600
P -2.74120600 -0.41530900 -0.08839300	P 2.66266200 0.59168500 0.03353700
P 3.80703000 -0.10707300 0.49919300	P -4.10157400 0.19608700 0.53744400
C 3.97778900 1.57039400 -0.36045100	C -4.31182300 -1.51319100 -0.24732000
C -3.67888800 -0.82898100 -1.66847100	C 3.67623700 1.07729200 -1.47671800
C 4.80974100 -1.25822700 -0.62253500	C -5.07956900 1.32629700 -0.62524700
C -4.04237200 0.29384700 1.07221700	C 3.90482200 -0.04605700 1.28888000
O -0.62768400 1.81222600 2.28275700	O 0.44582200 -1.81921900 2.39014700
C -2.41762400 -2.15253800 0.56239100	C 2.15303300 2.29873800 0.65258100
C 2.04632200 -0.48143900 -0.06033700	C -2.33395600 0.50183100 -0.04487500
H -2.41503800 -2.81878800 -0.30621800	H 2.15440000 2.96085800 -0.21895800
H 1.53422500 0.50077800 -0.06107000	H -1.84832200 -0.49033900 -0.03412500
H -3.20476300 -2.50423600 1.23136300	H 2.87100300 2.70816700 1.36575900
H 2.04177100 -0.85533400 -1.08707000	H -2.32610600 0.86002400 -1.07750800
C -1.05676100 -2.19841500 1.24372300	C 0.76033500 2.25661800 1.26620200
C 1.29302400 -1.41942300 0.87422000	C -1.54802500 1.42786800 0.87123800
H -0.77358400 -3.23390400 1.47941300	H 0.41239900 3.27257900 1.49733700
H 1.79530100 -2.39002500 0.97100200	H -2.03854400 2.40268600 0.97967100
H -1.07169800 -1.63231400 2.17734700	H 0.76634400 1.68300600 2.19492100
H 1.23303200 -0.97483200 1.86995400	H -1.47470700 0.98185400 1.86554100
H -2.93503400 -1.45433900 -2.17535600	H 2.92234200 1.63697200 -2.04223600
H -4.97998700 -0.21501800 0.82535900	H 4.81904200 0.53074800 1.11189300
H 4.79644200 -0.84067200 -1.63644300	H -5.07032400 0.87764300 -1.62579000
C -4.21320500 1.79309500 0.82532500	C 4.19559500 -1.52750500 1.05180500
C 6.25193400 -1.32553800 -0.11564700	C -6.52210100 1.43763100 -0.12708100
H -4.46841900 2.02359300 -0.20951800	H 4.55311800 -1.73204100 0.04238700
H 6.72474300 -0.34589200 -0.04657800	H -7.01575800 0.47050800 -0.03302800
H -3.29688800 2.33394300 1.06823800	H 3.29810100 -2.12712300 1.21145500
H 6.28525900 -1.77585000 0.88027700	H -6.55043800 1.91680100 0.85544200
H -5.01296600 2.18578600 1.46049900	H 4.96175900 -1.86957500 1.75379700
H 6.86136800 -1.94318100 -0.78298800	H -7.11541000 2.04861500 -0.81467500
C 5.42815500 1.97786000 -0.60050000	C -5.77021200 -1.89905300 -0.47300000
C -3.93333900 0.37976800 -2.56344800	C 4.09864800 -0.10763000 -2.33865600
H 5.93923900 1.31451000 -1.29993700	H -6.26404500 -1.25804900 -1.20486700
H -4.68925800 1.04634900 -2.14198900	H 4.88115700 -0.70092800 -1.86019400
H 5.99802300 1.99848500 0.33321700	H -6.34280500 -1.86302400 0.45850600
H -3.02366500 0.95378800 -2.73469300	H 3.25668100 -0.76102000 -2.56382800
H 5.46141200 2.98588500 -1.02463700	H -5.82497700 -2.92489400 -0.84942200
2Re-P_{dis}-singlet	
	

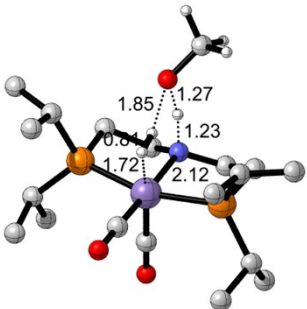
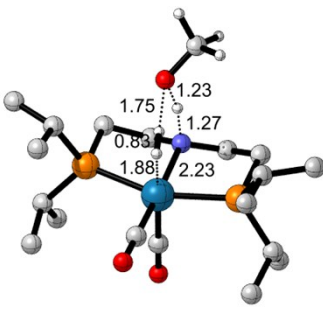
H -4.30754600 0.04446300 -3.53555800	H 4.50538400 0.25704700 -3.28666200
C -4.95391100 -1.64390300 -1.46301600	C 4.85810800 1.99663400 -1.17355400
H -4.80326800 -2.51638200 -0.82298600	H 4.58553900 2.85389000 -0.55368600
H -5.75347500 -1.04003400 -1.02659800	H 5.66739100 1.46074300 -0.67131600
H -5.32009200 -2.00633500 -2.42844300	H 5.26816300 2.38842300 -2.10918900
C -3.73204800 0.02998000 2.54465600	C 3.46036900 0.18752000 2.73118200
H -3.68691700 -1.03473300 2.78248200	H 3.32524600 1.24529000 2.96643000
H -2.79142900 0.49202400 2.84712700	H 2.53199500 -0.33970400 2.95417700
H -4.52159300 0.46463400 3.16511300	H 4.22527100 -0.19791700 3.41175000
C 4.22754700 -2.66948000 -0.66833600	C -4.46887000 2.72385700 -0.70970300
H 4.16839700 -3.10504900 0.33392400	H -4.40419500 3.18652800 0.28007200
H 3.23271400 -2.70381300 -1.11562900	H -3.47234500 2.72597300 -1.15466300
H 4.87361900 -3.31975700 -1.26587600	H -5.09982500 3.36956900 -1.32784400
C -0.62651800 1.17445000 1.31128700	C 0.54133500 -1.25294500 1.37589700
Mn -0.66576700 0.33961600 -0.26343800	Re 0.63650000 -0.38997900 -0.34724300
C 3.26619700 2.63082500 0.48020400	C -3.62527500 -2.54937900 0.64327100
H 2.21671300 2.39601800 0.66764300	H -2.57420400 -2.32355000 0.83476700
H 3.75700400 2.74997300 1.44985600	H -4.12793300 -2.62081400 1.61148800
H 3.29317000 3.59711400 -0.03193600	H -3.66206400 -3.53553900 0.17130100
H 3.47546900 1.48818100 -1.33188300	H -3.80654000 -1.48595700 -1.22036700
C -0.99571700 1.81831000 -1.16201100	C 1.29496400 -1.96749700 -1.16820800
O -1.19655400 2.76601100 -1.79528800	O 1.69278100 -2.92538400 -1.69258800
H -0.71479500 -0.29201400 -1.73617300	H 0.50990900 0.37350500 -1.92978500
2Mn-P_{dis}-triplet	
	
N -0.02867100 -1.24137900 -0.06005300	N -0.26297500 1.28116700 0.20787500
H 0.06106700 -1.55891300 -1.02247600	H -0.33009100 1.68148300 -0.72604400
P -3.03495300 -0.45918200 -0.08715300	P 2.72838500 0.82671000 -0.01026900
P 3.98813600 -0.26197100 0.52132900	P -4.30328500 0.21505900 0.43018100
C 4.47473800 1.42574200 -0.18295500	C -4.75553300 -1.32604500 -0.57058900
C -4.16871600 -0.59931400 -1.57833700	C 3.71103200 1.33109200 -1.53841800
C 4.96312900 -1.46993900 -0.56468700	C -5.23410700 1.59072200 -0.48265000
C -4.16987600 -0.34268600 1.40737800	C 3.98295200 0.53626400 1.35747800
O -0.80367100 2.11469600 2.13279400	O -0.22564000 -2.44646800 2.09010500
C -2.32423000 -2.18509200 0.03392000	C 1.91699300 2.45256200 0.45737100
C 2.27366200 -0.34552900 -0.24711700	C -2.55598600 0.41707400 -0.23546300
H -2.27612600 -2.58084300 -0.98473400	H 1.83822700 3.05442200 -0.45359000
H 1.87540100 0.67276000 -0.26556300	H -2.14722300 -0.58363300 -0.39686200
H -2.97315200 -2.85024600 0.60969000	H 2.52711700 3.02132000 1.16338900
H 2.33885400 -0.67755000 -1.28874800	H -2.57395800 0.90493500 -1.21590900
C -0.93010700 -2.16354800 0.64916900	C 0.53350700 2.20951000 1.04290600
C 1.31586200 -1.21515500 0.54703800	C -1.64830100 1.16052100 0.72650600
H -0.51090100 -3.17997700 0.65689700	H 0.00086400 3.16369900 1.15463900
H 1.70349800 -2.23874100 0.63829100	H -2.04144500 2.16405700 0.93257300
H -0.97708600 -1.82541600 1.68631500	H 0.60800600 1.75661700 2.03359600
H 1.21218100 -0.81695300 1.55904300	H -1.59527800 0.62850100 1.67879100
H -3.50572400 -1.10887000 -2.28615700	H 2.94868400 1.88388000 -2.10041300
H -4.95281700 -1.09605200 1.26769700	H 4.64682100 1.40778900 1.34418800
H 5.11711500 -0.99886400 -1.54317700	H -5.35269700 1.28259300 -1.52857900
C -4.81504500 1.04029100 1.47813300	C 4.79953200 -0.72711700 1.09978300
C 6.31916800 -1.75729200 0.08297300	C -6.61294900 1.78014100 0.15279500
H -5.44587800 1.25000500 0.61307700	H 5.39262100 -0.66349500 0.18666700
H 6.90147900 -0.85468700 0.26792900	H -7.20038800 0.86225500 0.17324800
H -4.05544100 1.82350900 1.53837500	H 4.14992900 -1.60127500 1.02001600
H 6.18285200 -2.26083400 1.04408000	H -6.51211600 2.12610600 1.18526400
2Re-P_{dis}-triplet	
	

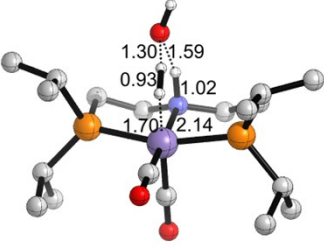
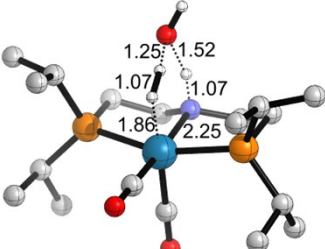
H	-5.44465700	1.11439700	2.36975200	H	5.49130500	-0.89421000	1.93045000
H	6.91673600	-2.41400400	-0.55746600	H	-7.18781000	2.53170900	-0.39791600
C	5.98251700	1.65088500	-0.23301300	C	-6.26042200	-1.53384700	-0.70974800
C	-4.48670600	0.76857200	-2.17824300	C	4.12442100	0.14058200	-2.39845900
H	6.48406400	0.97122900	-0.92378300	H	-6.74061400	-0.74390400	-1.28949600
H	-5.15179800	1.35466200	-1.54050700	H	4.88699100	-0.47366200	-1.91658200
H	6.43732600	1.53363700	0.75516100	H	-6.74842500	-1.58739000	0.26803100
H	-3.57225400	1.34188900	-2.33869600	H	3.27101500	-0.49963000	-2.62390900
H	6.19270000	2.67069300	-0.56957700	H	-6.45634200	-2.47969700	-1.22394500
H	-4.98610200	0.64433100	-3.14377100	H	4.54221300	0.49945900	-3.34375500
C	-5.42013400	-1.44620200	-1.37227700	C	4.87728900	2.27263800	-1.24949900
H	-5.19437000	-2.43446500	-0.96341200	H	4.58118000	3.13775800	-0.65072900
H	-6.13423800	-0.95925600	-0.70355900	H	5.68758100	1.76002900	-0.72590400
H	-5.92845400	-1.59649500	-2.32953800	H	5.28963900	2.65117700	-2.18952400
C	-3.42680000	-0.65536200	2.70395600	C	3.29119300	0.46346800	2.71590400
H	-3.04535800	-1.67825200	2.73053600	H	2.77700900	1.39147800	2.97566000
H	-2.59163600	0.02995000	2.86221500	H	2.56194700	-0.35040000	2.73708500
H	-4.10836600	-0.54419300	3.55250500	H	4.03334400	0.27365000	3.49652900
C	4.21685200	-2.78662200	-0.76987600	C	-4.48053200	2.91861600	-0.45002500
H	3.99300500	-3.26612600	0.18815100	H	-4.29218500	3.24031400	0.57906600
H	3.28038000	-2.66260100	-1.31642100	H	-3.52477000	2.87610200	-0.97542400
H	4.83734800	-3.48247000	-1.34290700	H	-5.07916500	3.70001800	-0.92825100
C	-0.86809000	1.49726900	1.15237400	C	0.16259100	-1.75359200	1.24204700
Mn	-1.00594700	0.66260200	-0.45404100	Re	0.86864300	-0.65826200	-0.19847500
C	3.80810900	2.51615400	0.65627500	C	-4.11492700	-2.54773000	0.08843000
H	2.72440000	2.40108100	0.72184900	H	-3.03276000	-2.45587600	0.19712500
H	4.20287300	2.51435500	1.67589600	H	-4.53438300	-2.71569500	1.08401200
H	4.00368600	3.50088800	0.22151800	H	-4.30545500	-3.44268400	-0.51150800
H	4.08277000	1.47354500	-1.20613900	H	-4.32844800	-1.19659900	-1.57245900
C	-0.54269400	2.27864700	-1.17597800	C	1.82964400	-2.16504500	-0.81569100
O	-0.26246600	3.30382000	-1.61825500	O	2.40965300	-3.08495200	-1.22624700
H	-1.32249000	0.11771400	-1.94229600	H	0.19468300	-0.60376700	-1.74458900
1Mn+H₂(ads)				1Re+H₂(ads)			
							
P	-0.03488700	-0.32590200	2.27234200	P	0.06182400	-0.34628300	2.38003300
P	-0.03488700	-0.32590200	-2.27234200	P	0.06182400	-0.34628300	-2.38003300
C	1.15451000	-1.74077000	2.41874100	C	1.29878600	-1.73130400	2.43951900
C	1.15451000	-1.74077000	-2.41874100	C	1.29878600	-1.73130400	-2.43951900
H	0.54644100	-2.65010500	2.40793200	H	0.71739300	-2.65812900	2.44311300
H	0.54644100	-2.65010500	-2.40793200	H	0.71739300	-2.65812900	-2.44311300
H	1.72555600	-1.72361200	3.34918000	H	1.90241400	-1.70736300	3.34975600
H	1.72555600	-1.72361200	-3.34918000	H	1.90241400	-1.70736300	-3.34975600
C	2.03395500	-1.72160000	1.17840500	C	2.15039100	-1.68411500	1.17883100
C	2.03395500	-1.72160000	-1.17840500	C	2.15039100	-1.68411500	-1.17883100
H	2.60871500	-2.66412000	1.14502400	H	2.74375200	-2.61412900	1.13354400
H	2.60871500	-2.66412000	-1.14502400	H	2.74375200	-2.61412900	-1.13354400
H	2.79520200	-0.91915100	1.28115400	H	2.89308000	-0.86463500	1.27078700
H	2.79520200	-0.91915100	-1.28115400	H	2.89308000	-0.86463500	-1.27078700
N	1.21366600	-1.59440500	0.00000000	N	1.32597800	-1.56067000	0.00000000
C	-1.55500800	-1.01256800	-3.15465700	C	-1.39250900	-1.10658700	-3.30709500
C	-1.55500800	-1.01256800	3.15465700	C	-1.39250900	-1.10658700	3.30709500
H	-1.79810600	-1.87667600	-2.52349700	H	-1.57180200	-2.00304100	-2.69968000
H	-1.79810600	-1.87667600	2.52349700	H	-1.57180200	-2.00304100	2.69968000
C	0.57176000	1.03541500	-3.42439500	C	0.71745100	0.99644800	-3.51695100
C	0.57176000	1.03541500	3.42439500	C	0.71745100	0.99644800	3.51695100

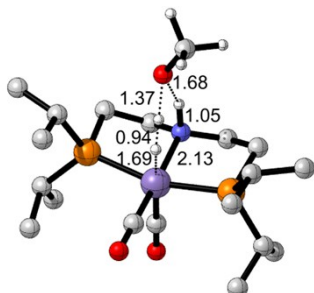
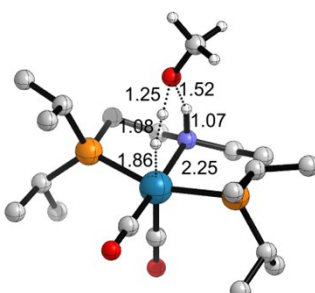
C	2.09376300	1.16734100	-3.46196500	C	2.21037600	1.25374900	-3.31983700
C	2.09376300	1.16734100	3.46196500	C	2.21037600	1.25374900	3.31983700
H	0.23806200	0.72857200	4.42109300	H	0.57348000	0.60273500	4.52872100
H	0.23806200	0.72857200	-4.42109300	H	0.57348000	0.60273500	-4.52872100
C	-0.07575700	2.37907200	3.08994100	C	-0.07963200	2.29219100	3.37424200
C	-0.07575700	2.37907200	-3.08994100	C	-0.07963200	2.29219100	-3.37424200
H	-1.16397700	2.32755700	3.04808400	H	-1.14748300	2.15246400	3.54294000
H	-1.16397700	2.32755700	-3.04808400	H	-1.14748300	2.15246400	-3.54294000
H	0.27272700	2.75418100	2.12673500	H	0.04368800	2.72169800	2.37922800
H	0.27272700	2.75418100	-2.12673500	H	0.04368800	2.72169800	-2.37922800
H	0.19483500	3.11730600	3.85105100	H	0.27926700	3.02611800	4.10203800
H	0.19483500	3.11730600	-3.85105100	H	0.27926700	3.02611800	-4.10203800
C	-2.75296100	-0.06706600	-3.13743700	C	-2.66375300	-0.26300300	-3.27553500
C	-2.75296100	-0.06706600	3.13743700	C	-2.66375300	-0.26300300	3.27553500
H	-2.59925100	0.78295100	-3.80638200	H	-2.59088100	0.59682300	-3.94480600
H	-2.59925100	0.78295100	3.80638200	H	-2.59088100	0.59682300	3.94480600
H	-2.95953900	0.32205300	-2.13979300	H	-2.88720500	0.10742300	-2.27460600
H	-2.95953900	0.32205300	2.13979300	H	-2.88720500	0.10742300	2.27460600
H	-3.64705600	-0.59234700	-3.48641900	H	-3.51441600	-0.86177300	-3.61449200
H	-3.64705600	-0.59234700	3.48641900	H	-3.51441600	-0.86177300	3.61449200
C	-1.28353900	-1.52957100	-4.56597100	C	-1.06232300	-1.56030900	-4.72722500
C	-1.28353900	-1.52957100	4.56597100	C	-1.06232300	-1.56030900	4.72722500
H	-0.44616700	-2.22849500	-4.60190100	H	-0.16230100	-2.17657000	-4.77230900
H	-0.44616700	-2.22849500	4.60190100	H	-0.16230100	-2.17657000	4.77230900
H	-1.07556200	-0.71431500	-5.26339400	H	-0.92688800	-0.70985900	-5.39987100
H	-1.07556200	-0.71431500	5.26339400	H	-0.92688800	-0.70985900	5.39987100
H	-2.16699400	-2.05350500	-4.94350900	H	-1.88905600	-2.15474900	-5.12763200
H	-2.16699400	-2.05350500	4.94350900	H	-1.88905600	-2.15474900	5.12763200
H	-1.30722800	-1.28201100	-0.40180400	H	-1.33372900	-1.45501700	-0.40995000
H	-1.30722800	-1.28201100	0.40180400	H	-1.33372900	-1.45501700	0.40995000
H	2.36799800	1.95071300	-4.17529900	H	2.53917600	2.02044100	-4.02793100
H	2.50100900	1.45310000	-2.49171100	H	2.42825600	1.62124600	-2.31675200
H	2.58696200	0.24827300	-3.78086100	H	2.81547700	0.36337100	-3.49597600
H	2.36799800	1.95071300	4.17529900	H	2.53917600	2.02044100	4.02793100
H	2.58696200	0.24827300	3.78086100	H	2.81547700	0.36337100	3.49597600
H	2.50100900	1.45310000	2.49171100	H	2.42825600	1.62124600	2.31675200
C	1.13960100	1.13873300	0.00000000	C	0.93038200	1.52668300	0.00000000
C	-1.40741600	1.21533400	0.00000000	C	-1.70255500	1.17665700	0.00000000
O	2.00986900	1.90111600	0.00000000	O	1.57893100	2.49026000	0.00000000
O	-2.18623400	2.07477900	0.00000000	O	-2.60919900	1.90650100	0.00000000
Mn	-0.16076700	-0.04309700	0.00000000	Re	-0.18975000	-0.00613200	0.00000000
1Mn + H₂-TS(1M/2M)				1Re + H₂-TS(1M/2M)			
							
P	-2.26649700	0.04398700	-0.30252600	P	-2.37233200	-0.04338600	-0.33673400
P	2.26649900	0.04398300	-0.30252600	P	2.37233700	-0.04339700	-0.33672900
C	-2.42398800	-1.04117000	-1.80776500	C	-2.44418700	-1.24820700	-1.76190900
C	2.42399000	-1.04118100	-1.80776000	C	2.44419700	-1.24824200	-1.76188500
H	-2.42461200	-0.37195000	-2.67326900	H	-2.45896400	-0.64367800	-2.67394500
H	2.42462100	-0.37196400	-2.67326700	H	2.45900100	-0.64373100	-2.67393200
H	-3.35518700	-1.61027800	-1.82619200	H	-3.35792000	-1.84627800	-1.74843500
H	3.35518600	-1.61029300	-1.82618100	H	3.35791900	-1.84632900	-1.74838300
C	-1.19758100	-1.93801000	-1.87004000	C	-1.20008200	-2.12672900	-1.76103400
C	1.19757900	-1.93801500	-1.87003600	C	1.20007800	-2.12674700	-1.76101600
H	-1.18195000	-2.45209800	-2.84638600	H	-1.17445800	-2.69563400	-2.70555800

H 1.18194800 -2.45210500 -2.84638100	H 1.17445500 -2.69565700 -2.70553700
H -1.28552700 -2.73411300 -1.10607600	H -1.28030200 -2.87571200 -0.95203200
H 1.28552000 -2.73411800 -1.10607000	H 1.28027900 -2.87572500 -0.95200900
N 0.00000100 -1.15620500 -1.69510200	N 0.00000300 -1.33395700 -1.62112100
C 3.07752800 1.62659900 -0.92874200	C 3.25133800 1.43965600 -1.09652500
C -3.07752900 1.62660700 -0.92873100	C -3.25133700 1.43968200 -1.09649400
H 2.41327300 1.87937100 -1.76379200	H 2.61711300 1.61920700 -1.97316800
H -2.41326500 1.87939800 -1.76376600	H -2.61708500 1.61929500 -1.97310600
C 3.47056400 -0.63869900 0.96977000	C 3.54713700 -0.72479900 0.95798500
C -3.47055800 -0.63869800 0.96977300	C -3.54713500 -0.72480000 0.95797400
C 3.45504300 -2.16470700 1.04522800	C 3.32128300 -2.21425100 1.21071000
C -3.45506000 -2.16470700 1.04520900	C -3.32133200 -2.21426900 1.21064400
H -4.46302300 -0.32681600 0.62765700	H -4.54944200 -0.59782100 0.53484200
H 4.46303000 -0.32683700 0.62763600	H 4.54944300 -0.59787200 0.53483300
C -3.21389800 -0.03344300 2.34995600	C -3.45415300 0.06383100 2.26310900
C 3.21393200 -0.03342000 2.34994900	C 3.45420100 0.06388000 2.26309300
H -3.22256800 1.05673900 2.34357100	H -3.66397000 1.12529200 2.13024100
H 3.22262500 1.05676100 2.34354800	H 3.66406800 1.12532500 2.13019000
H -2.24754000 -0.35323000 2.74274000	H -2.45998300 -0.02559200 2.70356800
H 2.24757200 -0.35318200 2.74274700	H 2.46002800 -0.02548200 2.70356100
H -3.98525200 -0.36905200 3.04980000	H -4.17695600 -0.33035100 2.98369800
H 3.98528700 -0.36903700 3.04978800	H 4.17698800 -0.33031200 2.98369200
C 3.03530500 2.78630200 0.06230700	C 3.20967500 2.69951300 -0.23672100
C -3.03533000 2.78629200 0.06234000	C -3.20973400 2.69949200 -0.23661700
H 3.72646900 2.62936200 0.89371000	H 3.88760400 2.62847500 0.61651000
H -3.72650500 2.62933000 0.89373000	H -3.88768200 2.62838400 0.61659200
H 2.03911100 2.94362700 0.47430800	H 2.20906200 2.90607000 0.14175100
H -2.03914400 2.94362000 0.47435900	H -2.20913600 2.90605900 0.14189200
H 3.34183100 3.70992200 -0.43806900	H 3.53130100 3.56045600 -0.83049300
H -3.34185700 3.70991900 -0.43802300	H -3.53137100 3.56046000 -0.83034800
C 4.48908500 1.43457200 -1.48041700	C 4.66994100 1.14632800 -1.57989700
C -4.48907700 1.43457900 -1.48042600	C -4.66991600 1.14634800 -1.57992900
H 4.55055100 0.62757700 -2.21280600	H 4.72530700 0.25803400 -2.21229900
H -4.55052500 0.62760000 -2.21283700	H -4.72523400 0.25811100 -2.21241400
H 5.20846100 1.22539800 -0.68459800	H 5.35924700 1.01050300 -0.74279300
H -5.20846000 1.22537700 -0.68462200	H -5.35924100 1.01042000 -0.74285600
H 4.82023300 2.35293900 -1.97498100	H 5.04338700 1.99106600 -2.16662600
H -4.82022900 2.35295400 -1.97497200	H -5.04337700 1.99112800 -2.16658900
H 0.00000200 1.21150700 -1.27042900	H 0.00000800 1.09212600 -1.59651400
H 0.00000200 0.37761400 -1.66043000	H 0.00000600 0.20204600 -1.85332300
H 4.18919000 -2.49659600 1.78572400	H 4.04096200 -2.56722500 1.95540100
H 2.48156300 -2.54330900 1.35927300	H 2.32246100 -2.40747100 1.60392700
H 3.71463200 -2.63530100 0.09574300	H 3.45878400 -2.81760500 0.31188800
H -4.18919300 -2.49659400 1.78571900	H -4.04101100 -2.56724200 1.95533400
H -3.71468200 -2.63528400 0.09572400	H -3.45886900 -2.81758600 0.31180300
H -2.48157800 -2.54333100 1.35922400	H -2.32251000 -2.40754000 1.60383800
Mn 0.00000000 0.08128600 0.01590000	Re 0.00000300 0.14346800 0.04412200
C 0.00000100 1.34223200 1.25368500	C 0.00000500 1.70385700 1.14467200
C -0.00000400 -1.20028900 1.22843200	C -0.00000500 -0.91595600 1.61902200
O 0.00000100 2.15450200 2.08078400	O 0.00000700 2.66571700 1.79900100
O -0.00000900 -2.04710600 2.01993400	O -0.00001500 -1.55943800 2.58929300
1Mn + H₂-TS(H₂O-H⁺)	1Re + H₂-TS(H₂O-H⁺)
	

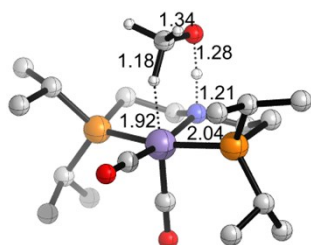
O	-0.06202200	2.95442100	-0.49040900	O	-0.05502600	2.99066800	-0.84601100
P	2.26566800	-0.11918400	-0.09686100	P	2.36937000	-0.17616500	-0.13028700
P	-2.27276500	-0.18046200	-0.09245900	P	-2.37384200	-0.23219600	-0.12063800
C	2.44181500	-0.47619300	-1.91444900	C	2.46288700	-0.88123800	-1.85447700
C	-2.40891500	-0.68342800	-1.87920500	C	-2.42937200	-1.05865600	-1.79347300
H	2.47442900	-1.56441300	-2.00416000	H	2.49835400	-1.96639700	-1.73249800
H	-2.35723100	-1.77537000	-1.89177200	H	-2.39559600	-2.13468300	-1.60080000
H	3.35505000	-0.05921700	-2.34153300	H	3.36216800	-0.56205500	-2.38402500
H	-3.35487000	-0.38793100	-2.33630600	H	-3.35597200	-0.84919400	-2.33156000
C	1.19448300	0.02887400	-2.62097000	C	1.20075000	-0.52009300	-2.62481700
C	-1.21077100	-0.11926000	-2.62451600	C	-1.20738100	-0.65671700	-2.60696300
H	1.18016400	-0.35686100	-3.65179000	H	1.18477500	-1.08892100	-3.56692000
H	-1.17302100	-0.55087800	-3.63683100	H	-1.16878900	-1.26862000	-3.52151900
H	1.19917400	1.12477700	-2.69162000	H	1.20016300	0.54446300	-2.89418300
H	-1.31483800	0.96691600	-2.75051700	H	-1.29504400	0.38882500	-2.93158000
N	0.01263200	-0.43523600	-1.89596500	N	0.01500900	-0.84553700	-1.82867900
C	-3.02118300	-1.68369100	0.75834600	C	-3.18928400	-1.54378200	0.95395400
C	3.00561900	-1.67787600	0.64674100	C	3.17565900	-1.54985400	0.86456500
H	-2.33303200	-2.46864600	0.42261400	H	-2.50520000	-2.38656000	0.79756700
H	2.35595200	-2.43284700	0.18589900	H	2.52348200	-2.38988900	0.59591900
C	-3.52252400	1.20116500	0.15890600	C	-3.59647400	1.19032800	-0.19842000
C	3.48426300	1.26200500	0.27623200	C	3.56073400	1.27352800	-0.09009200
C	-3.54834300	2.20034400	-0.99689600	C	-3.49506700	1.97867200	-1.50305000
C	3.46377400	2.37582600	-0.76956900	C	3.44753700	2.16045300	-1.32854300
O	-0.01872200	0.80146500	2.99463900	O	-0.01598900	1.22936400	3.04982700
H	4.47035800	0.78646400	0.24517800	H	4.55946000	0.82390500	-0.08071900
H	-4.49837600	0.70591700	0.20003800	H	-4.58722500	0.72534000	-0.15551100
C	3.26133600	1.84117100	1.67238400	C	3.37748400	2.10228800	1.18010900
C	-3.28232300	1.92507600	1.48350600	C	-3.43073300	2.11975500	1.00305100
H	3.27259700	1.08109000	2.45393600	H	3.47166900	1.50876200	2.08975700
H	-3.25358200	1.24856100	2.33799600	H	-3.51624300	1.59871500	1.95676000
H	2.30316100	2.36070300	1.73110300	H	2.39453600	2.57643200	1.19577600
H	-2.33803400	2.47182200	1.46417000	H	-2.45667500	2.61098100	0.98221500
H	4.04710900	2.56707100	1.90248000	H	4.13289000	2.89292400	1.21781200
H	-4.08271700	2.65010000	1.65913800	H	-4.20036700	2.89690100	0.97681500
C	-2.95787700	-1.62442200	2.28216100	C	-3.17824700	-1.20534400	2.44227500
C	2.85884400	-1.77580100	2.16247000	C	3.09368800	-1.34407000	2.37446700
H	-3.67112900	-0.90257200	2.68699400	H	-3.91307600	-0.43402900	2.68385800
H	3.53297100	-1.09115700	2.68304700	H	3.79129100	-0.57650600	2.71805600
H	-1.96489500	-1.35882800	2.64594600	H	-2.20013500	-0.85848900	2.77755600
H	1.84164900	-1.56498900	2.49473600	H	2.09147600	-1.05759500	2.69582500
H	-3.21666600	-2.60137700	2.70083400	H	-3.44038000	-2.09288700	3.02551000
H	3.11218300	-2.78818800	2.49083800	H	3.35906500	-2.27313100	2.88750700
C	-4.42728500	-2.04210100	0.28252700	C	-4.58300100	-1.96321000	0.49204800
C	4.44524900	-1.95099900	0.21711700	C	4.59982400	-1.88385800	0.42715700
H	-4.49959500	-2.10906300	-0.80462900	H	-4.61348500	-2.23435100	-0.56512300
H	4.57677200	-1.89817200	-0.86539900	H	4.68066900	-2.04833600	-0.64916600
H	-5.16897800	-1.31741900	0.62802500	H	-5.31895200	-1.17317900	0.66117500
H	5.14955200	-1.25517300	0.68131900	H	5.30616400	-1.09759500	0.70662900
H	-4.71784800	-3.01488400	0.69059300	H	-4.91463800	-2.83541200	1.06336700
H	4.73633800	-2.95801000	0.53087400	H	4.93042000	-2.80177300	0.92231500
H	-0.02742200	-1.45753800	0.84480300	H	-0.03734700	-1.50183300	1.13512300
H	0.12780700	-1.64027700	-1.75926400	H	0.13563900	-2.03934200	-1.45725900
H	-4.30998200	2.96059700	-0.79925300	H	-4.24161100	2.77841600	-1.49979700
H	-2.59406200	2.71775700	-1.10510800	H	-2.51659300	2.44820800	-1.61368700
H	-3.79623900	1.73386700	-1.95159300	H	-3.68380300	1.36225900	-2.38358100
H	4.22391800	3.12152600	-0.51757000	H	4.18355000	2.96737600	-1.26298900
H	3.68510200	2.01455400	-1.77496500	H	3.64269400	1.61769300	-2.25478000
H	2.50144000	2.88861900	-0.79509800	H	2.46291500	2.62380500	-1.40276200
H	0.04887500	-1.75643300	0.08858700	H	0.07577000	-1.92844200	0.42449900

O 0.40181600 -2.81844900 -1.32289400 C -0.03832800 1.82168200 -0.25069700 C -0.01430100 0.51021800 1.87465400 Mn -0.01263200 0.10737100 0.14994700 H -0.09804200 -3.52806600 -1.73199400	O 0.40848400 -3.07239800 -0.81486800 C -0.03476900 1.88859000 -0.47447500 C -0.01341900 0.80446400 1.96890200 Re -0.01061300 0.11283700 0.18495900 H -0.13270300 -3.83302600 -1.03777000
1Mn + H₂-TS(CH₃OH-H⁺) 	1Re + H₂-TS(CH₃OH-H⁺) 
O 0.01664000 -2.74153700 -1.46739300 P -2.27852400 0.02293100 -0.03539000 P 2.26574100 0.02355300 -0.00566300 C -2.44207700 0.98618600 -1.61857600 C 2.41856600 1.11068800 -1.50796300 H -2.47372000 2.03845200 -1.32730000 H 2.39450800 2.14232000 -1.14717100 H -3.35295900 0.74586500 -2.16884400 H 3.35945200 0.96851700 -2.04251800 C -1.19109500 0.75118000 -2.44930700 C 1.21292600 0.85978100 -2.39797000 H -1.17000300 1.46828400 -3.28399800 H 1.18877400 1.61027900 -3.20270100 H -1.19987000 -0.25294200 -2.89458300 H 1.29894100 -0.12050900 -2.88692700 N -0.01025300 0.92897500 -1.60490800 C 3.03578100 1.12336800 1.31388100 C -3.01138500 1.23553900 1.19889100 H 2.36695100 1.99087400 1.27235100 H -2.35456800 2.09778900 1.02707200 C 3.49177200 -1.38029300 -0.24900000 C -3.51063900 -1.39026600 -0.16338700 C 3.50895800 -1.92080700 -1.67827400 C -3.49615400 -2.07676300 -1.52845300 O -0.01762200 -1.93864000 2.54690800 H -4.49204900 -0.92255600 -0.03085900 H 4.47433000 -0.94381200 -0.04127700 C -3.30117500 -2.41666800 0.94887700 C 3.23743600 -2.51318100 0.74513300 H -3.30845500 -1.97156200 1.94410700 H 3.21814600 -2.17338100 1.78089200 H -2.34912500 -2.93640500 0.82670000 H 2.28481600 -3.00510700 0.54160300 H -4.09597900 -3.16788400 0.91435400 H 4.02587500 -3.26655200 0.65641300 C 2.96037300 0.54104100 2.72269900 C -2.86909300 0.80480300 2.65580200 H 3.65833800 -0.28926600 2.85285300 H -3.55123300 -0.01044600 2.90898700 H 1.96056900 0.18372000 2.97111700 H -1.85512400 0.48205300 2.89472600 H 3.23267300 1.30753400 3.45407000 H -3.11390800 1.64472500 3.31264400 C 4.45168900 1.59700500 0.99236900	O 0.02278900 -2.88601900 -1.38467800 P -2.37973200 0.09430300 -0.09158700 P 2.37001600 0.10208200 -0.06399100 C -2.46429000 1.10761000 -1.65453800 C 2.43787900 1.24517400 -1.53737300 H -2.51049600 2.15048500 -1.33272200 H 2.42339300 2.26272000 -1.13675000 H -3.35651000 0.88663200 -2.24271500 H 3.36129800 1.13215100 -2.10884000 C -1.19348900 0.90397600 -2.46743700 C 1.21192200 1.02820400 -2.41264800 H -1.17354700 1.64021300 -3.28525000 H 1.18497900 1.80537000 -3.19154300 H -1.18660800 -0.09055000 -2.93344800 H 1.28755200 0.06406600 -2.93400700 N -0.01314500 1.07533300 -1.61579700 C 3.22402100 1.14730700 1.24691800 C -3.19424800 1.25850400 1.13693500 H 2.55940000 2.01856600 1.28029500 H -2.53947100 2.13267300 1.03537100 C 3.55872000 -1.30490400 -0.43149900 C -3.57155500 -1.33624200 -0.32755600 C 3.45538000 -1.80188300 -1.87227100 C -3.45975500 -1.97443500 -1.71091000 O -0.01692700 -1.89925700 2.77393700 H -4.56957400 -0.89481700 -0.23427500 H 4.55920300 -0.88372100 -0.28633200 C -3.39045900 -2.38904600 0.76445000 C 3.36015600 -2.45986200 0.54930900 H -3.48696300 -1.97718900 1.76927600 H 3.44700600 -2.15078000 1.59105700 H -2.40698500 -2.85671100 0.69307600 H 2.37653600 -2.91417600 0.42117000 H -4.14507800 -3.17313100 0.65111200 H 4.11355700 -3.23177200 0.36615600 C 3.22144500 0.50589900 2.63194700 C -3.12563600 0.77287500 2.58193200 H 3.94081700 -0.31370000 2.69536900 H -3.82568200 -0.04493000 2.76898500 H 2.23947100 0.11646200 2.90324300 H -2.12613600 0.43037100 2.85276100 H 3.51086400 1.24635300 3.38325800 H -3.39640100 1.58920400 3.25800400 C 4.62161800 1.62624500 0.86087200

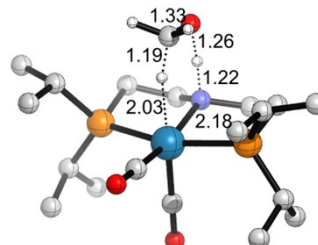
C -4.44725500 1.65161500 0.88798100 H 4.53270300 2.03774600 -0.00298800 H -4.57589900 1.97263900 -0.14755300 H 5.17741500 0.78290800 1.06413000 H -5.15837900 0.84514100 1.08655600 H 4.75679400 2.36092600 1.71374700 H -4.73142600 2.49326900 1.52679300 H 0.03481500 0.92526900 1.32905800 H -0.12180500 2.02511000 -1.05016300 H 4.26272100 -2.71013400 -1.75530200 H 2.55001100 -2.36017500 -1.95634400 H 3.76337600 -1.15723200 -2.41492100 H -4.26634800 -2.85375100 -1.54926800 H -3.70752900 -1.38922300 -2.34871400 H -2.53983400 -2.56189900 -1.72758700 H -0.05428100 1.45507800 0.71877800 O -0.39223800 2.98235900 -0.26715500 C 0.28406100 4.17721700 -0.45758200 H -0.29462800 5.03039500 -0.07135200 H 1.26417500 4.21695300 0.05721900 H 0.48471800 4.39583400 -1.52305700 C 0.00561800 -1.76261000 -0.84939300 C -0.01357000 -1.27472300 1.59928400 Mn -0.00248500 -0.29460200 0.12321800	C -4.61450300 1.67094400 0.75762300 H 4.64585000 2.11225200 -0.11636600 H -4.68572300 2.03519400 -0.26915400 H 5.34172800 0.80426400 0.84988700 H -5.32318900 0.84719300 0.87770700 H 4.97865500 2.35306400 1.59655800 H -4.94981500 2.47964600 1.41383500 H 0.07650300 1.14869400 1.41630800 H -0.15317100 2.18256600 -1.00930800 H 4.18208100 -2.60448200 -2.02928600 H 2.46756000 -2.21214600 -2.08615000 H 3.67105900 -1.02134100 -2.60365800 H -4.19800900 -2.77722900 -1.79816300 H -3.65342300 -1.26674000 -2.51856200 H -2.47655200 -2.41831600 -1.87147100 H -0.11636900 1.68225600 0.80497400 O -0.45874700 3.06594800 -0.20875200 C 0.29828600 4.23190600 -0.23115400 H 1.19589300 4.18147800 0.41308300 H 0.65128600 4.49095700 -1.24443000 H -0.28973600 5.08915700 0.12558900 C 0.01021700 -1.87457900 -0.81072500 C -0.01107100 -1.27651400 1.79378400 Re -0.00043000 -0.25674400 0.17412800
1Mn + H₂-TS(H₂O-H-H)  O 0.06163700 3.02402300 0.07693200 P -2.25733900 -0.10466800 0.12060700 P 2.26265100 -0.16373000 0.12108300 C -2.43770500 -0.21174100 1.97195300 C 2.40788500 -0.40088300 1.96164000 H -2.45421400 -1.27832600 2.21227700 H 2.34065600 -1.47847600 2.14024500 H -3.35741100 0.24636400 2.33873400 H 3.36447700 -0.05955900 2.37037400 C -1.20791200 0.41432000 2.61347600 C 1.23233600 0.28579800 2.63880600 H -1.19774300 0.18613000 3.69378300 H 1.19662800 0.01178400 3.70169500 H -1.21474600 1.50586600 2.50955100 H 1.32993600 1.36966600 2.58058700 N -0.00446400 -0.12632100 1.97211600 C 2.99020800 -1.78809900 -0.50221400 C -2.97923300 -1.76416800 -0.39648600 H 2.29239400 -2.49972200 -0.04468900 H -2.31717100 -2.43678000 0.16591100 C 3.53654800 1.14824800 -0.32971100 C -3.50307800 1.19370600 -0.43264300 C 3.56910900 2.30994500 0.66226300 C -3.47751800 2.44955900 0.43728500 O 0.01898900 0.41560600 -3.05876000 H -4.48374000 0.71984400 -0.31634700 H 4.50683600 0.64190600 -0.29129600	1Re + H₂-TS(H₂O-H-H)  O 0.13297700 3.12932500 0.44919900 P -2.36494900 -0.13717300 0.18279600 P 2.36858200 -0.22545300 0.13753900 C -2.46664600 -0.44417600 2.02872500 C 2.44722900 -0.74713300 1.93335900 H -2.60572300 -1.51870200 2.16103800 H 2.41438300 -1.84020300 1.93609900 H -3.32478700 0.06889300 2.46765300 H 3.38096800 -0.44686100 2.41251800 C -1.17967100 -0.00915400 2.71579000 C 1.24821900 -0.20679900 2.69738900 H -1.16569300 -0.40038600 3.74262700 H 1.21979400 -0.65839400 3.69885500 H -1.12317200 1.08138400 2.77960400 H 1.33041500 0.87591700 2.83115200 N -0.00117700 -0.49861600 1.98137000 C 3.11293400 -1.74115100 -0.69113300 C -3.10732500 -1.72822900 -0.48158700 H 2.41540000 -2.51753300 -0.35742300 H -2.47048500 -2.45739400 0.03646100 C 3.63872500 1.14108100 -0.06702100 C -3.63146000 1.21015600 -0.12157000 C 3.58812200 2.15868800 1.07113000 C -3.34381900 2.46211400 0.70342300 O -0.00564400 0.83710700 -3.16561800 H -4.58112900 0.78367000 0.22099000

C -3.30502000 1.56206900 -1.90213300 C 3.30727700 1.66692300 -1.74894900 H -3.32136800 0.69467300 -2.56238500 H 3.27617800 0.87004000 -2.49238100 H -2.35183400 2.07269600 -2.05158600 H 2.36703400 2.21699900 -1.81571300 H -4.09992800 2.24123200 -2.22483200 H 4.11393000 2.35150900 -2.02782100 C 2.90211500 -1.95642000 -2.01688200 C -2.82214200 -2.07172700 -1.88332600 H 3.61541100 -1.31692700 -2.53379600 H -3.50631300 -1.47990800 -2.49587000 H 1.90218700 -1.73099900 -2.39901900 H -1.80352600 -1.88485000 -2.23111200 H 3.13898400 -2.98991200 -2.28610100 H -3.04863200 -3.12684600 -2.06311300 C 4.39660300 -2.09430900 0.00780500 C -4.41411400 -2.00137100 0.06865200 H 4.48138300 -2.00017200 1.09212800 H -4.54858400 -1.80363600 1.13402300 H 5.13882100 -1.44184900 -0.44940400 H -5.13128500 -1.38912200 -0.48530700 H 4.66724700 -3.12191500 -0.25300300 H -4.68606300 -3.04720600 -0.10336500 H 0.04213700 -1.56217800 -0.44540600 H -0.06910000 -1.14292800 2.02927600 H 4.34150300 3.02283800 0.35847200 H 2.62077600 2.84897800 0.68327700 H 3.80547500 1.99001300 1.67839400 H -4.24802100 3.14526300 0.09134300 H -3.68030300 2.23863100 1.48852600 H -2.51932800 2.96678400 0.37120600 H -0.08384400 -1.97993800 0.37077800 O -0.36206100 -2.60164500 1.47713600 C 0.03818400 1.86820900 0.00221400 C 0.01461600 0.26962800 -1.91003500 Mn 0.01208700 0.11408800 -0.14952900 H -0.00692700 -3.49394900 1.45727800	H 4.61418000 0.64393900 -0.04133200 C -3.74208900 1.55576400 -1.60392900 C 3.46815800 1.83843500 -1.41561400 H -4.06921700 0.70910800 -2.20745700 H 3.51174000 1.14777600 -2.25791600 H -2.78309900 1.89859900 -1.99861500 H 2.50924500 2.35696400 -1.46375800 H -4.46871200 2.36174400 -1.74295200 H 4.26076100 2.58039800 -1.55035200 C 3.05665400 -1.68748900 -2.21528900 C -2.91518400 -1.93056900 -1.98268400 H 3.80749600 -1.00599900 -2.62183400 H -3.62917700 -1.35152500 -2.57247900 H 2.07793900 -1.37068900 -2.57698500 H -1.91066100 -1.65739000 -2.30666500 H 3.26460500 -2.67888100 -2.62794400 H -3.07093800 -2.98465400 -2.23024900 C 4.51220600 -2.10490200 -0.20023600 C -4.56090100 -1.95078200 -0.07150800 H 4.57355500 -2.17268700 0.88779000 H -4.72552000 -1.80264300 0.99847300 H 5.25978600 -1.38300500 -0.53832900 H -5.24173400 -1.28948000 -0.61458800 H 4.80326200 -3.07879800 -0.60486200 H -4.85585700 -2.97839600 -0.30421400 H 0.01157300 -1.61113400 -0.81595800 H -0.10638000 -1.55401000 1.84622000 H 4.35395900 2.92259300 0.90755700 H 2.62422300 2.66811500 1.11052500 H 3.78287100 1.70998000 2.04692300 H -4.17628000 3.16455900 0.59984400 H -3.23155800 2.24947800 1.76883200 H -2.44020700 2.96729800 0.36300600 H -0.17469000 -2.09850200 0.12317100 O -0.41218400 -2.84317500 1.10380000 C 0.07506300 1.98572500 0.23695000 C 0.00156900 0.56900300 -2.03607800 Re 0.01263300 0.13453700 -0.17895400 H 0.01323600 -3.70329000 1.14174000
1Mn + H₂-TS(CH₃OH-H-H)  O 0.04559100 -3.06164400 -0.69532700 P -2.27076100 -0.00220500 -0.08729700 P 2.26216600 0.03028200 -0.06308200 C -2.45026800 0.49448900 -1.87945200 C 2.41583500 0.71602300 -1.79382500 H -2.50267100 1.58581400 -1.88444600 H 2.37934300 1.80544700 -1.70114900 H -3.35767500 0.10211300 -2.34043700 H 3.36336800 0.46065500 -2.27131300 C -1.20500900 0.05616800 -2.63280600 C 1.23086400 0.23933600 -2.61659400	1Re + H₂-TS(CH₃OH-H-H)  O 0.11102400 -3.12124300 -0.96994800 P -2.37092900 0.06207700 -0.15151500 P 2.36611300 0.10727300 -0.08493000 C -2.46696100 0.67910200 -1.91867600 C 2.45152700 0.93600400 -1.76074000 H -2.60928100 1.75998300 -1.86688100 H 2.42655400 2.01269700 -1.57061500 H -3.32227100 0.24594000 -2.44132900 H 3.38400300 0.71818000 -2.28481200 C -1.17774900 0.36911500 -2.66665200

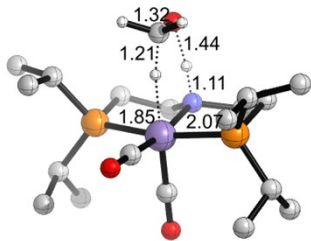
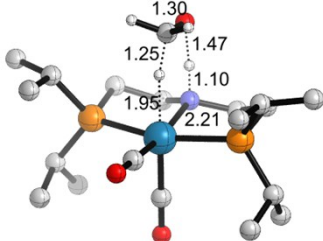
H	-1.19476400	0.50457100	-3.63640200	C	1.25072300	0.54653500	-2.60872300
H	1.20631100	0.76324200	-3.58261900	H	-1.15952700	0.93387300	-3.60909700
H	-1.18294300	-1.03012700	-2.75929600	H	1.22844900	1.16500300	-3.51672900
H	1.31636800	-0.83013100	-2.83055100	H	-1.12297700	-0.69346200	-2.92014900
N	-0.01385000	0.47034200	-1.87742900	H	1.32497300	-0.49722000	-2.92786500
C	3.05704200	1.41212600	0.93690000	N	0.00075100	0.71841300	-1.85528300
C	-3.04559100	1.48036800	0.76963200	C	3.12684600	1.44365200	0.99741900
H	2.38568000	2.24649000	0.71035200	C	-3.11246300	1.51867700	0.77249200
H	-2.40752000	2.28103100	0.37601400	H	2.43925300	2.27529500	0.80761500
C	3.48728600	-1.39397500	0.04406500	H	-2.47608200	2.32432400	0.38366900
C	-3.48008700	-1.41823700	0.17180500	C	3.61935700	-1.28948700	-0.12276500
C	3.50806800	-2.26425100	-1.21162900	C	-3.64341400	-1.31196300	-0.08445700
C	-3.44800500	-2.45259100	-0.95231200	C	3.56648100	-2.08659400	-1.42487900
O	-0.01030400	-1.10957700	2.91913900	C	-3.35291800	-2.41196800	-1.10241700
H	-4.47019300	-0.95026700	0.17091200	O	-0.02960600	-1.48494500	2.98371300
H	4.47219600	-0.92692800	0.14810800	H	-4.58823700	-0.82999400	-0.36044900
C	-3.25543600	-2.09587300	1.52249800	H	4.60025100	-0.80745200	-0.05399600
C	3.21613400	-2.25134300	1.28025400	C	-3.76968000	-1.89586900	1.31981800
H	-3.27133700	-1.39460600	2.35691500	C	3.43232500	-2.21476600	1.07865300
H	3.19052000	-1.67075800	2.20258600	H	-4.10166400	-1.15840000	2.05060600
H	-2.29417700	-2.61257200	1.54363600	H	3.47453200	-1.68598400	2.03102500
H	2.26129000	-2.77184300	1.19153000	H	-2.81549400	-2.30210500	1.66251300
H	-4.03762400	-2.84070100	1.69791500	H	2.46936400	-2.72544000	1.02743000
H	3.99971600	-3.00798300	1.38411100	H	-4.49897000	-2.71134900	1.31757500
C	3.00908000	1.17738500	2.44420200	H	4.21829400	-2.97576600	1.08383600
C	-2.89820400	1.45712400	2.28792000	C	3.06873500	1.12032400	2.48778900
H	3.71396400	0.40238300	2.75441800	C	-2.91806200	1.46651600	2.28606300
H	-3.56824400	0.73123500	2.75542800	H	3.81061000	0.36794100	2.76533400
H	2.01399900	0.89067600	2.78498800	H	-3.63150500	0.79713800	2.77168600
H	-1.87745800	1.22767000	2.59534600	H	2.08582300	0.75660600	2.78912700
H	3.29014300	2.09554800	2.96835300	H	-1.91328300	1.14274000	2.55872900
H	-3.15479000	2.43974400	2.69513600	H	3.28899400	2.01980300	3.06980300
C	4.46567600	1.79331700	0.48615300	H	-3.07275300	2.46440000	2.70669000
C	-4.48944100	1.75966300	0.35898800	C	4.53081400	1.87272900	0.57747800
H	4.52577100	1.99846400	-0.58448200	C	-4.56622500	1.80770000	0.40708700
H	-4.61720100	1.80682700	-0.72464900	H	4.59372400	2.13518900	-0.48051600
H	5.19434600	1.01423400	0.72400300	H	-4.73204800	1.84010700	-0.67245400
H	-5.18206700	1.01020600	0.75174500	H	5.26983500	1.09324500	0.77897700
H	4.78599200	2.69915300	1.00969300	H	-5.24735200	1.06593400	0.83317800
H	-4.80324700	2.72693400	0.76334700	H	4.83280500	2.75440500	1.15042100
H	0.09098700	1.27351800	0.84377200	H	-4.85970600	2.78249100	0.80806900
H	-0.12050000	1.49697600	-1.66770500	H	0.04593300	1.33705300	1.08840000
H	4.25437600	-3.05521900	-1.09082000	H	-0.10057400	1.73313300	-1.53961400
H	2.54614400	-2.75050700	-1.38058100	H	4.32283000	-2.87648000	-1.39613900
H	3.77515900	-1.70365800	-2.10926200	H	2.59766200	-2.56963000	-1.56013500
H	-4.20689000	-3.21753300	-0.76141500	H	3.77367700	-1.47308500	-2.30360000
H	-3.66603400	-2.01958500	-1.93017500	H	-4.19117900	-3.11472500	-1.12675200
H	-2.48359500	-2.95860800	-1.00882500	H	-3.22569800	-2.02612400	-2.11626100
H	-0.14391400	1.85904400	0.14711900	H	-2.45685000	-2.97430400	-0.84098400
O	-0.45119900	2.85987900	-0.74119800	H	-0.19939900	1.96632100	0.24721200
C	0.01924500	-1.93820500	-0.40137100	O	-0.42370000	2.87140500	-0.57937300
C	-0.00617800	-0.76716500	1.81354500	C	0.05486100	-2.03105800	-0.56425800
Mn	0.00493400	-0.25672600	0.12288300	C	-0.01665300	-1.02644600	1.91733200
C	0.20536700	4.04485900	-0.43260100	Re	0.00382000	-0.27910800	0.16286900
H	0.46691800	4.11897000	0.63833000	C	0.18209800	4.09809900	-0.36093400
H	1.14607400	4.18200600	-0.99719000	H	1.05232000	4.04414200	0.32385300
H	-0.42426500	4.91808100	-0.65999000	H	0.55614600	4.55833400	-1.29304000
				H	-0.51031900	4.82761300	0.09122800
Mn-TS1-H ⁺				Re-TS1-H ⁺			

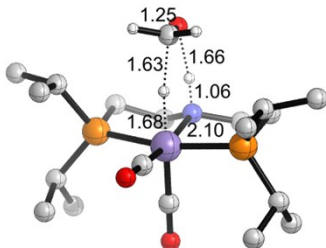
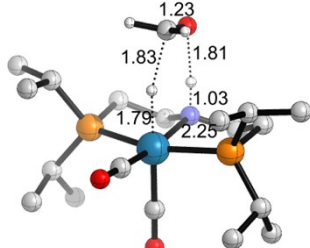


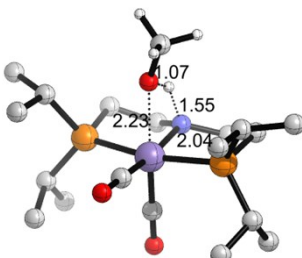
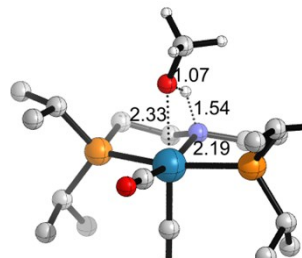
O	0.03412000	2.96494400	-0.21079100
P	2.29390100	-0.09671600	-0.08319200
P	-2.29737300	-0.04307700	-0.09747700
C	2.41060200	-0.72369400	-1.82892500
C	-2.46033300	-0.48145300	-1.89773500
H	2.35171300	-1.81418900	-1.76871900
H	-2.52499700	-1.57159900	-1.94069800
H	3.35089500	-0.46208300	-2.31773600
H	-3.35610900	-0.06513800	-2.36104200
C	1.20698000	-0.21421600	-2.60159800
C	-1.19412000	-0.04125100	-2.61081800
H	1.14740300	-0.73463400	-3.56822100
H	-1.16018500	-0.49992000	-3.60945400
H	1.30656000	0.85552900	-2.81977300
H	-1.18192600	1.04528000	-2.75670500
N	-0.01942200	-0.45353600	-1.83044900
C	-3.22986000	-1.47288800	0.69651500
C	3.22653000	-1.43106800	0.86426100
H	-2.66486000	-2.32654600	0.30967100
H	2.56674000	-2.29371400	0.73145200
C	-3.40717400	1.45111200	0.18182300
C	3.43723400	1.39624000	0.01426100
C	-3.33655000	2.48143200	-0.94459600
C	3.37489800	2.29044300	-1.22302000
O	-0.00103600	0.36457700	3.05703300
H	4.44459300	0.96983300	0.06841900
H	-4.42342000	1.04489500	0.19778400
C	3.19022600	2.21668500	1.28136200
C	-3.12600600	2.10773200	1.53338900
H	3.20038700	1.61164800	2.18775600
H	-3.17384400	1.40250500	2.36363400
H	2.23055400	2.73182500	1.23617400
H	-2.13837800	2.57056400	1.54876800
H	3.96937100	2.97849900	1.38148400
H	-3.86349900	2.89372800	1.72199500
C	-3.14280600	-1.50323800	2.21936200
C	3.33929400	-1.15905900	2.36253100
H	-3.73378500	-0.70520700	2.67484800
H	4.06351900	-0.36857600	2.57288400
H	-2.11709800	-1.41064800	2.57635100
H	2.38616700	-0.87759300	2.81050500
H	-3.54273900	-2.45102400	2.59191300
H	3.69326600	-2.06020500	2.87188900
C	-4.67500300	-1.61892200	0.22303100
C	4.58948300	-1.78348600	0.27113400
H	-4.76530000	-1.60403500	-0.86483400
H	4.53393800	-2.04508700	-0.78659100
H	-5.31882200	-0.83516100	0.62994600
H	5.30721800	-0.96661400	0.38281600
H	-5.07808400	-2.57493200	0.57045400
H	5.00491800	-2.64689700	0.79957600
H	0.02847300	-1.81392800	0.39618100



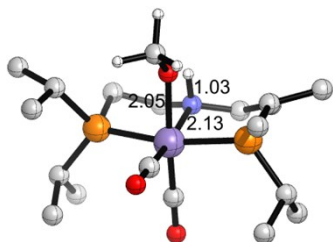
O	3.11883500	-0.20272800	0.00000000
P	-0.10110500	-0.15127000	2.38574000
P	-0.10110500	-0.15127000	-2.38574000
C	-0.82496500	-1.86826800	2.45559500
C	-0.82496500	-1.86826800	-2.45559500
H	-1.91137100	-1.74410100	2.46578300
H	-1.91137100	-1.74410100	-2.46578300
H	-0.53796600	-2.40389400	3.36266500
H	-0.53796600	-2.40389400	-3.36266500
C	-0.43554800	-2.64428600	1.20776200
C	-0.43554800	-2.64428600	-1.20776200
H	-1.02787800	-3.56901400	1.16163700
H	-1.02787800	-3.56901400	-1.16163700
H	0.61951600	-2.93767600	1.24241100
H	0.61951600	-2.93767600	-1.24241100
N	-0.68482900	-1.84035900	0.00000000
C	-1.39832900	0.82356400	-3.33818500
C	-1.39832900	0.82356400	3.33818500
H	-2.29057500	0.61948700	-2.73666900
H	-2.29057500	0.61948700	2.73666900
C	1.40775700	-0.19364700	-3.50237500
C	1.40775700	-0.19364700	3.50237500
C	2.27543800	-1.42851900	-3.26452800
C	2.27543800	-1.42851900	3.26452800
O	0.54250100	3.23197600	0.00000000
H	1.00597200	-0.25267300	4.51945100
H	1.00597200	-0.25267300	-4.51945100
C	2.23645500	1.08353000	3.37247500
C	2.23645500	1.08353000	-3.37247500
H	1.65772600	1.98413700	3.57750500
H	1.65772600	1.98413700	-3.57750500
H	2.65600100	1.17903200	2.37037200
H	2.65600100	1.17903200	-2.37037200
H	3.06850300	1.05455000	4.08232000
H	3.06850300	1.05455000	-4.08232000
C	-1.17032000	2.33247400	-3.32836800
C	-1.17032000	2.33247400	3.32836800
H	-0.35368800	2.62151900	-3.99342300
H	-0.35368800	2.62151900	3.99342300
H	-0.94487300	2.70924600	-2.33072600
H	-0.94487300	2.70924600	2.33072600
H	-2.06998300	2.84203200	-3.68578300
H	-2.06998300	2.84203200	3.68578300
C	-1.65451400	0.30855200	-4.75289600
C	-1.65451400	0.30855200	4.75289600
H	-1.84246600	-0.76643900	-4.78235600
H	-1.84246600	-0.76643900	4.78235600
H	-0.81770800	0.52722800	-5.42085900
H	-0.81770800	0.52722800	5.42085900
H	-2.53496800	0.80557300	-5.17088200
H	-2.53496800	0.80557300	5.17088200
H	-1.89229900	0.53032100	0.00000000

H -0.11217500 -1.65112200 -1.70964900 C -0.04437200 -2.89242000 -0.07812300 H -4.03725800 3.29441700 -0.73137300 H -2.34388200 2.92382700 -1.03081700 H -3.61314300 2.06269700 -1.91346500 H 4.08877400 3.11194900 -1.10978200 H 3.63599500 1.75807700 -2.13899700 H 2.38736600 2.73588300 -1.35074600 O -0.21663300 -2.89063300 -1.40277000 H -0.86993700 -3.33116700 0.50885400 C 0.01805200 1.81254100 -0.06276000 Mn 0.00109400 0.08680200 0.14050600 C -0.00110500 0.24329200 1.90539700 H 0.89484100 -3.35735800 0.27504700	H -1.88583500 -1.61711500 0.00000000 C -3.00785500 0.10479100 0.00000000 H 3.12488200 -1.40977900 -3.95375800 H 2.67977900 -1.44860500 -2.25176500 H 1.73525100 -2.36013200 -3.44146400 H 3.12488200 -1.40977900 3.95375800 H 1.73525100 -2.36013200 3.44146400 H 2.67977900 -1.44860500 2.25176500 O -3.08597600 -1.22454200 0.00000000 H -3.41528800 0.60924600 -0.89337200 C 1.96088900 -0.05162800 0.00000000 Re 0.10795000 0.18925000 0.00000000 C 0.39239200 2.07946500 0.00000000 H -3.41528800 0.60924600 0.89337200
3Mn⁺-OCH₃⁻  O -0.05057500 2.97607600 -0.15688300 P 2.29325500 -0.03369700 -0.09873900 P -2.29222000 -0.10566400 -0.08469800 C 2.46137900 -0.39884600 -1.91671500 C -2.40214200 -0.70890000 -1.84100100 H 2.53202700 -1.48623100 -2.00148100 H -2.32066600 -1.79899600 -1.79847100 H 3.35472800 0.04156500 -2.36173800 H -3.34941700 -0.45971000 -2.32278700 C 1.19573000 0.06034400 -2.61761900 C -1.21537200 -0.16262600 -2.61408800 H 1.17087200 -0.34594800 -3.63825500 H -1.15833300 -0.65035600 -3.59693300 H 1.16013000 1.15125300 -2.69994200 H -1.32191500 0.91231900 -2.79041300 N 0.02350900 -0.40872300 -1.86128100 C -3.21970900 -1.45809700 0.84068800 C 3.22664700 -1.49543000 0.63181800 H -2.55049900 -2.31303900 0.70481000 H 2.67101500 -2.33064500 0.19429200 C -3.44877400 1.37648500 0.02781400 C 3.40330100 1.44874900 0.23793400 C -3.39322300 2.28651500 -1.19811200 C 3.33268200 2.52294700 -0.84658500 O -0.00031700 0.31156000 3.06459200 H 4.41980700 1.04307200 0.23852600 H -4.45284000 0.94172700 0.07655000 C 3.12018700 2.05099300 1.61409000 C -3.20833000 2.18397800 1.30452700 H 3.17155700 1.31386300 2.41607600 H -3.21389000 1.56821100 2.20368100 H 2.13005900 2.50778000 1.64768100 H -2.25256000 2.70682300 1.26541500 H 3.85395000 2.83249900 1.83336200 H -3.99334600 2.93851100 1.41354000 C -3.34515500 -1.20082700 2.34060800 C 3.12054700 -1.60103100 2.14994200	3Re⁺-OCH₃⁻  O 0.00003600 3.12481900 0.20735700 P -2.38272500 -0.10240400 0.15050600 P 2.38272400 -0.10245300 0.15048000 C -2.45346000 -0.75159700 1.89943300 C 2.45341000 -0.75181900 1.89934000 H -2.44887800 -1.84263300 1.82279900 H 2.44868900 -1.84284800 1.82258800 H -3.36605700 -0.45292300 2.41884900 H 3.36605500 -0.45332400 2.41877500 C -1.21709500 -0.31444400 2.66779300 C 1.21711200 -0.31460100 2.66776800 H -1.18016200 -0.84226100 3.63019300 H 1.18016100 -0.84247000 3.63013900 H -1.24164800 0.75800000 2.88015400 H 1.24176800 0.75782800 2.88018900 N -0.00001900 -0.61885700 1.89143200 C 3.32625100 -1.44639300 -0.76594000 C -3.32624900 -1.44644400 -0.76577400 H 2.72660300 -2.32720700 -0.51330700 H -2.72682400 -2.32728400 -0.51270200 C 3.51097700 1.39891600 0.12405500 C -3.51096500 1.39896600 0.12398800 C 3.30057900 2.31355500 1.32940800 C -3.30041700 2.31378700 1.32917300 O 0.00000900 0.53052600 -3.23550500 H -4.52658700 0.99347300 0.18001100 H 4.52660500 0.99341000 0.17989000 C -3.36220800 2.17995700 -1.18090000 C 3.36208200 2.18011500 -1.18069400 H -3.54865500 1.56641100 -2.06248000 H 3.54835300 1.56669300 -2.06239500 H -2.35931000 2.59843900 -1.27431800 H 2.35920800 2.59869200 -1.27390500 H -4.07510000 3.00973300 -1.19630900 H 4.07503700 3.00983900 -1.19607400 C 3.29839600 -1.28899500 -2.28351100 C -3.29795400 -1.28953900 -2.28338500

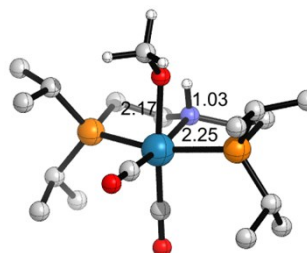
H -4.07852900 -0.41945700 2.55352000 H 3.69764700 -0.82110700 2.65235400 H -2.39762600 -0.91467400 2.79744100 H 2.08891600 -1.53485600 2.49578800 H -3.69344300 -2.11018500 2.83910600 H 3.52364600 -2.56267600 2.48121300 C -4.57519200 -1.81757300 0.23497900 C 4.67806000 -1.60874400 0.16917100 H -4.50943000 -2.07371000 -0.82351100 H 4.78149500 -1.53336700 -0.91509900 H -5.30044500 -1.00707300 0.34491100 H 5.31352700 -0.84638300 0.62680700 H -4.98788400 -2.68696400 0.75567800 H 5.08101900 -2.58115500 0.46767000 H -0.02788200 -1.74806400 0.34766800 H 0.13451300 -1.51272700 -1.77757300 C 0.07370400 -2.86410300 -0.11708700 H -4.11317100 3.10124400 -1.07500400 H -2.40906300 2.74145100 -1.31940100 H -3.65055100 1.76403600 -2.12097500 H 4.03423800 3.32629100 -0.60194400 H 3.60871800 2.14308900 -1.83160200 H 2.34044500 2.96945500 -0.91452700 O 0.30308200 -2.89598100 -1.41232400 H -0.88708500 -3.30134500 0.22244200 C -0.02784300 1.82040100 -0.03678800 Mn -0.00468400 0.08811600 0.14570300 C -0.00166200 0.21764300 1.91072900 H 0.87072400 -3.26045200 0.54013900	H 3.95487400 -0.48291000 -2.61843400 H -3.95407900 -0.48335500 -2.61875800 H 2.29440800 -1.08642200 -2.65669900 H -2.29380200 -1.08739500 -2.65635900 H 3.65431700 -2.20963400 -2.75516200 H -3.65403200 -2.21022300 -2.75483100 C 4.74629200 -1.67940800 -0.25483700 C -4.74646500 -1.67905500 -0.25496800 H 4.78798100 -1.81421100 0.82782700 H -4.78847900 -1.81335600 0.82774800 H 5.41372200 -0.85648700 -0.52239900 H -5.41371100 -0.85617100 -0.52309900 H 5.15663300 -2.58471800 -0.71193400 H -5.15678600 -2.58452300 -0.71176600 H -0.00003000 -1.82908800 -0.46414500 H -0.00010100 -1.70800700 1.73495000 C -0.00009100 -3.00135000 -0.02980800 H 3.99866600 3.15384200 1.26986300 H 2.29294900 2.73049500 1.34889600 H 3.48610600 1.80612700 2.27778600 H -3.99854100 3.15404100 1.26960500 H -3.48579400 1.80649200 2.27765200 H -2.29279800 2.73076100 1.34846100 O -0.00029100 -3.10162400 1.27004500 H 0.89796600 -3.36129300 -0.56798400 C 0.00001900 1.96671000 0.06028800 Re 0.00000100 0.10626300 -0.19501400 C 0.00000200 0.38349000 -2.08293300 H -0.89798600 -3.36127200 -0.56826400
Mn-TS1-H⁻  O -0.05537000 3.00711800 -0.17496000 P 2.27696000 -0.02629900 -0.09407100 P -2.27930200 -0.09408500 -0.08235500 C 2.45641300 -0.40857100 -1.91094500 C -2.41113400 -0.66074400 -1.85326700 H 2.52161800 -1.49680300 -1.99264700 H -2.35443000 -1.75320100 -1.83734300 H 3.35710900 0.02075600 -2.35225900 H -3.35596200 -0.38321700 -2.32407300 C 1.20387000 0.06258400 -2.62717900 C -1.22246800 -0.11621600 -2.62448700 H 1.18811400 -0.32956000 -3.65340100 H -1.18232200 -0.57061200 -3.62390600 H 1.16939900 1.15366700 -2.68984200 H -1.30429600 0.96578700 -2.75859300 N 0.01841100 -0.40333200 -1.88754900 C -3.20485400 -1.47002700 0.81104300 C 3.20977100 -1.48376500 0.64910500 H -2.55213000 -2.32654100 0.61765800 H 2.67510300 -2.32071400 0.18935400 C -3.44631100 1.37874000 0.06370600 C 3.40316500 1.45094500 0.21723700	Re-TS1-H⁻  O 0.00000500 -3.16097600 -0.37034100 P -2.36486300 0.09543800 -0.13654800 P 2.36486500 0.09545900 -0.13650700 C -2.45507500 0.71568100 -1.90224100 C 2.45506900 0.71580700 -1.90216000 H -2.46716700 1.80848200 -1.85298200 H 2.46708000 1.80860600 -1.85282500 H -3.36859200 0.39950500 -2.40956000 H 3.36861900 0.39973600 -2.40948500 C -1.22638600 0.26637100 -2.67682900 C 1.22642600 0.26646500 -2.67680100 H -1.20845600 0.74806900 -3.66367300 H 1.20850300 0.74819800 -3.66362800 H -1.23280300 -0.81466900 -2.83133600 H 1.23290400 -0.81456800 -2.83134600 N -0.00000100 0.60942800 -1.92804900 C 3.29253200 1.46744400 0.75781200 C -3.29249800 1.46749300 0.75770200 H 2.71535900 2.34125800 0.43737300 H -2.71546000 2.34130500 0.43700900 C 3.52800800 -1.38178200 -0.08545900 C -3.52803300 -1.38177600 -0.08544600

C -3.39947200 2.31590400 -1.14212300 C 3.31843000 2.52172300 -0.86956900 O -0.00192400 0.33721600 3.05764100 H 4.41853500 1.04294800 0.20310100 H -4.44942600 0.94189600 0.10873300 C 3.14200000 2.05977200 1.59466500 C -3.19856700 2.15906900 1.35564700 H 3.21639700 1.32809100 2.39997300 H -3.21056800 1.52548000 2.24247400 H 2.14769700 2.50606300 1.64449200 H -2.23643400 2.67112500 1.32700300 H 3.87208100 2.84981800 1.79508800 H -3.97538200 2.91980500 1.47986400 C -3.27666500 -1.27817300 2.32400200 C 3.05764200 -1.60542200 2.16205500 H -3.98423800 -0.49126200 2.59562200 H 3.60516000 -0.82125100 2.69005800 H -2.30807100 -1.03216200 2.75919000 H 2.01394700 -1.55633400 2.47239400 H -3.62963300 -2.20091600 2.79416000 H 3.46492700 -2.56370300 2.49856400 C -4.58367900 -1.78747000 0.23543500 C 4.67492100 -1.58229900 0.22883100 H -4.55913000 -1.98054200 -0.83839300 H 4.81121700 -1.48551600 -0.85037300 H -5.29875500 -0.98159200 0.41947000 H 5.29140400 -0.82509100 0.71956400 H -4.98387800 -2.68394900 0.71880000 H 5.07498100 -2.55776600 0.52153800 H -0.00829900 -1.55115700 0.38001400 H 0.10425500 -1.45642400 -1.82156000 C 0.09843700 -3.07506400 -0.18116200 H -4.12046300 3.12623000 -0.99739800 H -2.41713800 2.77579700 -1.25862700 H -3.66163400 1.81408900 -2.07531500 H 4.02767600 3.32290900 -0.64019200 H 3.57637400 2.13767000 -1.85809700 H 2.32716100 2.97227000 -0.92168600 O 0.31606400 -3.05369900 -1.40803900 H -0.89563900 -3.34750700 0.21835200 C -0.03111300 1.84920500 -0.06536700 Mn -0.00613400 0.11088500 0.14389400 C -0.00365300 0.25219400 1.90218800 H 0.89371000 -3.32100500 0.54409200	C 3.34710100 -2.31814800 -1.27856100 C -3.34701700 -2.31828500 -1.27841900 O -0.00003900 -0.68456700 3.21020700 H -4.53796500 -0.96197900 -0.13461500 H 4.53795400 -0.96199900 -0.13447100 C -3.37288400 -2.14795500 1.22738800 C 3.37271400 -2.14811200 1.22727100 H -3.54483000 -1.52136600 2.10315800 H 3.54447800 -1.52160500 2.10313300 H -2.37055400 -2.57014500 1.31475500 H 2.37040400 -2.57038200 1.31444200 H -4.09125200 -2.97254700 1.26195500 H 4.09113700 -2.97265500 1.26185400 C 3.18154900 1.37842100 2.27675800 C -3.18124400 1.37874700 2.27664400 H 3.78561100 0.56294300 2.68046600 H -3.78507700 0.56322500 2.68059900 H 2.15028500 1.22812700 2.59660400 H -2.14989500 1.22869700 2.59633400 H 3.54817100 2.30451800 2.72996100 H -3.54796200 2.30485200 2.72974900 C 4.73865900 1.66409400 0.30947600 C -4.73871800 1.66393800 0.30957400 H 4.83884800 1.72987400 -0.77629300 H -4.83910200 1.72944500 -0.77619600 H 5.38467200 0.85631700 0.66182000 H -5.38461100 0.85620000 0.66222900 H 5.13281000 2.59395000 0.73057500 H -5.13285800 2.59387000 0.73051300 H -0.00005800 1.61770400 0.57014400 H -0.00004900 1.63642300 -1.81532100 C -0.00003800 3.34247900 -0.05619500 H 4.05925100 -3.14503700 -1.19901000 H 2.34731500 -2.75286800 -1.30192100 H 3.53491900 -1.82329900 -2.23349200 H -4.05925000 -3.14510500 -1.19888900 H -3.53464700 -1.82352600 -2.23343300 H -2.34726300 -2.75308900 -1.30157800 O -0.00015200 3.36231700 -1.28584200 H 0.92481600 3.48018100 0.52652200 C 0.00001400 -2.00878200 -0.18083100 Re 0.00000000 -0.13696200 0.19503600 C -0.00001900 -0.49348900 2.06305400 H -0.92477600 3.48023000 0.52669600
Mn-TS(CH₃OH)  P 2.30339100 0.04393400 0.15966400 P -2.28719900 0.01901200 0.16045900 C 2.44219000 0.04301600 2.01402400 C -2.44014500 0.01040100 2.01415900 H 2.45667800 1.09526600 2.31144800 H -2.48435400 1.06064700 2.31998500 H 3.36358500 -0.41397700 2.37929400	Re-TS(CH₃OH)  P -2.39710500 -0.01501100 0.22447100 P 2.37241900 -0.00928000 0.22509600 C -2.46854900 -0.07147600 2.08965800 C 2.44721900 -0.11418000 2.08841500 H -2.52561100 -1.13001400 2.35804300 H 2.49867700 -1.17935300 2.33613000

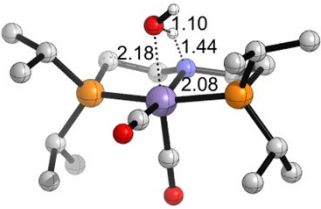
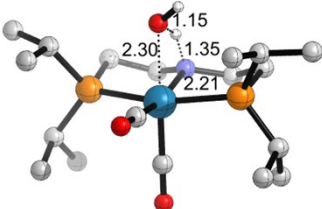
H	-3.35245600	-0.47041500	2.37215400	H	-3.36531500	0.41539100	2.47897700
C	1.19972100	-0.62576000	2.58491400	H	3.34811600	0.35580600	2.48981100
C	-1.18736000	-0.63686800	2.58624000	C	-1.20284300	0.53312100	2.68375800
H	1.16887300	-0.44133100	3.67179400	C	1.18818700	0.49102300	2.69602600
H	-1.15865900	-0.45156800	3.67304700	H	-1.16998200	0.28982600	3.75831200
H	1.27265000	-1.71939500	2.46691100	H	1.15004200	0.22341000	3.76466700
H	-1.24842500	-1.73143700	2.46963600	H	-1.24610800	1.63187500	2.62142000
N	0.00204700	-0.10444600	1.94531400	H	1.25173400	1.58975800	2.66076700
C	-3.23854800	1.58100200	-0.28989500	N	-0.01125900	0.02019300	2.01836700
C	3.19373100	1.63590700	-0.29863100	C	3.41258800	-1.50756100	-0.25805600
H	-2.62474100	2.35429100	0.17852500	C	-3.35059600	-1.57458200	-0.21730500
H	2.51466600	2.37899500	0.12820000	H	2.86597400	-2.30881200	0.24892900
C	-3.39792400	-1.35947400	-0.48760700	H	-2.71534900	-2.32663300	0.26209500
C	3.44778500	-1.30872300	-0.47953500	C	3.44632000	1.47026200	-0.21026000
C	-3.38387900	-2.61342000	0.38599800	C	-3.50218200	1.41862900	-0.26719200
C	3.46755400	-2.55561400	0.40364000	C	3.12909300	2.69795900	0.64195300
O	0.00765800	0.43735600	-2.99175800	C	-3.22460200	2.67575400	0.55594300
H	4.44998300	-0.86648700	-0.46660800	O	-0.00853800	-0.78981700	-3.14336600
H	-4.41093300	-0.94381100	-0.46598600	H	-4.52076400	1.08309300	-0.04276700
C	3.10670100	-1.68602800	-1.92156900	H	4.46778400	1.15377200	0.02599400
C	-3.05427000	-1.71615300	-1.93378800	C	-3.39898600	1.72217100	-1.76156100
H	3.09784400	-0.82733800	-2.59283800	C	3.36877400	1.81016700	-1.69794900
H	-3.09851200	-0.85744000	-2.60354600	H	-3.61685800	0.85508700	-2.38484700
H	2.12823600	-2.16335500	-1.98182200	H	3.63365700	0.96808600	-2.33723300
H	-2.05351200	-2.14182000	-2.00770800	H	-2.40046200	2.07631800	-2.02018000
H	3.84757300	-2.39744800	-2.29976400	H	2.36641100	2.13719000	-1.97508800
H	-3.76218800	-2.46439000	-2.30390100	H	-4.11186900	2.50921500	-2.02573900
C	-3.26883600	1.85940300	-1.79092000	H	4.06082700	2.62739600	-1.92294200
C	3.26998700	1.87408600	-1.80454200	C	3.39124600	-1.81952000	-1.75198000
H	-3.94089000	1.17193000	-2.30985500	C	-3.38131000	-1.87949400	-1.71235200
H	3.99704600	1.21048200	-2.27962500	H	3.99651400	-1.11158500	-2.32168400
H	-2.28252600	1.77922300	-2.24839700	H	-4.07478000	-1.22471700	-2.24489000
H	2.30745800	1.73423000	-2.29667400	H	2.38103900	-1.80348300	-2.16082300
H	-3.64378800	2.87112700	-1.97396100	H	-2.39860400	-1.78137800	-2.17319600
H	3.59860800	2.89963300	-1.99946000	H	3.81342200	-2.81381400	-1.92725100
C	-4.64315800	1.66776000	0.30591300	H	-3.72664500	-2.90580900	-1.87030700
C	4.57037700	1.79511500	0.34374200	C	4.83909100	-1.49524100	0.28734000
H	-4.66753200	1.43530000	1.37189400	C	-4.74946800	-1.64997100	0.39035100
H	4.55632000	1.63524700	1.42318900	H	4.87821200	-1.30105600	1.36130800
H	-5.34010500	0.99671200	-0.20209600	H	-4.75128700	-1.48472500	1.46961000
H	5.30322700	1.10917900	-0.08985400	H	5.45725900	-0.74758800	-0.21532300
H	-5.03342900	2.68286600	0.18255400	H	-5.42851400	-0.92393500	-0.06435800
H	4.94231800	2.80963500	0.16857700	H	5.31043000	-2.46723200	0.11200800
H	0.06268500	1.38962300	1.55325500	H	-5.17694700	-2.64134300	0.21058600
H	-4.10932700	-3.33375300	-0.00433400	H	-0.10488000	-1.47035200	1.65424600
H	4.19901900	-3.26781300	0.00950900	H	3.81251000	3.50860900	0.37136400
H	-2.40619500	-3.09723300	0.37643000	H	-3.91566900	3.46701900	0.24993500
H	2.49730000	-3.05502000	0.41103700	H	2.11369100	3.05620000	0.47132400
H	-3.65504100	-2.40923100	1.42277000	H	-2.21171000	3.04581700	0.39258800
H	3.74866400	-2.33830400	1.43511300	H	3.25520400	2.50971800	1.70939300
O	0.21221900	2.02125300	0.70378800	H	-3.36602400	2.51618500	1.62619600
C	0.00606300	0.25846800	-1.84565400	O	-0.26516000	-2.09400100	0.79987000
C	-0.30350700	3.32916600	0.74106600	C	-0.00982100	-0.47437700	-2.02260000
H	0.46516700	4.04022100	1.06951300	C	0.37175200	-3.35129600	0.76651100
H	-0.63356500	3.62976900	-0.25675900	H	-0.25915700	-4.10948000	1.24411600
H	-1.15416900	3.42062300	1.42826300	H	0.53889900	-3.64659800	-0.27071800
C	0.01015900	-1.77981800	-0.31752300	H	1.33754400	-3.34004300	1.28595800
O	0.02413500	-2.93781100	-0.42996700	C	0.00584800	1.80252300	-0.68030900
Mn	0.00373200	-0.05310700	-0.09502600	O	-0.00123700	2.92968100	-0.99436800
				Re	-0.00897800	0.00601100	-0.17463900

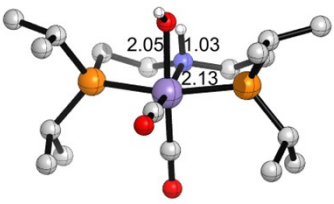
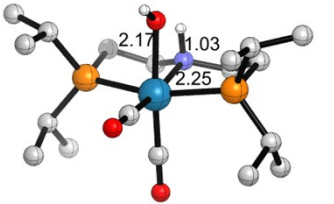
2Mn-OCH₃

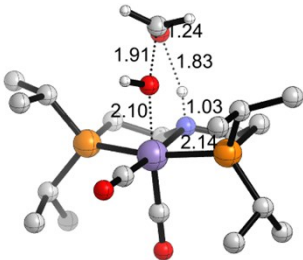
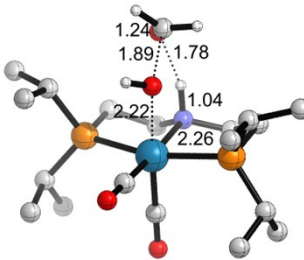
N	-0.64050800	1.92746800	0.00000000
H	3.25522600	-0.09226900	0.87738900
H	0.34937100	2.21713200	0.00000000
C	3.00902900	0.53155300	0.00000000
P	0.00539400	0.19278600	2.29199500
P	0.00539400	0.19278600	-2.29199500
C	1.64055500	0.18688500	-3.21843900
C	1.64055500	0.18688500	3.21843900
C	-1.17680000	-0.70633000	-3.45156500
C	-1.17680000	-0.70633000	3.45156500
O	-2.68777900	-1.26053800	0.00000000
C	-0.45526300	1.99800800	2.42537700
C	-0.45526300	1.99800800	-2.42537700
H	0.48913000	2.54898000	2.40124700
H	0.48913000	2.54898000	-2.40124700
H	-0.95742500	2.24319600	3.36262800
H	-0.95742500	2.24319600	-3.36262800
C	-1.29424700	2.39741200	1.22484900
C	-1.29424700	2.39741200	-1.22484900
H	-1.42546700	3.48896900	1.20030500
H	-1.42546700	3.48896900	-1.20030500
H	-2.29126400	1.95182500	1.27503900
H	-2.29126400	1.95182500	-1.27503900
H	2.26251900	0.77350300	-2.53593900
H	2.26251900	0.77350300	2.53593900
O	1.19209900	-2.76828600	0.00000000
H	-0.79016600	-0.52200400	4.45981700
H	-0.79016600	-0.52200400	-4.45981700
C	-1.15659100	-2.21357800	3.19046300
C	-1.15659100	-2.21357800	-3.19046300
H	-0.15099700	-2.63354800	3.21402500
H	-0.15099700	-2.63354800	-3.21402500
H	-1.59046600	-2.44804100	2.21764500
H	-1.59046600	-2.44804100	-2.21764500
H	-1.75039000	-2.72831200	3.95220600
H	-1.75039000	-2.72831200	-3.95220600
C	2.25089300	-1.20685300	-3.34676800
C	2.25089300	-1.20685300	3.34676800
H	1.71929700	-1.80986400	-4.08749500
H	1.71929700	-1.80986400	4.08749500
H	2.25201000	-1.75001300	-2.40145500
H	2.25201000	-1.75001300	2.40145500
H	3.28828400	-1.12514200	-3.68479700
H	3.28828400	-1.12514200	3.68479700
C	1.61014800	0.88708900	-4.57586900
C	1.61014800	0.88708900	4.57586900
H	1.24197200	1.91273500	-4.51706800
H	1.24197200	1.91273500	4.51706800
H	0.99474600	0.34782300	-5.30113900
H	0.99474600	0.34782300	5.30113900
H	2.62334000	0.92920100	-4.98764900

2Re-OCH₃

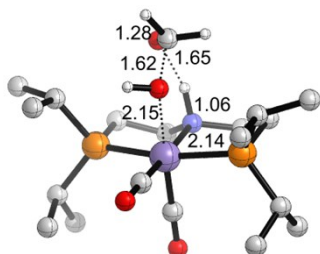
N	-0.52014000	2.02659500	0.00000000
H	3.35313500	-0.13247700	0.87962500
H	0.47428700	2.30083400	0.00000000
C	3.12595600	0.49383700	0.00000000
P	0.00412100	0.24677700	2.37737100
P	0.00412100	0.24677700	-2.37737100
C	1.64099300	0.18986400	-3.29525800
C	1.64099300	0.18986400	3.29525800
C	-1.24368800	-0.55175000	-3.53178300
C	-1.24368800	-0.55175000	3.53178300
O	-2.84129500	-1.30438100	0.00000000
C	-0.36013300	2.08303300	2.44545700
C	-0.36013300	2.08303300	-2.44545700
H	0.61390200	2.58068400	2.42960800
H	0.61390200	2.58068400	-2.42960800
H	-0.86369000	2.37626700	3.36838800
H	-0.86369000	2.37626700	-3.36838800
C	-1.16175100	2.51913700	1.22964700
C	-1.16175100	2.51913700	-1.22964700
H	-1.23900700	3.61505600	1.20432800
H	-1.23900700	3.61505600	-1.20432800
H	-2.17695700	2.11757100	1.26273300
H	-2.17695700	2.11757100	-1.26273300
H	2.27279000	0.76266300	-2.60827300
H	2.27279000	0.76266300	2.60827300
O	1.12542500	-3.00742000	0.00000000
H	-0.89423100	-0.32232900	4.54454800
H	-0.89423100	-0.32232900	-4.54454800
C	-1.26411100	-2.06917300	3.34612900
C	-1.26411100	-2.06917300	-3.34612900
H	-0.27994200	-2.52286700	3.46233800
H	-0.27994200	-2.52286700	-3.46233800
H	-1.63591500	-2.33305800	2.35536100
H	-1.63591500	-2.33305800	-2.35536100
H	-1.92997800	-2.52107900	4.08764700
H	-1.92997800	-2.52107900	-4.08764700
C	2.21263700	-1.22192700	-3.40017000
C	2.21263700	-1.22192700	3.40017000
H	1.68306700	-1.81407200	-4.15066000
H	1.68306700	-1.81407200	4.15066000
H	2.16873700	-1.75573700	-2.45021200
H	2.16873700	-1.75573700	2.45021200
H	3.26073900	-1.17387200	-3.70998700
H	3.26073900	-1.17387200	3.70998700
C	1.63720200	0.88182600	-4.65649800
C	1.63720200	0.88182600	4.65649800
H	1.28228200	1.91303800	-4.60797600
H	1.28228200	1.91303800	4.60797600
H	1.02106200	0.34570500	-5.38326300
H	1.02106200	0.34570500	5.38326300
H	2.65469700	0.90700300	-5.05856500

H 2.62334000 0.92920100 4.98764900	H 2.65469700 0.90700300 5.05856500
C -2.60962700 -0.17858800 3.39368400	C -2.65052400 0.02151900 3.36908100
H -2.68110400 0.87708900 3.66224600	H -2.69728000 1.09125200 3.58266200
H -3.04934000 -0.31650700 2.40460200	H -3.03780900 -0.15263400 2.36381000
H -3.22968700 -0.73474800 4.10347700	H -3.32771500 -0.47720700 4.06890800
C -2.60962700 -0.17858800 -3.39368400	C -2.65052400 0.02151900 -3.36908100
H -3.04934000 -0.31650700 -2.40460200	H -3.03780900 -0.15263400 -2.36381000
H -2.68110400 0.87708900 -3.66224600	H -2.69728000 1.09125200 -3.58266200
H -3.22968700 -0.73474800 -4.10347700	H -3.32771500 -0.47720700 -4.06890800
O 1.71038600 1.00558700 0.00000000	O 1.83304900 0.99394900 0.00000000
H 3.25522600 -0.09226900 -0.87738900	H 3.35313500 -0.13247700 -0.87962500
C -1.61861400 -0.79637300 0.00000000	C -1.75160100 -0.87212500 0.00000000
Mn -0.01089900 -0.10488000 0.00000000	Re -0.00420500 -0.16085000 0.00000000
C 0.72136500 -1.70984300 0.00000000	C 0.68937000 -1.92860700 0.00000000
H 3.72726700 1.36859000 0.00000000	H 3.85537800 1.31942500 0.00000000
Mn-TS(H₂O)	Re-TS(H₂O)
	
P -2.28593700 0.06638000 -0.21797100	P 2.37798200 0.01133700 0.26060800
P 2.29137400 0.05397600 -0.22708600	P -2.37409400 -0.00255100 0.30194800
C -2.41139900 -0.58603500 -1.95772200	C 2.45193200 -0.68564100 1.99326400
C 2.45127800 -0.69051400 -1.92967500	C -2.45351000 -0.77456000 2.00637000
H -2.37960300 0.29322800 -2.60671400	H 2.45786200 0.17988500 2.66149600
H 2.50373900 0.14827400 -2.63107300	H -2.52867300 0.04755800 2.72448000
H -3.34976300 -1.10864100 -2.15224300	H 3.37183300 -1.24621300 2.17198000
H 3.36338900 -1.27664700 -2.05512500	H -3.34673600 -1.39126500 2.12929500
C -1.19438300 -1.45339400 -2.24188800	C 1.21940000 -1.53301000 2.28140300
C 1.19956700 -1.50790900 -2.21426100	C -1.18675000 -1.57726600 2.27869800
H -1.16270400 -1.68371800 -3.31974300	H 1.19004400 -1.75790100 3.35948000
H 1.17237000 -1.75877700 -3.28756400	H -1.14437800 -1.81663300 3.35318700
H -1.29075100 -2.42211100 -1.72569100	H 1.29576300 -2.50064500 1.76499400
H 1.25293900 -2.46976400 -1.67889600	H -1.23301100 -2.54016800 1.74966100
N 0.01580200 -0.75959400 -1.83378700	N 0.00242300 -0.83548100 1.88085000
C 3.21364800 1.68389200 -0.48228700	C -3.28733400 1.62185500 0.62012300
C -3.15547700 1.72651700 -0.37097900	C 3.25847200 1.65336900 0.50140200
H 2.63376300 2.14408300 -1.29250700	H -2.81943800 1.95456100 1.55558300
H -2.42528700 2.28272300 -0.96693200	H 2.57546100 2.13446100 1.21007700
C 3.43285100 -0.93972800 0.89103800	C -3.55253200 -1.03749100 -0.72687100
C -3.44647400 -0.98022000 0.82989600	C 3.52645700 -1.05839500 -0.76495700
C 3.38469200 -2.44203300 0.61331800	C -3.23066200 -2.52829200 -0.63799200
C -3.42529900 -2.46153200 0.45515400	C 3.30297800 -2.54849500 -0.51185100
O -0.00258000 1.69389400 2.51595700	O -0.01609200 1.98517800 -2.54171900
H -4.44928500 -0.59061900 0.62093900	H 4.53778100 -0.80039100 -0.43123900
H 4.44344700 -0.58849000 0.65988900	H -4.53926700 -0.87823300 -0.27992300
C -3.16110600 -0.80561600 2.32223400	C 3.39877400 -0.74314300 -2.25502400
C 3.14277600 -0.65616900 2.36551800	C -3.58175500 -0.56785400 -2.17940200
H -3.18905100 0.23670700 2.63890200	H 3.58352800 0.30667400 -2.48184300
H 3.16727900 0.40713400 2.60554600	H -3.96288900 0.44960300 -2.28007000
H -2.18203800 -1.20709900 2.58473500	H 2.40259600 -0.99311500 -2.62233800
H 2.16163600 -1.03633300 2.65256400	H -2.58503000 -0.59943600 -2.62345100
H -3.90986200 -1.35152900 2.90475400	H 4.12319600 -1.33840500 -2.81913400
H 3.88933600 -1.15602700 2.99014000	H -4.23228100 -1.22219800 -2.76705200
C 3.15457200 2.62133400 0.72037500	C -3.01472200 2.69155900 -0.43276600
C -3.32853400 2.44528400 0.96496700	C 3.30790000 2.51731300 -0.75598100
H 3.75621500 2.24437400 1.55026500	H -3.40125800 2.41173500 -1.41419200

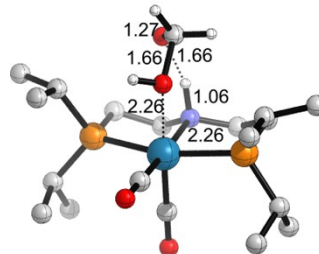
H	-4.11140600	1.98276900	1.57180400	H	4.05236700	2.15284700	-1.46779200
H	2.13632700	2.76594600	1.08100500	H	-1.94770800	2.88204200	-0.54636500
H	-2.40875000	2.46735700	1.54972200	H	2.34439100	2.56517600	-1.26280400
H	3.56080900	3.60069500	0.44975000	H	-3.50260400	3.62782800	-0.14453800
H	-3.63302500	3.48092400	0.78615500	H	3.59583900	3.53804700	-0.48692300
C	4.64630700	1.52815800	-0.99071500	C	-4.78065400	1.45959100	0.89367500
C	-4.48069100	1.67153600	-1.12951900	C	4.64022200	1.53573900	1.14091300
H	4.72209400	0.83957500	-1.83445400	H	-4.98832900	0.68844800	1.63961800
H	-4.36417500	1.31837900	-2.15517700	H	4.63063100	0.95902400	2.06773200
H	5.31497800	1.17346200	-0.20284600	H	-5.32908100	1.20730100	-0.01696300
H	-5.21356000	1.02916300	-0.63296500	H	5.36234800	1.07398400	0.46211000
H	5.03066000	2.49800100	-1.32112700	H	-5.19533200	2.40001800	1.26875100
H	-4.91765300	2.67395500	-1.17721700	H	5.02115200	2.53314600	1.38119000
H	0.00124700	0.67067700	-1.97659300	H	0.01562000	0.49886600	2.10333000
H	4.07748000	-2.95410000	1.28802100	H	-3.98914000	-3.09170000	-1.18980200
H	-4.14982600	-3.00162300	1.07229100	H	4.00116500	-3.12838500	-1.12285600
H	2.39173400	-2.85579800	0.79178700	H	-2.26194800	-2.76047700	-1.07956200
H	-2.44607900	-2.90717400	0.63791200	H	2.29333300	-2.85345000	-0.79164100
H	3.68295900	-2.68981700	-0.40657500	H	-3.23792900	-2.89643300	0.38962100
H	-3.69262600	-2.63564300	-0.58818600	H	3.47246000	-2.82724200	0.52962600
O	-0.14655400	1.63559400	-1.46055300	O	0.15141700	1.54249000	1.64224800
C	0.00074600	1.07442200	1.53580100	C	-0.01212000	1.26055400	-1.63122400
H	0.61158800	2.21518600	-1.56581300	H	-0.58675300	2.13451300	1.80585800
C	0.01148000	-1.39310000	0.97464600	C	-0.01966000	-1.36026300	-1.31443800
O	0.00243900	-2.39883100	1.55877900	O	-0.01599200	-2.26719700	-2.05240200
Mn	0.00702100	0.09114000	0.06419000	Re	-0.00592200	0.08768000	-0.12694600
2Mn-OH				2Re-OH			
							
N	0.90404900	-1.81262700	0.00000000	N	0.82638100	-1.91925400	0.00000000
H	-0.01483200	-2.27345300	0.00000000	H	-0.09351800	-2.38008900	0.00000000
P	-0.06281200	-0.22738600	2.27831400	P	-0.04760200	-0.27707200	2.36990000
P	-0.06281200	-0.22738600	-2.27831400	P	-0.04760200	-0.27707200	-2.36990000
C	-1.72427000	-0.54530100	-3.09558600	C	-1.70595900	-0.55992800	-3.20121300
C	-1.72427000	-0.54530100	3.09558600	C	-1.70595900	-0.55992800	3.20121300
C	0.88558000	0.84722300	-3.49755400	C	0.97675600	0.73829600	-3.56977900
C	0.88558000	0.84722300	3.49755400	C	0.97675600	0.73829600	3.56977900
O	2.42094000	1.66476700	0.00000000	O	2.53561100	1.75403000	0.00000000
C	0.71419400	-1.92202000	2.42241900	C	0.66953400	-2.00797400	2.44538000
C	0.71419400	-1.92202000	-2.42241900	C	0.66953400	-2.00797400	-2.44538000
H	-0.11234900	-2.63755000	2.39361800	H	-0.18659900	-2.68864900	2.43034300
H	-0.11234900	-2.63755000	-2.39361800	H	-0.18659900	-2.68864900	-2.43034300
H	1.24550300	-2.06952800	3.36401800	H	1.21882800	-2.19321500	3.37023300
H	1.24550300	-2.06952800	-3.36401800	H	1.21882800	-2.19321500	-3.37023300
C	1.62368300	-2.16162700	1.22907800	C	1.54600500	-2.28225600	1.23255200
C	1.62368300	-2.16162700	-1.22907800	C	1.54600500	-2.28225600	-1.23255200
H	1.95026300	-3.21137000	1.20438400	H	1.83086500	-3.34333000	1.20751900
H	1.95026300	-3.21137000	-1.20438400	H	1.83086500	-3.34333000	-1.20751900
H	2.52162800	-1.54115600	1.28778200	H	2.46542500	-1.69387000	1.26914700
H	2.52162800	-1.54115600	-1.28778200	H	2.46542500	-1.69387000	-1.26914700
H	-2.13721300	-1.27511300	-2.39101500	H	-2.14864400	-1.26820700	-2.49150300
H	-2.13721300	-1.27511300	2.39101500	H	-2.14864400	-1.26820700	2.49150300
O	-1.63764100	2.53712900	0.00000000	O	-1.67910700	2.74484100	0.00000000
H	0.52838000	0.55701000	4.49161100	H	0.66858600	0.41869600	4.57148000
H	0.52838000	0.55701000	-4.49161100	H	0.66858600	0.41869600	-4.57148000

C	0.56813200	2.32638900	3.27314300	C	0.67592100	2.22792900	3.40546300
C	0.56813200	2.32638900	-3.27314300	C	0.67592100	2.22792900	-3.40546300
H	-0.50108600	2.53794600	3.29770300	H	-0.38064200	2.46221900	3.53638800
H	-0.50108600	2.53794600	-3.29770300	H	-0.38064200	2.46221900	-3.53638800
H	0.94971500	2.66439100	2.30830600	H	0.97156400	2.57403300	2.41375500
H	0.94971500	2.66439100	-2.30830600	H	0.97156400	2.57403300	-2.41375500
H	1.04539500	2.93076200	4.05071600	H	1.23962200	2.80239600	4.14673700
H	1.04539500	2.93076200	-4.05071600	H	1.23962200	2.80239600	-4.14673700
C	-2.64417000	0.67270300	-3.10223300	C	-2.58487800	0.68785100	-3.22350800
C	-2.64417000	0.67270300	3.10223300	C	-2.58487800	0.68785100	3.22350800
H	-2.32085800	1.42146500	-3.82972600	H	-2.25079600	1.40478600	-3.97743200
H	-2.32085800	1.42146500	3.82972600	H	-2.25079600	1.40478600	3.97743200
H	-2.70235700	1.15228300	-2.12510500	H	-2.60209000	1.19371900	-2.25765200
H	-2.70235700	1.15228300	2.12510500	H	-2.60209000	1.19371900	2.25765200
H	-3.65602100	0.36761800	-3.38640400	H	-3.61234200	0.41070400	-3.47807500
H	-3.65602100	0.36761800	3.38640400	H	-3.61234200	0.41070400	3.47807500
C	-1.64336400	-1.17351900	-4.48464600	C	-1.62826600	-1.20640900	-4.58157800
C	-1.64336400	-1.17351900	4.48464600	C	-1.62826600	-1.20640900	4.58157800
H	-1.02274900	-2.07138500	-4.50918800	H	-1.03724300	-2.12456900	-4.58770800
H	-1.02274900	-2.07138500	4.50918800	H	-1.03724300	-2.12456900	4.58770800
H	-1.25246300	-0.47282800	-5.22765600	H	-1.20302100	-0.52630600	-5.32467400
H	-1.25246300	-0.47282800	5.22765600	H	-1.20302100	-0.52630600	5.32467400
H	-2.64555300	-1.46265100	-4.81651200	H	-2.63441500	-1.46565700	-4.92550000
H	-2.64555300	-1.46265100	4.81651200	H	-2.63441500	-1.46565700	4.92550000
C	2.39577600	0.61855000	3.45074800	C	2.47514200	0.47968800	3.42030900
H	2.67419100	-0.40909500	3.69202400	H	2.74477400	-0.56064100	3.61340200
H	2.80953200	0.86935900	2.47257200	H	2.82893600	0.75346100	2.42487300
H	2.88435300	1.26609700	4.18526300	H	3.02275100	1.09405300	4.14123000
C	2.39577600	0.61855000	-3.45074800	C	2.47514200	0.47968800	-3.42030900
H	2.80953200	0.86935900	-2.47257200	H	2.82893600	0.75346100	-2.42487300
H	2.67419100	-0.40909500	-3.69202400	H	2.74477400	-0.56064100	-3.61340200
H	2.88435300	1.26609700	-4.18526300	H	3.02275100	1.09405300	-4.14123000
O	-1.57075600	-1.26180500	0.00000000	O	-1.68318000	-1.31052200	0.00000000
C	1.44099200	1.03389200	0.00000000	C	1.53467100	1.14409900	0.00000000
Mn	-0.03672000	0.09450900	0.00000000	Re	-0.06556200	0.14273800	0.00000000
C	-1.00580300	1.56444800	0.00000000	C	-1.05595000	1.76089000	0.00000000
H	-2.44598900	-0.87134400	0.00000000	H	-2.56700600	-0.94069000	0.00000000
Mn-TS2-OH⁻				Re-TS2-OH⁻			
							
P	-2.27217600	-0.07571600	-0.06900200	P	-2.36424700	-0.02017400	-0.13538900
P	2.31389500	0.05627100	-0.07361900	P	2.39514100	0.10640500	-0.13827500
C	-2.45416800	0.49048000	-1.83569900	C	-2.47668900	0.56074000	-1.90872700
C	2.40380800	0.81805900	-1.77412700	C	2.42422700	0.88724300	-1.83876300
H	-2.51072800	1.58158100	-1.80148500	H	-2.55121500	1.65013500	-1.86673700
H	2.31761700	1.89949300	-1.63433800	H	2.35751100	1.96827600	-1.68348100
H	-3.35790100	0.11230000	-2.31541200	H	-3.36163500	0.17577800	-2.41780800
H	3.35252200	0.62811700	-2.27947300	H	3.35645700	0.69475100	-2.37356300
C	-1.20567500	0.09640400	-2.60647000	C	-1.21006600	0.18753300	-2.66300600
C	1.22704600	0.32575900	-2.59910300	C	1.22720400	0.42180400	-2.65356100
H	-1.21880800	0.55893900	-3.60278700	H	-1.22066600	0.65376100	-3.65723700
H	1.19208500	0.85339300	-3.56215800	H	1.19367000	0.95955100	-3.61049900
H	-1.14556400	-0.98662200	-2.74395000	H	-1.13186300	-0.89374300	-2.80037300

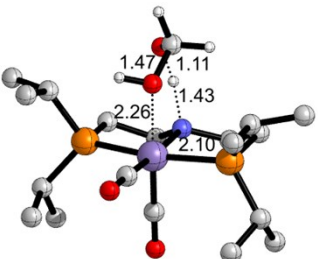
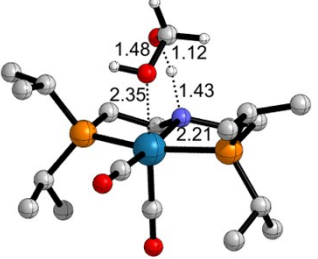
H	1.32224700	-0.74204100	-2.81372600	H	1.30291300	-0.64526300	-2.87658200
N	-0.02040200	0.53696700	-1.85332900	N	-0.02465500	0.64240900	-1.90820000
C	3.16559600	1.36435100	0.96904300	C	3.25457100	1.41700200	0.89103700
C	-3.17842200	1.29260200	0.84560700	C	-3.27691600	1.36404500	0.74735200
H	2.43607100	2.17645000	0.89742600	H	2.52247300	2.22864100	0.83146400
H	-2.55057700	2.15242200	0.59481600	H	-2.64781300	2.21914900	0.47883500
C	3.52514600	-1.38499100	-0.09976500	C	3.59173400	-1.33927500	-0.21418200
C	-3.38974900	-1.58121500	0.11099800	C	-3.48667600	-1.52112300	-0.00257900
C	3.51614100	-2.17072500	-1.41016800	C	3.49751400	-2.12641700	-1.52020400
C	-3.37623700	-2.50494100	-1.10640300	C	-3.37624200	-2.45991000	-1.20284800
O	0.06610100	-1.04553300	2.95509700	O	0.07006500	-1.14908900	3.10413200
H	-4.40189200	-1.17591600	0.21367900	H	-4.50483200	-1.11824700	0.02307400
H	4.51562600	-0.93116100	0.01454400	H	4.59016800	-0.89214000	-0.15409600
C	-3.04989800	-2.36819200	1.37715600	C	-3.22248300	-2.28245900	1.29579200
C	3.27965100	-2.32406200	1.08260300	C	3.39313300	-2.27055200	0.98194400
H	-3.04001300	-1.74683600	2.27299700	H	-3.30874200	-1.65234800	2.18139800
H	3.26779700	-1.80456600	2.04079700	H	3.45786500	-1.75164700	1.93811500
H	-2.06999500	-2.84060700	1.29255400	H	-2.22002400	-2.71288000	1.29414600
H	2.32717000	-2.84514000	0.97663000	H	2.41862700	-2.75826000	0.93516700
H	-3.78873800	-3.16091800	1.52959800	H	-3.94156400	-3.10093700	1.39685600
H	4.06932900	-3.08055700	1.12352300	H	4.16084100	-3.05016000	0.97174100
C	3.28111200	0.97435800	2.44051200	C	3.37572900	1.02399000	2.36102700
C	-3.16297600	1.11051500	2.36128800	C	-3.26530000	1.20919200	2.26621300
H	4.04151300	0.20499200	2.59682300	H	4.14956200	0.26796300	2.51553700
H	-3.83924400	0.31246900	2.67766000	H	-3.96873300	0.44122600	2.59679600
H	2.33751100	0.60884700	2.84683700	H	2.43546100	0.64061900	2.75874500
H	-2.16809700	0.87325500	2.74191200	H	-2.27886100	0.93785800	2.64746700
H	3.58269100	1.84606600	3.02906900	H	3.65883700	1.89925000	2.95314900
H	-3.50101500	2.02906500	2.85031700	H	-3.56858100	2.14725500	2.74060200
C	4.50990400	1.83908200	0.42288800	C	4.59258300	1.89266800	0.33147100
C	-4.59298500	1.56804500	0.34129400	C	-4.68847900	1.62966500	0.23003500
H	4.44827000	2.18749500	-0.60966100	H	4.52157800	2.23797100	-0.70180500
H	-5.27858600	0.74969600	0.57708600	H	-4.71776400	1.77543500	-0.85125700
H	5.27220000	1.05642900	0.47049000	H	5.35473000	1.10980400	0.37440200
H	-4.98800600	2.46536400	0.82755000	H	-5.37501900	0.81771400	0.48384600
H	4.87551300	2.67581300	1.02632600	H	4.96368500	2.73104300	0.92899100
H	-4.62693500	1.74160900	-0.73548300	H	-5.08489400	2.53949200	0.69100300
H	4.25985800	-2.97156900	-1.35659400	H	4.22866000	-2.94011400	-1.50427600
H	-4.06610300	-3.33693000	-0.93511300	H	-4.07256800	-3.29372400	-1.07221900
H	2.54830900	-2.64146600	-1.59061200	H	2.51236400	-2.57957500	-1.64331800
H	-2.38815600	-2.93454000	-1.27714200	H	-2.37517800	-2.88384900	-1.29101000
H	3.76906200	-1.55351600	-2.27411800	H	3.71439100	-1.51567900	-2.39864200
H	-3.69788800	-2.00296200	-2.02034000	H	-3.63166500	-1.97206300	-2.14520200
C	0.04884200	-0.71259100	1.84565100	C	0.05173500	-0.79372300	1.99676800
C	0.06549100	-1.87751800	-0.35358200	C	0.05574200	-1.98985200	-0.37423000
O	0.10234100	-2.99698400	-0.67054500	O	0.08880600	-3.11003200	-0.71313600
H	-0.19752400	1.94400000	1.59926200	H	-0.35466400	2.05189900	1.65644400
O	0.07884500	1.82339900	0.68771000	O	0.10070700	1.93574400	0.81914200
C	-0.25798800	3.46838000	-0.22718100	C	-0.19108300	3.51008800	-0.18666800
H	0.80565800	3.75040600	-0.14869900	H	0.89096400	3.72263700	-0.19500300
H	-0.87524100	3.87797400	0.59476100	H	-0.72229300	4.02299900	0.63577800
O	-0.76704600	3.22339800	-1.33048600	O	-0.78949600	3.23704500	-1.24092000
H	-0.13748900	1.55202300	-1.71014100	H	-0.15176600	1.66247800	-1.77024100
Mn	0.02618900	-0.20508000	0.15550900	Re	0.02302200	-0.19758200	0.19289600
3Mn⁺-O(H)CH₂O⁻				3Re⁺-O(H)CH₂O⁻			

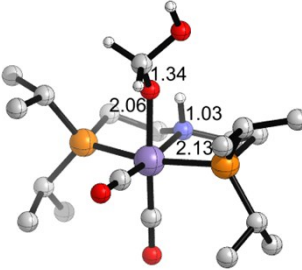
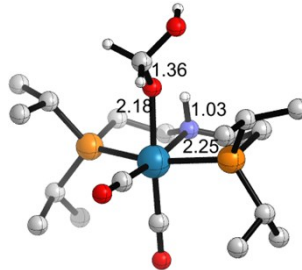


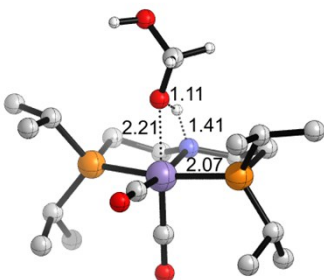
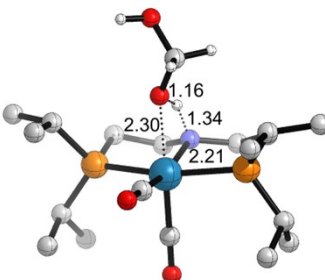
P	-2.28756200	-0.06117900	-0.09360100
P	2.31163300	0.06244500	-0.09334300
C	-2.46526400	0.28366100	-1.91512100
C	2.39794700	0.71046700	-1.83952600
H	-2.55987200	1.36807000	-2.00335300
H	2.31789700	1.79903100	-1.76947500
H	-3.34747900	-0.18420300	-2.35356700
H	3.34485400	0.48437800	-2.33377300
C	-1.19126700	-0.15211400	-2.61888900
C	1.21826400	0.16783900	-2.62809900
H	-1.19872100	0.21002800	-3.65632900
H	1.17625300	0.64587100	-3.61663200
H	-1.10683700	-1.24262700	-2.65260800
H	1.33168500	-0.90799300	-2.79391800
N	-0.03262500	0.39626500	-1.89785000
C	3.19581500	1.41740400	0.86222300
C	-3.20921400	1.40519600	0.63766500
H	2.48860900	2.24443700	0.75601800
H	-2.61638800	2.23154700	0.22872600
C	3.49994300	-1.39637200	-0.02726200
C	-3.39358600	-1.54213400	0.26928200
C	3.48379900	-2.26195200	-1.28610000
C	-3.36995100	-2.61231200	-0.82141500
O	0.07525500	-0.81000400	3.01717000
H	-4.40791600	-1.13217900	0.31215800
H	4.49467400	-0.94572600	0.05764500
C	-3.06150600	-2.15881100	1.62800300
C	3.24930300	-2.25679100	1.21248700
H	-3.06434100	-1.42810200	2.43751700
H	3.23441000	-1.67701400	2.13529700
H	-2.07799600	-2.63119300	1.61391500
H	2.29822100	-2.78521100	1.13704700
H	-3.79700200	-2.93073700	1.87410500
H	4.03922400	-3.00850800	1.30421000
C	3.32360300	1.11324800	2.35267500
C	-3.16068200	1.44985100	2.16347000
H	4.06842600	0.33693100	2.54499300
H	-3.82265100	0.70272500	2.60837500
H	2.37700000	0.79824600	2.79229800
H	-2.16004100	1.26960200	2.56411200
H	3.65358900	2.01190200	2.88218200
H	-3.49515600	2.42827200	2.52067600
C	4.54074900	1.83242900	0.27035500
C	-4.64208900	1.56995700	0.13588800
H	4.46960400	2.11962300	-0.78013700
H	-5.30524000	0.79044400	0.52045100
H	5.28934500	1.03996100	0.35495500
H	-5.04196800	2.52875500	0.47978500
H	4.92929600	2.69672500	0.81771400
H	-4.70519500	1.56595600	-0.95352200
H	4.22297100	-3.06208300	-1.18279000
H	-4.06166100	-3.41596100	-0.55094800



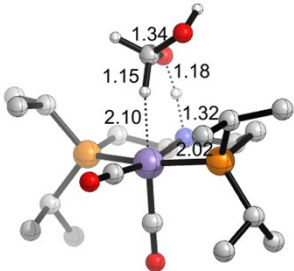
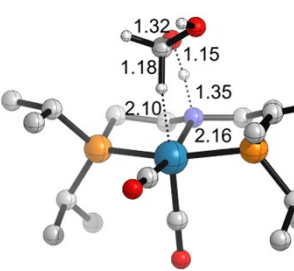
P	2.37296800	-0.01394500	0.15541600
P	-2.39193700	0.10012500	0.15581600
C	2.48123200	0.42849400	1.96655100
C	-2.42262200	0.79387100	1.89276700
H	2.56780100	1.51668100	2.00311700
H	-2.36620000	1.88177300	1.79154500
H	3.35732600	-0.00693200	2.44936800
H	-3.35257900	0.56645300	2.41797500
C	1.20303800	0.01586500	2.67999000
C	-1.22123900	0.29646500	2.68242000
H	1.20765600	0.41733700	3.70238400
H	-1.18292800	0.80167100	3.65685700
H	1.11948500	-1.07216400	2.74979200
H	-1.30767200	-0.77680300	2.87339400
N	0.03098500	0.53114900	1.94625300
C	-3.28260600	1.44504000	-0.80406800
C	3.28845300	1.43282200	-0.61663600
H	-2.58061500	2.27754800	-0.69652900
H	2.67636900	2.26609400	-0.25199600
C	-3.56866500	-1.36445700	0.16114700
C	3.49039900	-1.50359700	-0.09404100
C	-3.46053500	-2.21543300	1.42515800
C	3.37989200	-2.53297600	1.02959800
O	-0.07060000	-0.93625100	-3.16550100
H	4.50881600	-1.10094100	-0.08730700
H	-4.57188800	-0.92561600	0.12935000
C	3.22785800	-2.15974500	-1.44880800
C	-3.36927900	-2.23079600	-1.08268500
H	3.31575500	-1.46125500	-2.28153900
H	-3.44363500	-1.66377500	-2.01038200
H	2.22554400	-2.58925900	-1.48371700
H	-2.39170200	-2.71412900	-1.06723200
H	3.94717700	-2.96754900	-1.61368900
H	-4.13150300	-3.01538400	-1.10860000
C	-3.39092700	1.13319800	-2.29422300
C	3.25570100	1.41654400	-2.14337400
H	-4.14356200	0.36637100	-2.49296600
H	3.94931000	0.67775000	-2.55203000
H	-2.43988400	0.79941600	-2.71015900
H	2.26514200	1.18140300	-2.54049100
H	-3.69726300	2.03269300	-2.83612200
H	3.55843100	2.39190400	-2.53570100
C	-4.63300400	1.85245800	-0.22052600
C	4.71102800	1.63433800	-0.09997900
H	-4.57152900	2.13292500	0.83271900
H	4.75782200	1.67533000	0.98974900
H	-5.37608300	1.05634100	-0.31624300
H	5.38609900	0.84546900	-0.44208000
H	-5.02191400	2.71810700	-0.76526200
H	5.10813200	2.58169500	-0.47693400
H	-4.18461000	-3.03378000	1.37105100
H	4.07481000	-3.35495800	0.83309900

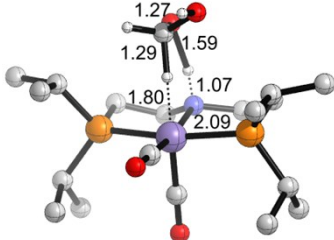
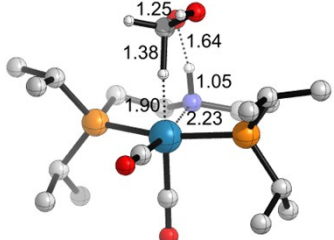
H	2.51322100	-2.73719900	-1.43642600
H	-2.38139400	-3.05940500	-0.93125000
H	3.73933700	-1.70104400	-2.18668400
H	-3.68528400	-2.22986200	-1.79338000
C	0.05036600	-0.54342000	1.89121300
C	0.05457800	-1.86271700	-0.21337800
O	0.09046800	-3.00178300	-0.44405400
H	-0.54410000	2.07244200	1.37541400
O	0.09732100	1.92974700	0.67548900
C	-0.05890500	3.17621200	-0.34274400
H	1.01975800	3.33745900	-0.55000000
H	-0.40869100	3.96201300	0.35847700
O	-0.81708900	2.89703600	-1.33831600
H	-0.22125200	1.43326500	-1.81174700
Mn	0.02116200	-0.15797100	0.16411700
Mn-TS2-H⁺			
			
P	2.30325000	-0.04832200	-0.10244700
P	-2.29253300	0.05408500	-0.10621400
C	2.41176300	-0.69484000	-1.84396500
C	-2.47454800	-0.29859300	-1.92298300
H	2.39139000	-1.78582200	-1.77452600
H	-2.63508700	-1.37485300	-2.01101600
H	3.34196700	-0.41892400	-2.34474700
H	-3.32943800	0.21069900	-2.36937700
C	1.18989300	-0.20942900	-2.60731200
C	-1.16737600	0.07556300	-2.60654300
H	1.15180200	-0.71796700	-3.58463700
H	-1.17345800	-0.33178400	-3.63054700
H	1.30050500	0.86458600	-2.82903400
H	-1.09502500	1.16967700	-2.71288100
N	-0.03364100	-0.45833700	-1.85655000
C	-3.25516000	-1.38614400	0.64005900
C	3.24340200	-1.35642400	0.87355900
H	-2.69717400	-2.23854400	0.23532700
H	2.56903500	-2.21418800	0.80536400
C	-3.37153300	1.55379400	0.26928000
C	3.44409500	1.44999800	-0.02461400
C	-3.37968500	2.60403800	-0.84118300
C	3.43748400	2.29945100	-1.29462900
O	0.06550000	0.76051800	3.01956700
H	4.44791400	1.02649400	0.08915900
H	-4.38715300	1.15454100	0.35559100
C	3.14635300	2.31935400	1.19837100
C	-2.98759700	2.19173000	1.60424600
H	3.11660900	1.75089400	2.12763700
H	-2.96003800	1.47507500	2.42575800
H	2.18998000	2.83183000	1.09241400
H	-2.00498800	2.66210000	1.54604300
H	3.92176600	3.08489200	1.30066000
H	-3.71316500	2.96863600	1.86406200
C	-3.19886300	-1.42526300	2.16613400
C	3.39005000	-1.01147100	2.35363200
H	-2.47115300	-2.66531300	1.52164700
H	2.37866900	-2.96132100	1.08775600
H	-3.67873800	-1.65154300	2.33390600
H	3.63787700	-2.12003600	2.00630500
C	-0.04994300	-0.64730800	-2.03970800
C	-0.04559000	-1.98954500	0.25007600
O	-0.07316500	-3.12910600	0.51210100
H	0.55272600	2.16903200	-1.47869000
O	-0.09242200	2.01809300	-0.78298100
C	0.04378700	3.29039100	0.27028400
H	-1.04198400	3.41912400	0.45231100
H	0.39626400	4.06588600	-0.43814300
O	0.78976200	3.01008900	1.26516900
H	0.20098700	1.56803700	1.83362400
Re	-0.01892800	-0.16820500	-0.19808500
Re-TS2-H⁺			
			
P	2.37879300	-0.01454900	0.17359200
P	-2.38913800	0.07888300	0.16632400
C	2.48763300	0.45731100	1.97386300
C	-2.43665700	0.79754100	1.88821800
H	2.63476900	1.53909100	1.99954200
H	-2.44133600	1.88528000	1.77255500
H	3.33793400	-0.01057400	2.47261600
H	-3.34824600	0.52844600	2.42627700
C	1.17557400	0.10898300	2.66514200
C	-1.19431400	0.36912700	2.65741200
H	1.17643800	0.56435500	3.66816900
H	-1.15794600	0.92484400	3.60790900
H	1.10564700	-0.97884400	2.81641300
H	-1.28243800	-0.69478000	2.92640700
N	0.03034800	0.59801200	1.89407500
C	-3.34074900	1.36623800	-0.82311800
C	3.33161600	1.40128500	-0.62470200
H	-2.68561400	2.23801600	-0.73204000
H	2.75977900	2.26148600	-0.25610500
C	-3.51891300	-1.42351300	0.19365400
C	3.47699200	-1.52258400	-0.05392100
C	-3.37981300	-2.25373100	1.46865700
C	3.34411000	-2.53775500	1.08056300
O	-0.05182000	-0.84654400	-3.18528400
H	4.50032800	-1.13323500	-0.04010100
H	-4.53408000	-1.01292900	0.16534000
C	3.22151000	-2.18938100	-1.40481400
C	-3.30975400	-2.30147100	-1.04052300
H	3.33041300	-1.50168700	-2.24407800
H	-3.39611000	-1.74805200	-1.97524300
H	2.21404400	-2.60517900	-1.44913700
H	-2.32613900	-2.77152000	-1.02337900
H	3.93137400	-3.00903800	-1.55130000
H	-4.06055100	-3.09747900	-1.05317800
C	-3.43851900	1.02859500	-2.30852600
C	3.27634300	1.38486100	-2.15127700

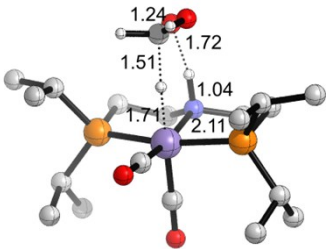
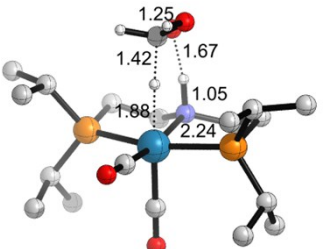
H -3.82479100 -0.64576200 2.60696700	H -4.16035100 0.22945000 -2.49203900
H 4.11260900 -0.20664100 2.50926400	H 3.93753500 0.62069300 -2.56591300
H -2.18959100 -1.28205600 2.56136900	H -2.47668900 0.72479700 -2.72268000
H 2.44288000 -0.71474900 2.80490600	H 2.27402400 1.17847400 -2.53592500
H -3.57455000 -2.38462400 2.53447400	H -3.78295400 1.90593300 -2.86400500
H 3.76073700 -1.88447500 2.89914000	H 3.60863400 2.34708700 -2.55268700
C -4.69533700 -1.51493000 0.14729700	C -4.70687600 1.72566800 -0.24336400
C 4.59033100 -1.74594300 0.26776200	C 4.76690900 1.56205100 -0.12854500
H -4.76554200 -1.49949000 -0.94153200	H -4.65617800 2.01439100 0.80817800
H 4.50963600 -2.05922100 -0.77441200	H 4.83110500 1.58448500 0.96089800
H -5.33442100 -0.72096900 0.54175300	H -5.41612600 0.89900600 -0.33336500
H 5.31316300 -0.92734300 0.31906100	H 5.41365900 0.75966300 -0.49204600
H -5.11822900 -2.46486900 0.48861400	H -5.13094000 2.57024300 -0.79512000
H 5.01716100 -2.58287900 0.82922800	H 5.18435400 2.50299400 -0.49977800
H -4.04867900 3.42150200 -0.55518600	H -4.08039000 -3.09322600 1.42796700
H 4.15469400 3.11829900 -1.18215200	H 4.03288300 -3.36843800 0.89923400
H -2.39089500 3.03401900 -1.00231500	H -2.37740800 -2.67192500 1.56817000
H 2.45953500 2.74711500 -1.47569700	H 2.33838000 -2.95466000 1.13523700
H -3.74104600 2.20878600 -1.79146900	H -3.60879700 -1.68326800 2.37019400
H 3.72716100 1.73405000 -2.18152800	H 3.59616800 -2.11566700 2.05460400
O 0.05857300 -2.06555600 0.73978600	C -0.03569100 -0.57808200 -2.05304800
C 0.04079800 0.48527900 1.89410200	C -0.03210100 -1.96230700 0.20709600
C 0.10388300 -3.12183800 -0.27951800	O -0.05208800 -3.10793400 0.44026600
H -0.18092400 -4.06554200 0.20302100	H 0.74904200 2.27734700 -1.33360700
H 1.17468000 -3.16585200 -0.52658200	O -0.04698900 2.13216000 -0.81224200
C 0.03419400 1.81071400 -0.22745300	C -0.13279400 3.19812400 0.21074100
O 0.05938100 2.94219200 -0.49135600	H -1.20438500 3.19251700 0.45406000
Mn 0.01187200 0.11557600 0.15925600	H 0.11376100 4.14289800 -0.28828500
O -0.69232600 -2.84624500 -1.32961100	O 0.67333300 2.96103200 1.25666300
H -0.35843700 -1.83913000 -1.66834900	H 0.34418200 1.96695700 1.64825900
H -0.74457100 -2.18254500 1.25597700	Re -0.01135400 -0.13939300 -0.19220700
2Mn-OCH₂OH	
	
P -2.33791100 0.00873900 0.17129900	P 2.41446600 0.02684900 0.22915100
P 2.25380800 0.16239200 0.14458100	P -2.34548900 -0.13860800 0.20673100
C -2.46774000 0.11479000 2.03228800	C 2.47898200 0.00600600 2.10227300
C 2.38561100 0.22552600 2.00487600	C -2.41639300 -0.13642300 2.07836400
H -2.42173800 -0.91539900 2.39626900	H 2.43637600 1.05326500 2.41555500
H 2.38385800 -0.81695400 2.33623200	H -2.43717600 0.91738200 2.37194700
H -3.41262100 0.54306400 2.37056500	H 3.41186000 -0.41163300 2.48512800
H 3.31341800 0.68357800 2.35180700	H -3.32611700 -0.60096000 2.46311600
C -1.28144300 0.89043700 2.57931800	C 1.28094900 -0.73626600 2.67493500
C 1.17127800 0.93639200 2.57645700	C -1.18243400 -0.80035700 2.66961100
H -1.25115200 0.81260100 3.67559100	H 1.25008900 -0.61459000 3.76655300
H 1.15464500 0.83784500 3.67134300	H -1.16769900 -0.66424300 3.75988700
H -1.35678500 1.95230500 2.33049000	H 1.34373800 -1.80596500 2.46385300
H 1.19511500 2.00457700 2.34601100	H -1.18112200 -1.87422900 2.47138400
N -0.04555200 0.36622100 1.98914900	N 0.03664900 -0.22947500 2.07116200
C 3.25540800 -1.37943800 -0.23236600	C -3.34407500 1.39868100 -0.18871500
C -3.16350500 -1.65049900 -0.13685700	C 3.24469700 1.67195000 -0.12779300
H 2.63515500 -2.16151900 0.21666700	H -2.71383200 2.18560300 0.23953300
H -2.46248300 -2.31139100 0.38152600	H 2.52536700 2.35319000 0.33875600
2Re-OCH₂OH	
	

C	3.33789200	1.57216500	-0.47838600
C	-3.56142500	1.28145000	-0.48137100
C	3.22581200	2.84980300	0.35183300
C	-3.54164100	2.59844600	0.29361800
O	-0.02819800	-0.45788300	-2.98665700
H	-4.55022600	0.82848800	-0.35163600
H	4.36454100	1.20182200	-0.38658400
C	-3.33349900	1.53899600	-1.97187000
C	3.05993400	1.86896600	-1.95287400
H	-3.33742300	0.62384600	-2.56431500
H	3.12517800	0.98106500	-2.58176400
H	-2.37846400	2.03848300	-2.14097000
H	2.06596500	2.29725800	-2.08583700
H	-4.12277800	2.19017800	-2.35992400
H	3.78760100	2.59599000	-2.32674300
C	3.37591900	-1.66685600	-1.72757600
C	-3.18661200	-2.04884900	-1.60994200
H	4.07864600	-0.98648800	-2.21606400
H	-3.91729900	-1.46460900	-2.17493900
H	2.41883200	-1.59638600	-2.24548300
H	-2.21311400	-1.92896200	-2.08520400
H	3.75840900	-2.68148000	-1.87378300
H	-3.47681100	-3.09975200	-1.70260000
C	4.62887900	-1.42329300	0.43530300
C	-4.54702500	-1.80294300	0.49124300
H	4.57821000	-1.28410000	1.51656500
H	-4.55848200	-1.56430800	1.55647700
H	5.31312800	-0.67402400	0.02713900
H	-5.29233200	-1.17480700	-0.00409300
H	5.08528000	-2.40208100	0.25802700
H	-4.88470500	-2.83876700	0.38699900
H	-0.02444500	-0.65851600	2.08787100
H	3.90378600	3.60656500	-0.05477100
H	-4.28691200	3.27887700	-0.12955600
H	2.21845400	3.26750300	0.31614200
H	-2.57274400	3.09466600	0.21997800
H	3.50287100	2.69761700	1.39669600
H	-3.78670200	2.46965500	1.34956000
O	-0.06973300	-1.76316100	0.60872100
C	-0.03751600	-0.22261600	-1.85255600
C	-0.11003900	1.87002900	-0.47982900
O	-0.16260600	3.00936700	-0.71634700
Mn	-0.04849700	0.15831700	-0.12911100
C	0.16943200	-2.94914400	0.02988300
H	0.57606200	-2.85446100	-0.99438200
O	1.13463800	-3.67753500	0.83209500
H	-0.73991300	-3.58737000	-0.03202800
H	1.10969900	-4.59953300	0.55462800
Mn-TS(HOCH₂OH)			
			
P	2.28132700	-0.15223200	0.12339000
P	-2.31177100	-0.03894100	0.13891300
C	-3.42270200	-1.58017100	-0.33311400
C	3.62781600	-1.29271300	-0.32639000
C	-3.21622200	-2.83301100	0.51618900
C	3.51242900	-2.58077800	0.48720800
O	0.02243000	0.39435700	-3.18923000
H	4.62302600	-0.86678200	-0.15758800
H	-4.45342900	-1.23708600	-0.19163900
C	3.45931500	-1.58876800	-1.81677100
C	-3.20743500	-1.89778800	-1.81303700
H	3.55517000	-0.69835000	-2.43800700
H	-3.36033100	-1.03192600	-2.45701000
H	2.48071000	-2.02780400	-2.01534200
H	-2.19656800	-2.26755700	-1.98827100
H	4.22214000	-2.30418300	-2.13841800
H	-3.90974700	-2.67590500	-2.12727700
C	-3.46236100	1.65685500	-1.68950700
C	3.30144900	1.99926500	-1.61772000
H	-4.18991300	0.98918100	-2.15825800
H	4.06516200	1.40979700	-2.13084000
H	-2.50951200	1.53862800	-2.20742600
H	2.34572600	1.82625100	-2.11311100
H	-3.80766700	2.68091400	-1.85663300
H	3.56387900	3.05251200	-1.75356600
C	-4.71395500	1.45903200	0.48404300
C	4.61056400	1.85511900	0.52906500
H	-4.66092700	1.33153800	1.56712500
H	4.59327300	1.67117900	1.60520400
H	-5.40123300	0.70690900	0.08691000
H	5.36511100	1.19941100	0.08638300
H	-5.16663800	2.43723400	0.29632100
H	4.95564600	2.88292200	0.38051400
H	0.00900600	0.79423800	2.16630500
H	-3.88080100	-3.62541100	0.15902700
H	4.24930800	-3.30406000	0.12553800
H	-2.19441700	-3.20721600	0.43504500
H	2.52774100	-3.03712300	0.37362200
H	-3.44804900	-2.67014100	1.57069600
H	3.70728600	-2.42724500	1.55046600
O	0.04668500	1.90641500	0.58540300
C	0.03030600	0.18552100	-2.04503000
C	0.10378700	-1.98890800	-0.52616500
O	0.15221100	-3.14119200	-0.73345500
Re	0.04093000	-0.14050000	-0.17380400
C	-0.22164100	3.06981600	-0.07049600
H	-0.68002200	2.92190700	-1.05667200
O	-1.16928000	3.88110100	0.63551400
H	0.69848300	3.67041100	-0.21062800
H	-0.79969200	4.02232200	1.51320600
Re-TS(HOCH₂OH)			
			
P	2.39005700	-0.10084800	0.20152300
P	-2.38173600	-0.01958100	0.19794000

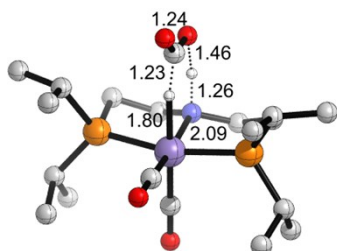
C	2.43277300	0.11045600	1.96061900	C	2.47119900	0.24091900	2.03737900
C	-2.44586600	0.26823900	1.97076100	C	-2.43570300	0.44993800	2.00571600
H	2.49565400	1.19222600	2.10586000	H	2.55216500	1.32653500	2.13830500
H	-2.45961000	1.35451100	2.10355000	H	-2.42881400	1.54385200	2.03908900
H	3.33822200	-0.33302300	2.37872200	H	3.35666300	-0.20073600	2.49882300
H	-3.37088400	-0.12334200	2.39879400	H	-3.35512400	0.11848800	2.49342300
C	1.17387200	-0.41660500	2.63370900	C	1.19523000	-0.23447600	2.71950100
C	-1.21533000	-0.31749500	2.64775700	C	-1.20479200	-0.08630200	2.72402000
H	1.15742700	-0.06769300	3.67925500	H	1.17622700	0.15715300	3.74846800
H	-1.16988400	0.05077500	3.68589100	H	-1.16078900	0.35522400	3.73197000
H	1.20150200	-1.51685000	2.68052400	H	1.19603700	-1.33043800	2.80328300
H	-1.31565300	-1.41220800	2.71914700	H	-1.30055900	-1.17153700	2.86595300
N	-0.00902000	0.04745000	1.92483700	N	0.01624400	0.21816200	1.98683300
C	-3.24445400	1.45620200	-0.53497000	C	-3.40374500	1.36785500	-0.57095800
C	3.22419200	1.34171900	-0.52663100	C	3.36083200	1.36818900	-0.45958400
H	-2.67218100	2.27417700	-0.08858200	H	-2.84229400	2.25200400	-0.25401500
H	2.60967400	2.14662200	-0.11259400	H	2.80254000	2.18770200	0.00439900
C	-3.46585000	-1.48413600	-0.20927500	C	-3.48417900	-1.53507400	0.06332800
C	3.38477700	-1.61916400	-0.28574500	C	3.48418200	-1.60030200	-0.06917900
C	-3.35403000	-2.61123600	0.81670000	C	-3.19628400	-2.56912500	1.15000900
C	3.28443700	-2.75529900	0.73135000	C	3.19287100	-2.71987600	0.92902200
O	-0.02511900	-0.07802000	-3.06066000	O	-0.00484300	0.05684100	-3.25809800
H	4.40615500	-1.22595400	-0.24856900	H	4.50380500	-1.24212800	0.10873300
H	-4.47411400	-1.06515500	-0.13215800	H	-4.49929100	-1.15591400	0.22184100
C	3.11410700	-2.13934700	-1.69831300	C	3.38427800	-2.11063200	-1.50561100
C	-3.26898800	-2.02542300	-1.62551900	C	-3.40898700	-2.16800100	-1.32563800
H	3.15599700	-1.35508700	-2.45440600	H	3.72261500	-1.37360400	-2.23476900
H	-3.36219500	-1.25416500	-2.39027600	H	-3.58805200	-1.45054800	-2.12642000
H	2.13126200	-2.60811300	-1.76194000	H	2.35867600	-2.38411700	-1.75720100
H	-2.28687700	-2.48610500	-1.73775600	H	-2.43378800	-2.62364600	-1.49781400
H	3.85972100	-2.89587900	-1.96169100	H	4.00728000	-3.00227300	-1.62318800
H	-4.02075300	-2.79273700	-1.83425200	H	-4.16524400	-2.95427400	-1.40999200
C	-3.16736900	1.61461900	-2.05086000	C	-3.40408300	1.35211500	-2.09804300
C	3.21860500	1.46965000	-2.04715100	C	3.26886000	1.54334600	-1.97205800
H	-3.78069500	0.87162500	-2.56530600	H	-4.06007300	0.57336000	-2.49269300
H	3.86999700	0.72849200	-2.51666200	H	3.83731400	0.78040700	-2.50802400
H	-2.14772300	1.52646300	-2.42458600	H	-2.40718100	1.19305100	-2.50929500
H	2.22026100	1.35972200	-2.46990500	H	2.23876700	1.50319600	-2.32482700
H	-3.55008600	2.59841900	-2.33967500	H	-3.77684300	2.30847800	-2.47682200
H	3.60025300	2.45412100	-2.33618900	H	3.68980600	2.51271900	-2.25771800
C	-4.68610000	1.58043300	-0.04335900	C	-4.82275300	1.49385100	-0.01967500
C	4.64157600	1.47792500	0.02596100	C	4.80810400	1.42824800	0.02328400
H	-4.77859500	1.43800600	1.03526500	H	-4.85171500	1.52228000	1.07148000
H	4.67703600	1.41925200	1.11528900	H	4.90491700	1.23827700	1.09445300
H	-5.34598100	0.86404000	-0.53834400	H	-5.46045600	0.67261800	-0.35561800
H	5.31225700	0.71436900	-0.37681600	H	5.43856400	0.71037700	-0.50764900
H	-5.06983000	2.57855500	-0.27602100	H	-5.27815800	2.42019200	-0.38280900
H	5.05680500	2.44880800	-0.26232000	H	5.22329700	2.42218300	-0.16976200
H	0.09955000	1.34331300	1.38244600	H	0.13346500	1.44382400	1.44885800
H	-4.08446700	-3.38946500	0.57484200	H	-3.82287100	-3.45044100	0.98310700
H	3.96968700	-3.55859100	0.44350100	H	3.87491300	-3.55478500	0.74255100
H	-2.36797000	-3.07546100	0.80451000	H	-2.15794700	-2.90142200	1.12930000
H	2.28083800	-3.18058700	0.76482300	H	2.17625500	-3.09999100	0.82379500
H	-3.56431400	-2.27478000	1.83321700	H	-3.42222600	-2.19416200	2.14983000
H	3.55882900	-2.44060000	1.73948600	H	3.33953900	-2.40561900	1.96383400
O	0.23108300	1.91828300	0.44570500	O	0.26012000	2.02875600	0.45570000
C	-0.02352300	-0.10613500	-1.90175200	C	-0.00111800	-0.03707400	-2.09818500
C	-0.27077500	3.21017200	0.33785400	C	-0.38503300	3.24170900	0.24953900
H	-0.62803000	3.37321500	-0.68537100	H	-0.67270100	3.30643400	-0.80711900
H	-1.09747900	3.38617300	1.03696400	H	-1.27915600	3.33134800	0.87865200

C	-0.06285900	-1.93441900	-0.17678700
O	-0.07603900	-3.09724000	-0.19658300
Mn	-0.02277900	-0.19589900	-0.13103900
O	0.70322400	4.18604900	0.66125000
H	1.35511600	4.21229800	-0.04488700
Mn-TS3-H⁺			
			
O	0.08291900	-3.08609000	0.19537800
P	2.33145300	-0.03088700	0.10325200
P	-2.27337200	-0.09196800	0.08423800
C	2.49636600	0.38536000	1.90909300
C	-2.39347600	0.63182600	1.79064600
H	2.60332300	1.47056800	1.96490000
H	-2.36962900	1.71630300	1.65156600
H	3.37357800	-0.06868800	2.37186400
H	-3.32540100	0.37707900	2.29954800
C	1.20980600	-0.02352700	2.60764100
C	-1.17696200	0.19771100	2.58902000
H	1.16742900	0.45759500	3.59610500
H	-1.11799700	0.79051800	3.51430000
H	1.19001600	-1.10676500	2.78375200
H	-1.27380600	-0.85166500	2.89640700
N	0.04803900	0.37836900	1.80315800
C	-3.25527700	1.15049300	-0.92935200
C	3.21533300	1.43640100	-0.68003200
H	-2.64512000	2.05117000	-0.81101000
H	2.63371900	2.26760300	-0.26847100
C	-3.35422300	-1.63290500	0.10176900
C	3.47581200	-1.49245700	-0.20721200
C	-3.20400400	-2.46857800	1.37180300
C	3.43226400	-2.54629600	0.89875000
O	0.05596200	-0.49645600	-3.04792500
H	4.48155800	-1.06056400	-0.21616300
H	-4.37773400	-1.24388200	0.07773600
C	3.20861200	-2.12913900	-1.57102700
C	-3.13762100	-2.49707200	-1.14141800
H	3.23681600	-1.40710500	-2.38752900
H	-3.22280000	-1.93197300	-2.06926100
H	2.23314400	-2.61673200	-1.59397500
H	-2.15600900	-2.97083600	-1.12817700
H	3.96546400	-2.89229000	-1.77586000
H	-3.88757700	-3.29358900	-1.16804300
C	-3.33660700	0.82146500	-2.41818200
C	3.10910600	1.49067300	-2.20115600
H	-4.02801900	-0.00145900	-2.61567300
H	3.71761200	0.71846700	-2.67745600
H	-2.36777000	0.56421900	-2.84594500
H	2.08293600	1.37432500	-2.54970800
H	-3.71479100	1.69342000	-2.95986400
H	3.47719900	2.45603100	-2.56115600
C	-4.64350400	1.44975700	-0.36523900
C	4.66247000	1.61159600	-0.22239600
C	-0.04571500	-2.02117400	-0.35488700
O	-0.05850200	-3.18658500	-0.45026500
Re	-0.00041900	-0.15885400	-0.19464100
O	0.41653200	4.34002600	0.62155200
H	1.07792300	4.47218000	-0.06507800
Re-TS3-H⁺			
			
O	0.08355900	-3.21153200	-0.25820000
P	2.41140200	0.01410000	0.17668200
P	-2.36775200	-0.07639900	0.18076700
C	2.49297300	0.50477000	1.97374500
C	-2.43231800	0.57329700	1.92537200
H	2.55777600	1.59519300	1.99496100
H	-2.46102600	1.66340200	1.84108000
H	3.37984500	0.10488000	2.46915400
H	-3.33492900	0.25468100	2.45155400
C	1.21935800	0.07012600	2.68233500
C	-1.18038500	0.16045200	2.68174900
H	1.16788000	0.57259400	3.65935300
H	-1.12825700	0.72888000	3.62192400
H	1.23613800	-1.00886800	2.88160100
H	-1.22874400	-0.90071300	2.95703000
N	0.02979400	0.41279800	1.88775100
C	-3.39717200	1.21144900	-0.71929100
C	3.34226400	1.44610800	-0.61706800
H	-2.84652500	2.12108800	-0.45670400
H	2.76937700	2.29731400	-0.23231800
C	-3.41546400	-1.63417800	0.19773900
C	3.54802300	-1.47165200	0.02242300
C	-3.06331500	-2.56534200	1.35615200
C	3.28631500	-2.51600000	1.10659400
O	0.03156500	-0.18113500	-3.26312100
H	4.55605300	-1.07170400	0.17480900
H	-4.43898400	-1.27637500	0.35251400
C	3.47008400	-2.09885500	-1.36820400
C	-3.35143200	-2.37510400	-1.13690600
H	3.70868400	-1.39106400	-2.16241800
H	-3.65967900	-1.75279300	-1.97697200
H	2.47392200	-2.49732300	-1.56470600
H	-2.34317200	-2.73680500	-1.34095700
H	4.18134600	-2.92720100	-1.43799600
H	-4.01692800	-3.24305300	-1.10633700
C	-3.37951500	1.08022600	-2.23992100
C	3.25792700	1.47983600	-2.14004700
H	-3.99793700	0.24951300	-2.58674300
H	3.87760900	0.70607000	-2.59776100
H	-2.37295100	0.93657000	-2.63229100
H	2.23741200	1.34717900	-2.49875000
H	-3.78953100	1.99031500	-2.68870800
H	3.62474000	2.44293600	-2.50763700
C	-4.82421900	1.34763100	-0.19216600
C	4.78367400	1.59736800	-0.13523000

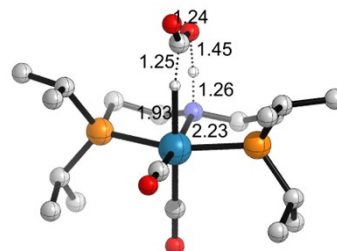
H -4.61836900 1.73568000 0.68767100 H 4.76838300 1.57630300 0.86364600 H -5.32525800 0.60160200 -0.47251400 H 5.32043500 0.85345900 -0.65445100 H -5.08457200 2.28502800 -0.91757600 H 5.03568800 2.58484000 -0.55501500 H -0.09488300 1.86197000 -0.43729100 H 0.21642800 1.67401100 1.63534800 C 0.05312200 2.88666100 0.06080200 H -3.88865200 -3.32099000 1.32524400 H -2.19499200 -2.86947100 1.47680000 H -3.44838800 -1.90546200 2.27398000 H 4.15099300 -3.33811400 0.66681000 H 3.70245700 -2.14137100 1.87515000 H 2.45048900 -3.01301400 0.97928800 O 0.43687800 2.79512400 1.33734500 C 0.06471200 -1.93337000 0.05085000 Mn 0.03421600 -0.20971500 -0.13002900 C 0.04466900 -0.36557900 -1.89782600 H 0.78956800 3.40494400 -0.57277400 O -1.21208000 3.53062300 -0.10689800 H -1.25139500 4.17221800 0.61166100	H -4.86364500 1.46566400 0.89258700 H 4.86748400 1.58469900 0.95342500 H -5.44438600 0.49006300 -0.46586500 H 5.42711600 0.81052200 -0.53635100 H -5.29240200 2.23366500 -0.63138300 H 5.19035000 2.55160500 -0.48309900 H 0.00251200 1.91119000 -0.33942500 H 0.11225700 1.74849600 1.74300400 C 0.04796800 2.97181600 0.18128000 H -3.71709500 -3.44213900 1.32555200 H -2.03544100 -2.92363700 1.28874200 H -3.20248100 -2.09053400 2.32889200 H 3.99606300 -3.34044000 0.99019900 H 3.41714500 -2.11557000 2.11330800 H 2.28351500 -2.93676900 1.02946400 O 0.24586400 2.86542600 1.48203600 C 0.06079800 -2.04400000 -0.23286600 Re 0.02732700 -0.18011100 -0.18874400 C 0.02870000 -0.20082000 -2.10024600 H 0.86691100 3.47616800 -0.35884700 O -1.17572200 3.62050500 -0.12683400 H -1.12058700 3.95667000 -1.02781000
3Mn⁺-HCH(OH)O⁻  O 0.05389500 -3.07305400 -0.12815200 P 2.31859000 -0.03807300 0.10799500 P -2.27581100 -0.08251600 0.10836000 C 2.48566000 0.16869300 1.95240500 C -2.39889300 0.35195600 1.91370300 H 2.54966400 1.24432700 2.13363600 H -2.37432700 1.44457600 1.96480200 H 3.38406900 -0.30084300 2.35555200 H -3.33039900 0.01464700 2.37230700 C 1.23046600 -0.36793800 2.61572200 C -1.19017500 -0.21062800 2.63724700 H 1.20834700 -0.06473800 3.67137700 H -1.15176000 0.17939300 3.66340300 H 1.20445400 -1.46102300 2.58825000 H -1.24660900 -1.30069600 2.70469000 N 0.04117900 0.14929400 1.91632100 C -3.28420200 1.30330200 -0.65987800 C 3.25768600 1.48156700 -0.48728500 H -2.69718800 2.17407900 -0.35235800 H 2.71302300 2.27588000 0.03212500 C -3.36019200 -1.60612800 -0.12124000 C 3.44455400 -1.47660200 -0.35088600 C -3.22871400 -2.63542400 0.99984900 C 3.38909800 -2.64242200 0.63551000 O 0.02872400 -0.11420000 -3.07406800 H 4.45612200 -1.06096000 -0.31422200 H -4.38333000 -1.21761100 -0.09472500 C 3.17117400 -1.95927500 -1.77545300 C -3.12845800 -2.25793300 -1.48513900	3Re⁺-HCH(OH)O⁻  O 0.06686400 -3.22752800 -0.18473500 P 2.39921700 0.01355100 0.16898300 P -2.36190700 -0.06353300 0.17252000 C 2.48608400 0.37964500 2.00011700 C -2.43021600 0.42990400 1.97259200 H 2.51576900 1.46802600 2.09774200 H -2.43514800 1.52413900 1.99048200 H 3.38963100 -0.02497400 2.45997300 H -3.34340500 0.08486500 2.46206900 C 1.24105700 -0.14161100 2.69891000 C -1.20052300 -0.07574800 2.70768200 H 1.21335600 0.23439600 3.73010700 H -1.17195700 0.35228700 3.71843000 H 1.23682700 -1.23358900 2.74048800 H -1.21992600 -1.16343900 2.80730400 N 0.02774900 0.29838900 1.97772200 C -3.36953600 1.31297900 -0.60886500 C 3.32998700 1.49729800 -0.51837400 H -2.79249900 2.18799800 -0.29179400 H 2.75589100 2.31929500 -0.07761000 C -3.44401500 -1.59532600 0.04719100 C 3.55069100 -1.44824100 -0.09395100 C -3.20456900 -2.58950600 1.18130800 C 3.36511300 -2.54387300 0.95441900 O 0.01816100 -0.20439000 -3.26807500 H 4.56101900 -1.04106700 0.02039800 H -4.46968100 -1.22265000 0.13828900 C 3.40401400 -2.01838800 -1.50398500 C -3.28758000 -2.27736600 -1.31149700

H 3.21671100 -1.15399800 -2.50945600	H 3.57707800 -1.27207700 -2.27968300
H -3.21796000 -1.55125600 -2.31035600	H -3.48674500 -1.60479100 -2.14562500
H 2.18655000 -2.42218700 -1.85334300	H 2.40565500 -2.43032500 -1.65741400
H -2.13982400 -2.71365400 -1.54376700	H -2.27931900 -2.67343200 -1.43792500
H 3.91444300 -2.71020400 -2.05987700	H 4.12748500 -2.82603300 -1.65225300
H -3.86729800 -3.04927400 -1.64465300	H -3.98784600 -3.11509500 -1.38472000
C -3.32052500 1.27319100 -2.18598800	C -3.36551400 1.28356500 -2.13552400
C 3.13950400 1.72857700 -1.98823700	C 3.23737300 1.62484900 -2.03613700
H -3.96668100 0.47666100 -2.56296600	H -4.01489400 0.49888700 -2.53014600
H 3.71392200 1.00021300 -2.56538600	H 3.86284000 0.88663200 -2.54284200
H -2.33149400 1.14187600 -2.62563200	H -2.36564100 1.13108700 -2.54366400
H 2.10548100 1.68827400 -2.33177100	H 2.21508100 1.50251400 -2.39512200
H -3.73011400 2.21677200 -2.55978100	H -3.74638200 2.23465800 -2.52063300
H 3.53783700 2.71785000 -2.23293900	H 3.59161000 2.61224600 -2.34676500
C -4.69149200 1.45394200 -0.08490100	C -4.78898400 1.44877900 -0.06230800
C 4.71315600 1.54825200 -0.02830700	C 4.77239900 1.62331300 -0.03319800
H -4.69836900 1.51061400 1.00500900	H -4.81864800 1.50272800 1.02780200
H 4.82580100 1.36447600 1.04205500	H 4.86078300 1.54211500 1.05224200
H -5.35326200 0.63849000 -0.38898100	H -5.43254600 0.62480400 -0.38078500
H 5.34419800 0.83588600 -0.56539900	H 5.41910100 0.86772200 -0.48544900
H -5.13669900 2.38107800 -0.45851000	H -5.23892000 2.37040900 -0.44335600
H 5.11438600 2.54574500 -0.23112800	H 5.17331300 2.60013700 -0.32061300
H -0.03887900 1.63825200 -0.19364800	H -0.01053700 1.72459700 -0.24445200
H 0.12578700 1.21199800 1.92504900	H 0.06503200 1.35170500 1.95428600
C 0.14631200 2.80066800 0.32251700	C 0.10074700 2.98299200 0.30073800
H -3.92064700 -3.46227400 0.81250900	H -3.87603100 -3.44457200 1.05886500
H -2.22526700 -3.05974100 1.04784300	H -2.18451100 -2.97564400 1.17189900
H -3.47897100 -2.22174500 1.97846900	H -3.40729900 -2.15927000 2.16407600
H 4.10298400 -3.41041200 0.32248300	H 4.07806700 -3.35064600 0.76091100
H 3.66031700 -2.34652700 1.65036400	H 3.55018200 -2.18870900 1.96974100
H 2.40425200 -3.10854000 0.66252800	H 2.36588300 -2.97861500 0.91416800
O 0.37298900 2.73758600 1.56953600	O 0.24891700 2.92896100 1.54353400
C 0.04444400 -1.91072100 -0.12350400	C 0.05272900 -2.06019500 -0.16942300
Mn 0.02357200 -0.16447400 -0.14985300	Re 0.02291300 -0.17073500 -0.20326200
C 0.02507300 -0.13570900 -1.91622600	C 0.02181800 -0.21101900 -2.10589000
H 0.96292500 3.14572900 -0.34297300	H 0.95018300 3.28958400 -0.33798400
O -1.03741100 3.50825800 -0.03622100	O -1.07617200 3.60272000 -0.15750800
H -0.97388800 3.73156000 -0.97201600	H -0.99380100 3.72982500 -1.11091300
Mn-TS3-H'	Re-TS3-H'
	
O -0.05592500 -3.09790900 0.17434600	O 0.08277900 -3.22943000 -0.11397700
P -2.30488400 -0.04127700 -0.10841700	P 2.39807900 0.02407900 0.16134300
P 2.26161100 -0.09860500 -0.10902800	P -2.36182300 -0.07137800 0.17430600
C -2.48074700 0.15696700 -1.95574600	C 2.48089600 0.40578700 1.98964700
C 2.40400900 0.26581700 -1.93134400	C -2.43202600 0.40611400 1.97992200
H -2.53710500 1.23120300 -2.14945800	H 2.48548600 1.49595900 2.07542900
H 2.40076800 1.35552300 -2.02889300	H -2.44130900 1.49981500 2.00823600
H -3.38709300 -0.30467400 -2.35065500	H 3.39315700 0.02829600 2.45498000
H 3.33149400 -0.10575800 -2.37104700	H -3.34209700 0.05324800 2.46926700
C -1.23828900 -0.40352500 -2.62281500	C 1.24698000 -0.13503600 2.69351200
C 1.19079900 -0.30588800 -2.63971700	C -1.19751800 -0.10036100 2.70706200
H -1.22211500 -0.12415100 -3.68527300	H 1.22301800 0.22878500 3.72935000
H 1.16663200 0.03292700 -3.68452000	H -1.17356900 0.30695900 3.72649500

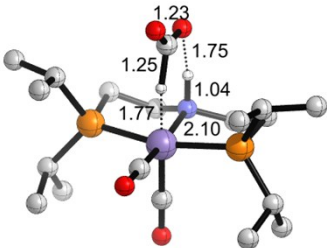
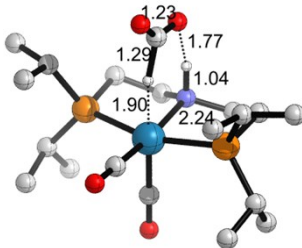
H	-1.22085500	-1.49518600	-2.56861600	H	1.25396300	-1.22711900	2.72349800
H	1.22269700	-1.39841600	-2.64953900	H	-1.20513200	-1.18999000	2.78479600
N	-0.03679400	0.10998900	-1.94228200	N	0.02613800	0.29864600	1.98378100
C	3.27080100	1.31896400	0.60217800	C	-3.36458000	1.31610300	-0.59457400
C	-3.24821700	1.48315700	0.47438700	C	3.33401400	1.49595500	-0.54295500
H	2.70404700	2.17692300	0.23053400	H	-2.79495000	2.18735600	-0.25556900
H	-2.72559900	2.27110400	-0.07665400	H	2.72260800	2.32610200	-0.17430200
C	3.35728400	-1.60610000	0.17697200	C	-3.44747800	-1.60030700	0.03373200
C	-3.44691300	-1.46999100	0.34547000	C	3.54870900	-1.43985600	-0.09972200
C	3.23031100	-2.67755300	-0.90455800	C	-3.19030000	-2.61994400	1.14146600
C	-3.37572000	-2.64716900	-0.62624900	C	3.39469200	-2.51680600	0.97286200
O	-0.02958500	-0.06510000	3.06736400	O	0.03268100	-0.24762400	-3.26696800
H	-4.45747400	-1.05477300	0.28639200	H	4.55961800	-1.02665800	-0.01998500
H	4.37985800	-1.21759800	0.13821800	H	-4.47145800	-1.22960600	0.14856200
C	-3.19747700	-1.93703100	1.77951000	C	3.36998800	-2.03777700	-1.49466000
C	3.12204800	-2.20747300	1.56314400	C	-3.31172400	-2.25076900	-1.34174200
H	-3.26646300	-1.12518200	2.50461100	H	3.50393300	-1.30280000	-2.28869700
H	3.21545400	-1.47190100	2.36257200	H	-3.56112000	-1.56849500	-2.15462200
H	-2.20917100	-2.38750400	1.88119800	H	2.37599900	-2.47179200	-1.60966500
H	2.12978500	-2.65336100	1.63708100	H	-2.29532600	-2.61005800	-1.50827000
H	-3.93819200	-2.69326100	2.05670200	H	4.10433300	-2.83378000	-1.65048900
H	3.85555000	-2.99742800	1.75191700	H	-3.98642900	-3.10945900	-1.41056400
C	3.26225100	1.38044900	2.12770100	C	-3.33667800	1.31696900	-2.12108600
C	-3.09262600	1.76795700	1.96516100	C	3.32224300	1.54651000	-2.06835900
H	3.87962100	0.59530100	2.57071900	H	-3.97036200	0.53367300	-2.54304300
H	-3.64299700	1.04762600	2.57462100	H	4.01265200	0.81796600	-2.49933400
H	2.25777900	1.29072000	2.54223600	H	-2.32844100	1.18094700	-2.51392300
H	-2.04916600	1.74200000	2.28025800	H	2.32992900	1.35560300	-2.47864300
H	3.68016600	2.33648600	2.45880600	H	-3.72046100	2.27182300	-2.49347600
H	-3.49434500	2.75878100	2.19876300	H	3.64615900	2.53465600	-2.40853600
C	4.69543000	1.42328000	0.06080000	C	-4.79157800	1.43711700	-0.06495400
C	-4.71524600	1.53200900	0.05124000	C	4.74601500	1.67814100	0.00951300
H	4.73598300	1.39386700	-1.02969900	H	-4.83684200	1.45097800	1.02604600
H	-4.85493400	1.31391000	-1.00968600	H	4.77175000	1.69526000	1.10082000
H	5.34306700	0.63200500	0.44727100	H	-5.43172900	0.62655100	-0.42278200
H	-5.32858000	0.83407000	0.62617000	H	5.42258100	0.89245700	-0.33540200
H	5.13427000	2.37529100	0.37484600	H	-5.23385400	2.37329800	-0.41855900
H	-5.11635600	2.53362600	0.23357700	H	5.15748000	2.62949700	-0.34089200
H	0.03587300	1.53221600	0.20095400	H	-0.07516300	1.70495400	-0.23523900
H	-0.08698500	1.14896700	-1.98387800	H	0.04931200	1.34490000	1.96017500
C	-0.14282600	2.91360400	-0.39316400	C	0.06595900	3.00993400	0.30235000
H	3.92373100	-3.49522800	-0.68485300	H	-3.87378600	-3.46541300	1.01824100
H	2.22801300	-3.10555800	-0.93821100	H	-2.17512100	-3.01590300	1.09912800
H	3.48197000	-2.30116000	-1.89790800	H	-3.36403400	-2.20898900	2.13781500
H	-4.09618100	-3.41077100	-0.31730400	H	4.10710100	-3.32383600	0.77733400
H	-3.62925000	-2.36269000	-1.64912800	H	3.60058100	-2.14207200	1.97729200
H	-2.39126300	-3.11460000	-0.63059000	H	2.39707600	-2.95713500	0.96283000
O	-0.29514700	2.81992300	-1.61976600	O	0.17752500	2.95932100	1.54384700
C	-0.04729400	-1.93492500	0.13529100	C	0.06444000	-2.06245300	-0.13120000
Mn	-0.02452000	-0.18036500	0.14941300	Re	0.02211800	-0.17043500	-0.20235500
C	-0.02630900	-0.12272900	1.90933400	C	0.02648500	-0.23813300	-2.10395300
H	-0.99335700	3.12844100	0.27355500	H	0.93803300	3.27177600	-0.32334400
O	1.00500800	3.55573000	0.06199500	O	-1.08515400	3.63040900	-0.19849900
H	0.93796100	3.64557100	1.02015500	H	-0.99310700	3.70532200	-1.15589100
Mn-TS4-H⁺				Re-TS4-H⁺			

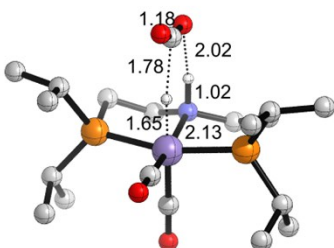
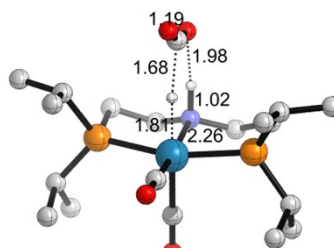


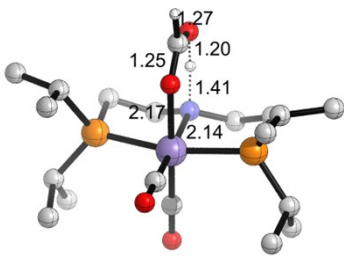
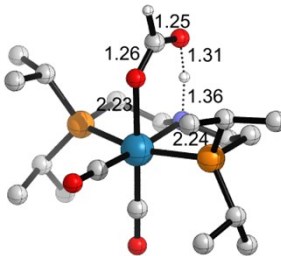
O	-0.00022200	-3.16551500	-0.36686000
P	2.25278700	-0.06966300	0.13139500
P	-2.25290900	-0.06946300	0.13141700
C	2.43669900	-0.01757400	1.99350900
C	-2.43677900	-0.01725300	1.99353300
H	2.46449600	1.03701000	2.28331700
H	-2.46442300	1.03735000	2.28329300
H	3.36396200	-0.47434100	2.34317800
H	-3.36410200	-0.47387200	2.34323600
C	1.22516800	-0.68545600	2.61967100
C	-1.22533100	-0.68527600	2.61970300
H	1.21503700	-0.52347400	3.70667500
H	-1.21516600	-0.52326600	3.70670300
H	1.24138900	-1.76377100	2.44513100
H	-1.24169600	-1.76359500	2.44519400
N	-0.00005100	-0.14934600	2.00499300
C	-3.12157900	1.53684500	-0.33553600
C	3.12177500	1.53648400	-0.33552900
H	-2.54255800	2.26013400	0.24824900
H	2.54288300	2.25991500	0.24820200
C	-3.44984800	-1.41472000	-0.42392000
C	3.44947200	-1.41510200	-0.42407400
C	-3.39255800	-2.67075600	0.44406700
C	3.39222100	-2.67108400	0.44399500
O	-0.00001700	0.03809600	-3.03062700
H	4.44889800	-0.98108300	-0.32028300
H	-4.44921100	-0.98060200	-0.31992200
C	3.21937300	-1.77190100	-1.89257600
C	-3.22003300	-1.77144900	-1.89248200
H	3.27441200	-0.90489900	-2.55157800
H	-3.27523700	-0.90441700	-2.55143100
H	2.24030800	-2.23240100	-2.03397900
H	-2.24097600	-2.23190400	-2.03410100
H	3.97670800	-2.48936000	-2.22286600
H	-3.97740700	-2.48891900	-2.22265700
C	-2.96619500	1.91146600	-1.80612700
C	2.96653200	1.91106800	-1.80614400
H	-3.54766100	1.25288100	-2.45525300
H	3.54779100	1.25225000	-2.45522000
H	-1.92530800	1.87944900	-2.12514300
H	1.92563900	1.87937800	-2.12517300
H	-3.33285400	2.92950300	-1.96654700
H	3.33352900	2.92897500	-1.96662200
C	-4.57912400	1.63195800	0.11063600
C	4.57931800	1.63134400	0.11071000
H	-4.72123600	1.35770900	1.15846200
H	4.72132300	1.35713700	1.15856200
H	-5.23079800	0.99920300	-0.49671100
H	5.23090700	0.99842800	-0.49656000
H	-4.93310700	2.66032200	-0.00906500
H	4.93350100	2.65963400	-0.00904000
H	-0.00059300	1.39858700	-0.07828600



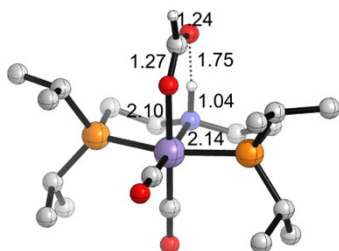
O	-0.00000600	-3.22288600	-0.34048200
P	2.37810200	-0.00823000	0.18986000
P	-2.37811500	-0.00817900	0.18990400
C	2.45878500	0.24076600	2.04250800
C	-2.45875400	0.24086200	2.04254600
H	2.48485400	1.32053900	2.21288600
H	-2.48476100	1.32064200	2.21289300
H	3.36810200	-0.18104900	2.47457500
H	-3.36808400	-0.18089000	2.47464400
C	1.22231100	-0.34558900	2.70699400
C	-1.22229200	-0.34552600	2.70702500
H	1.19293100	-0.04417100	3.76281500
H	-1.19288400	-0.04408000	3.76283800
H	1.24430800	-1.43841300	2.67796500
H	-1.24432900	-1.43835100	2.67802600
N	0.00001100	0.11627100	2.02236100
C	-3.26140200	1.53782800	-0.41709700
C	3.26140000	1.53778000	-0.41712700
H	-2.66164100	2.32258800	0.05688500
H	2.66171500	2.32253600	0.05695700
C	-3.54331200	-1.43643200	-0.16524400
C	3.54326100	-1.43650500	-0.16532400
C	-3.35057200	-2.60522300	0.79912400
C	3.35058700	-2.60526000	0.79909900
O	-0.00009000	-0.09924100	-3.25060300
H	4.54813200	-1.02973500	-0.01116600
H	-4.54816700	-1.02965900	-0.01099900
C	3.41496200	-1.90495100	-1.61387600
C	-3.41512900	-1.90482400	-1.61382500
H	3.58036400	-1.10216300	-2.33254900
H	-3.58057000	-1.10200200	-2.33245200
H	2.42488900	-2.32235600	-1.80379900
H	-2.42507900	-2.32224100	-1.80383900
H	4.15275600	-2.68750900	-1.81378900
H	-4.15295300	-2.68735900	-1.81371200
C	-3.16733300	1.74561900	-1.92584000
C	3.16719400	1.74567700	-1.92584500
H	-3.80221400	1.04536200	-2.47311300
H	3.80195300	1.04540200	-2.47323400
H	-2.14561400	1.64141200	-2.29010300
H	2.14542500	1.64158200	-2.29000300
H	-3.50612800	2.75481700	-2.17484900
H	3.50604600	2.75486200	-2.17482300
C	-4.69908500	1.67154100	0.07962600
C	4.69913200	1.67140700	0.07947700
H	-4.78912500	1.53193100	1.15918200
H	4.78926800	1.53169000	1.15901300
H	-5.36528100	0.95913600	-0.41315300
H	5.36526400	0.95903400	-0.41343300
H	-5.07362900	2.67269700	-0.15181300
H	5.07368000	2.67257700	-0.15189900
H	-0.00013700	1.75139800	-0.13158600

H 0.00003000 0.86218300 2.14625500	H 0.00004900 1.37811800 2.04922500
H -4.12722600 -3.39478200 0.07864500	H -4.07038300 -3.39280000 0.55764300
H -2.41473900 -3.15105600 0.39766800	H -2.35395700 -3.03953600 0.71277300
H -3.63238500 -2.47164900 1.49035900	H -3.51878400 -2.32395000 1.84032200
H 4.12670200 -3.39522900 0.07842900	H 4.07039100 -3.39284000 0.55760500
H 3.63233600 -2.47195700 1.49021700	H 3.51885900 -2.32394600 1.84027700
H 2.41432800 -3.15125900 0.39786100	H 2.35396900 -3.03958400 0.71282600
O 0.00049300 2.84447100 1.76085400	O 0.00033700 2.78020700 1.66781800
C -0.00005200 -0.08311200 -1.87889600	C -0.00004800 -0.13561200 -2.09170400
C 0.00061100 3.04768500 0.59394000	C 0.00015300 2.86969200 0.43269700
O 0.00096000 3.67963000 -0.39299000	O 0.00014100 3.74862300 -0.38935300
C -0.00012700 -2.00871100 -0.23398100	C -0.00003700 -2.05861900 -0.26836600
Mn -0.00009100 -0.24984400 -0.12609400	Re -0.00001400 -0.18161100 -0.18346900
3Mn⁺-OOCH⁻	3Re⁺-OOCH⁻
	
O -0.00015600 -3.10741200 -0.39896100	O -0.00004900 -3.22866200 -0.36903600
P 2.28163300 -0.04840600 0.13793900	P 2.37537700 -0.00902700 0.19194700
P -2.28167100 -0.04832300 0.13796300	P -2.37539300 -0.00897200 0.19201100
C 2.43961900 -0.01514200 1.99770500	C 2.45634900 0.16830300 2.05425100
C -2.43968500 -0.01518600 1.99773300	C -2.45629900 0.16838200 2.05431600
H 2.45401400 1.03808900 2.29099400	H 2.46964500 1.24125300 2.26534100
H -2.45412800 1.03801700 2.29111400	H -2.46954800 1.24133500 2.26539100
H 3.36509200 -0.47019100 2.35395300	H 3.37010300 -0.25892100 2.47123600
H -3.36515200 -0.47029800 2.35390900	H -3.37005600 -0.25879900 2.47133900
C 1.22203800 -0.69051100 2.60449600	C 1.22768600 -0.45547500 2.69784900
C -1.22209000 -0.69057700 2.60447600	C -1.22763700 -0.45542300 2.69789000
H 1.19758400 -0.52259200 3.68967600	H 1.20303900 -0.21305900 3.76843900
H -1.19761600 -0.52274800 3.68966700	H -1.20295600 -0.21298400 3.76847400
H 1.24973400 -1.77081400 2.43965100	H 1.24425500 -1.54366200 2.60361200
H -1.24976600 -1.77086400 2.43953500	H -1.24424000 -1.54361200 2.60367800
N -0.00003300 -0.15826200 1.97845800	N 0.00002300 0.04068300 2.04326500
C -3.13442400 1.56648900 -0.31877600	C -3.24951100 1.56507000 -0.35166100
C 3.13444100 1.56635400 -0.31889600	C 3.24952600 1.56499700 -0.35173900
H -2.55122200 2.28840800 0.26185300	H -2.65181800 2.32569700 0.16225400
H 2.55123500 2.28833700 0.26164600	H 2.65189900 2.32563400 0.16223700
C -3.45746600 -1.39738600 -0.44109600	C -3.55157300 -1.41325100 -0.21934100
C 3.45740100 -1.39756400 -0.44092700	C 3.55149000 -1.41335000 -0.21944700
C -3.40519600 -2.65839200 0.41996200	C -3.37782900 -2.61704900 0.70478200
C 3.40487800 -2.65851300 0.42020600	C 3.37785800 -2.61707500 0.70479000
O 0.00004800 0.04207800 -3.04067400	O -0.00009700 -0.05737900 -3.24840800
H 4.45740800 -0.96422900 -0.34039000	H 4.55431700 -1.00356400 -0.06077800
H -4.45745400 -0.96396700 -0.34070800	H -4.55437400 -1.00346600 -0.06051000
C 3.21845700 -1.74066500 -1.91117700	C 3.41284800 -1.83248200 -1.68210400
C -3.21834400 -1.74044800 -1.91133400	C -3.41313000 -1.83226400 -1.68205100
H 3.25906000 -0.86625200 -2.56109000	H 3.56566000 -1.00400800 -2.37400500
H -3.25853100 -0.86598200 -2.56120000	H -3.56603200 -1.00372900 -2.37386000
H 2.24485600 -2.21300600 -2.05122100	H 2.42341500 -2.24936400 -1.87673100
H -2.24487400 -2.21309800 -2.05122800	H -2.42372600 -2.24913700 -1.87684700
H 3.98166800 -2.44547800 -2.25417700	H 4.15380000 -2.60248700 -1.91616500
H -3.98172300 -2.44498400 -2.25453100	H -4.15411800 -2.60224400 -1.91607500
C -2.99120600 1.94675900 -1.78933700	C -3.13910500 1.83767000 -1.84887100
C 2.99129000 1.94653600 -1.78949100	C 3.13902600 1.83765400 -1.84893100
H -3.56815800 1.28570500 -2.44017900	H -3.75836500 1.15412900 -2.43396100

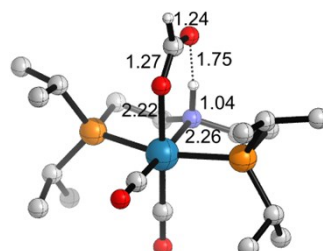
H	3.56825700	1.28543800	-2.44027600
H	-1.95170500	1.93776000	-2.11439700
H	1.95180300	1.93754100	-2.11459200
H	-3.36959100	2.96165100	-1.93829900
H	3.36968500	2.96141800	-1.93848500
C	-4.58817100	1.65706100	0.14129700
C	4.58817100	1.65692300	0.14122700
H	-4.71969900	1.38143000	1.18998200
H	4.71964300	1.38140300	1.18995000
H	-5.24642800	1.02711000	-0.46210700
H	5.24644000	1.02689100	-0.46207900
H	-4.94015900	2.68646600	0.02862800
H	4.94020100	2.68630400	0.02846400
H	-0.00040600	1.56055200	-0.01843600
H	-0.00003200	0.87525900	2.11098400
H	-4.14026600	-3.37790600	0.04714000
H	-2.42872600	-3.14166600	0.37458000
H	-3.64803300	-2.46440400	1.46620100
H	4.13999600	-3.37809600	0.04761100
H	3.64749200	-2.46445400	1.46648400
H	2.42839800	-3.14174200	0.37464900
O	0.00015900	2.58780900	1.77387300
C	0.00000300	-0.04441400	-1.88930100
C	0.00014600	2.67195500	0.54303400
O	0.00041500	3.55022700	-0.28832500
C	-0.00005800	-1.95271500	-0.27422800
Mn	-0.00002600	-0.21044900	-0.12487000
Mn-TS4-H⁻			
			
O	-0.00009900	-3.10738300	-0.34621200
P	2.28351300	-0.04789500	0.13577000
P	-2.28354500	-0.04782000	0.13579800
C	2.44187600	0.02476700	1.99344600
C	-2.44193100	0.02473900	1.99347800
H	2.46645900	1.08377700	2.26382700
H	-2.46654600	1.08372800	2.26393400
H	3.36353100	-0.43098500	2.35860700
H	-3.36358300	-0.43106000	2.35857900
C	1.21765900	-0.62695200	2.61312900
C	-1.21770400	-0.62700400	2.61311900
H	1.18980500	-0.42325500	3.69243600
H	-1.18983000	-0.42338200	3.69243800
H	1.24829000	-1.71333700	2.48759900
H	-1.24832300	-1.71337900	2.48750800
N	-0.00003000	-0.11246300	1.96727700
C	-3.13936100	1.55563700	-0.35580700
C	3.13936300	1.55552200	-0.35591700
H	-2.55930100	2.29116200	0.21089300
H	2.55929800	2.29109700	0.21070800
C	-3.45431000	-1.41140900	-0.41814300
C	3.45426200	-1.41155100	-0.41801700
C	-3.40058600	-2.65431700	0.46885900
C	3.40035400	-2.65440700	0.46905200
H	3.75821100	1.15410600	-2.43409000
H	-2.11111400	1.76102900	-2.20202900
H	2.11100400	1.76107400	-2.20201500
H	-3.48608600	2.85282600	-2.05945900
H	3.48603600	2.85280100	-2.05950900
C	-4.69151600	1.68144700	0.13668100
C	4.69156700	1.68130800	0.13651500
H	-4.79362300	1.48871900	1.20706500
H	4.79374000	1.48852400	1.20688300
H	-5.35624600	0.99825000	-0.39765100
H	5.35624200	0.99811900	-0.39789600
H	-5.05868500	2.69492600	-0.04825600
H	5.05875200	2.69478600	-0.04839600
H	-0.00015000	1.71733200	-0.09563300
H	0.00004600	1.07730300	2.12295200
H	-4.10165100	-3.38947300	0.42876400
H	-2.38404700	-3.05680200	0.61241700
H	-3.55442400	-2.37186700	1.75381400
H	4.10165000	-3.38951900	0.42874800
H	3.55457500	-2.37181000	1.75378300
H	2.38406500	-3.05683700	0.61257800
O	0.00046900	2.79312300	1.69233100
C	-0.00004700	-0.10977500	-2.09022500
C	0.00018400	2.88065700	0.46843400
O	0.00008200	3.72306800	-0.38921500
C	-0.00003800	-2.06516300	-0.28505100
Re	-0.00002000	-0.18324800	-0.18452300
Re-TS4-H⁻			
			
O	-0.00001000	-3.27385300	-0.29421200
P	2.36214700	-0.01906400	0.18501000
P	-2.36216200	-0.01904100	0.18500600
C	2.45623000	0.15470100	2.05079100
C	-2.45624300	0.15472200	2.05078700
H	2.47880000	1.22659700	2.26864000
H	-2.47880300	1.22661800	2.26863700
H	3.37013100	-0.27761400	2.46239200
H	-3.37014800	-0.27758400	2.46238800
C	1.23027000	-0.46886700	2.69996200
C	-1.23028800	-0.46885800	2.69995800
H	1.21522400	-0.24288600	3.77479100
H	-1.21524300	-0.24288100	3.77478800
H	1.23795800	-1.55482500	2.58635200
H	-1.23798600	-1.55481600	2.58634500
N	-0.00000600	0.03796100	2.05863300
C	-3.24586600	1.55358900	-0.35222300
C	3.24586700	1.55355400	-0.35222400
H	-2.65374900	2.31014300	0.17418900
H	2.65378300	2.31011500	0.17421400
C	-3.55269900	-1.41541600	-0.22286100
C	3.55267500	-1.41545100	-0.22284300
C	-3.38647800	-2.62101400	0.70020900
C	3.38643200	-2.62104900	0.70022300

O	-0.00004100	-0.00893600	-3.04551500
H	4.45528800	-0.97837300	-0.32740000
H	-4.45532500	-0.97817400	-0.32763600
C	3.21323100	-1.78373100	-1.88086000
C	-3.21314600	-1.78355100	-1.88098100
H	3.25343800	-0.92248300	-2.54815800
H	-3.25302600	-0.92225800	-2.54823800
H	2.23943400	-2.25858100	-2.01065700
H	-2.23945400	-2.25864200	-2.01066000
H	3.97588400	-2.49545200	-2.21057100
H	-3.97593400	-2.49505300	-2.21085100
C	-2.99576900	1.90727500	-1.83338100
C	2.99581400	1.90707800	-1.83351900
H	-3.56982400	1.23169100	-2.47168800
H	3.56988700	1.23146400	-2.47177900
H	-1.95606300	1.89419900	-2.15780600
H	1.95611700	1.89398900	-2.15797000
H	-3.37703900	2.91784800	-2.00300700
H	3.37707600	2.91764700	-2.00317800
C	-4.59387800	1.65132300	0.10082300
C	4.59386800	1.65121700	0.10074500
H	-4.72556200	1.39526000	1.15439500
H	4.72551400	1.39524600	1.15434600
H	-5.24959800	1.00799800	-0.49111600
H	5.24960000	1.00783300	-0.49111500
H	-4.94864800	2.67738200	-0.03187700
H	4.94866400	2.67725700	-0.03203300
H	-0.00038000	1.58567900	-0.05153500
H	-0.00001900	1.14510900	2.07983700
H	-4.13367200	-3.38280100	0.10980600
H	-2.42306700	-3.13632000	0.43524900
H	-3.64518000	-2.43904700	1.51045500
H	4.13348200	-3.38293800	0.11018100
H	3.64477400	-2.43907100	1.51067500
H	2.42283100	-3.13638700	0.43531100
O	0.00015000	2.56990900	1.76020200
C	-0.00003000	-0.07173300	-1.89245800
C	0.00013700	2.66828000	0.52279700
O	0.00040400	3.57564300	-0.27675000
C	-0.00003800	-1.95055800	-0.24579200
Mn	-0.00001900	-0.20808200	-0.12444800
Mn-TS(HCOOH)			
			
P	2.33891500	-0.01800800	-0.11265600
P	-2.33770900	-0.01594500	-0.12215200
C	2.45136400	-0.39361700	-1.93468700
C	-2.44594200	-0.40116600	-1.94154000
H	2.47241100	-1.48342600	-2.02555900
H	-2.46690700	-1.49116800	-2.02963600
H	3.36355900	-0.01061800	-2.39634100
H	-3.35749100	-0.01875800	-2.40542500
C	1.20708600	0.14790000	-2.62279200
C	-1.20054300	0.14050000	-2.62818800
O	0.00002000	-0.09678000	-3.24791500
H	4.55464000	-1.00253100	-0.06695400
H	-4.55466300	-1.00248600	-0.06698700
C	3.41061500	-1.83673900	-1.68463900
C	-3.41062300	-1.83670900	-1.68465400
H	3.56469600	-1.00967000	-2.37819800
H	-3.56467400	-1.00963800	-2.37821700
H	2.41807300	-2.24818000	-1.87556800
H	-2.41808700	-2.24817200	-1.87556500
H	4.14778500	-2.61021600	-1.91984500
H	-4.14780600	-2.61017000	-1.91987100
C	-3.11654300	1.83633500	-1.84585100
C	3.11650600	1.83632100	-1.84584500
H	-3.72632000	1.15408200	-2.44224900
H	3.72623700	1.15405200	-2.44227200
H	-2.08296300	1.75833200	-2.18233500
H	2.08291200	1.75835900	-2.18229500
H	-3.46335800	2.85152000	-2.05866900
H	3.46335100	2.85149600	-2.05866400
C	-4.69339400	1.66589200	0.11968200
C	4.69341100	1.66582300	0.11964200
H	-4.80844100	1.46162300	1.18681500
H	4.80848400	1.46153500	1.18676900
H	-5.35071000	0.98670700	-0.42858800
H	5.35069900	0.98663400	-0.42865800
H	-5.06144000	2.68027800	-0.06020800
H	5.06147100	2.68020500	-0.06024300
H	-0.00002800	1.60996700	-0.13489600
H	-0.00000100	1.05732800	2.15677300
H	-4.11119400	-3.39148000	0.42051700
H	-2.39331100	-3.06264000	0.61107600
H	-3.56689800	-2.37726900	1.74915200
H	4.11115000	-3.39151800	0.42054200
H	3.56683600	-2.37730600	1.74916900
H	2.39326400	-3.06267000	0.61107400
O	0.00006400	2.97973200	1.69097900
C	0.00000700	-0.14720600	-2.08755700
C	0.00007900	3.16234800	0.51490200
O	0.00012100	3.82743700	-0.45361300
C	-0.00001200	-2.10831000	-0.23202100
Re	-0.00000800	-0.20026000	-0.18586100
Re-TS(HCOOH)			
			
P	-2.37886700	-0.05166600	0.15723900
P	2.37784200	-0.05146000	0.18341900
C	-2.46395300	-0.47742500	1.97684600
C	2.45191500	-0.47258700	2.00419200
H	-2.47904100	-1.56940500	2.03788600
H	2.47710800	-1.56379100	2.07315200
H	-3.37678800	-0.11138800	2.45062200
H	3.35780700	-0.09335900	2.48176900
C	-1.22797400	0.04723800	2.69420700
C	1.20578300	0.04806900	2.70803700

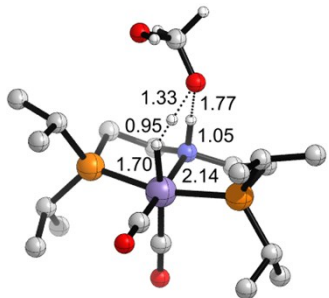
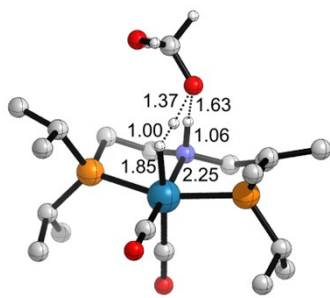
H	1.19110100	-0.19389100	-3.66891700	H	-1.22005100	-0.32312800	3.72926700
H	-1.18016200	-0.20540800	-3.67285600	H	1.18656800	-0.32283300	3.74272200
H	1.23065000	1.24522000	-2.64499400	H	-1.24453500	1.14131000	2.73907200
H	-1.22725900	1.23763000	-2.65484000	H	1.21920100	1.14215600	2.75358200
N	0.00311000	-0.30129800	-1.91988400	N	-0.00705100	-0.37943000	1.99506700
C	-3.22729200	-1.49289600	0.63066000	C	3.25052700	-1.53047600	-0.58002000
C	3.23617300	-1.49787700	0.62631400	C	-3.26606200	-1.52634300	-0.59913200
H	-2.62016800	-2.31664700	0.24492900	H	2.66768200	-2.35405500	-0.15808100
H	2.63947700	-2.32538500	0.23011900	H	-2.65168700	-2.35345700	-0.22950800
C	-3.49530800	1.43895100	0.15153700	C	3.56002500	1.38985700	-0.03103800
C	3.48552500	1.44217300	0.18421300	C	-3.53509000	1.40821700	-0.08567800
C	-3.34887500	2.52913500	-0.90927700	C	3.34523500	2.48987800	1.00686100
C	3.39062000	2.51179500	-0.90308000	C	-3.41543500	2.45213600	1.02355200
O	0.00052900	0.55472600	3.12801900	O	0.00917700	0.63790400	-3.21605700
H	4.49638400	1.02269200	0.15681200	H	-4.54465100	0.98589600	-0.04819700
H	-4.50331600	1.02026900	0.06460900	H	4.55676200	0.96521000	0.12819800
C	3.24276400	2.05645400	1.56265800	C	-3.31853500	2.05287200	-1.45434500
C	-3.31757800	2.02416200	1.55200400	C	3.48135800	1.95874800	-1.44652800
H	3.32270800	1.32849100	2.37037400	H	-3.41392400	1.34287700	-2.27619400
H	-3.46781000	1.28698400	2.34072000	H	3.70693500	1.21564200	-2.21182500
H	2.25029500	2.50571000	1.61987000	H	-2.32667700	2.50256000	-1.51954500
H	-2.31671500	2.44123000	1.67507000	H	2.48559600	2.35686400	-1.65115300
H	3.97835900	2.84448500	1.75002700	H	-4.05805500	2.84420500	-1.60927100
H	-4.03809000	2.83234300	1.70939600	H	4.19934800	2.77692500	-1.55592700
C	-3.15864600	-1.53427000	2.15997300	C	3.11185800	-1.58870400	-2.10778500
C	3.14649100	-1.55899400	2.14841400	C	-3.19325600	-1.55042900	-2.12324900
H	-3.49175900	-2.49930100	2.54785700	H	3.46046100	-2.53860500	-2.51608300
H	2.12157000	-1.43582400	2.49762900	H	-2.17359500	-1.40467600	-2.47993400
H	-3.81128600	-0.77906900	2.60183900	H	3.70873000	-0.80976300	-2.58434800
H	3.50803800	-2.52992000	2.50037000	H	-3.54516400	-2.51811000	-2.49311400
H	-2.14452000	-1.36081200	2.52304800	H	2.07224500	-1.45538300	-2.41406900
H	3.76767700	-0.79501200	2.62144900	H	-3.83028100	-0.78445200	-2.57134000
C	-4.65654200	-1.68835400	0.12751700	C	4.69952200	-1.70529700	-0.12929500
C	4.67319000	-1.67275700	0.14069800	C	-4.69415000	-1.72974600	-0.09897800
H	-4.72487700	-1.67625600	-0.96249000	H	4.81025800	-1.66919800	0.95713700
H	4.75649700	-1.64550100	-0.94789500	H	-4.76447100	-1.72796500	0.99090100
H	-5.33265000	-0.92436800	0.51903300	H	5.35333700	-0.94493800	-0.56328600
H	5.33635100	-0.90738500	0.55124300	H	-5.37163300	-0.96374400	-0.48428400
H	-5.03781600	-2.65594800	0.46793000	H	5.07407900	-2.67750100	-0.46331600
H	5.05957000	-2.64082000	0.47398600	H	-5.07258200	-2.69495700	-0.44876900
H	0.00593500	-1.70565900	-1.85807800	H	-0.00499800	-1.73262700	1.90941500
H	-4.07551900	3.32251300	-0.70928200	H	4.09759700	3.27092700	0.86140400
H	4.10265200	3.31237500	-0.68062000	H	-4.13057500	3.25857700	0.83561700
H	-2.35820900	2.98303400	-0.89315800	H	2.36561100	2.95679400	0.90565000
H	2.39861700	2.96215100	-0.94333900	H	-2.42128100	2.89983000	1.05017700
H	-3.54377000	2.16054500	-1.91796600	H	3.45247000	2.12703600	2.03092700
H	3.63724800	2.12679100	-1.89399900	H	-3.64087700	2.04527200	2.01096100
O	-0.00397300	-2.01165200	0.51695100	O	0.00692000	-2.06032600	-0.55208900
C	-0.00041800	0.37741100	1.98331900	C	0.00695800	0.44643100	-2.07075300
C	0.00585600	1.90695700	-0.04434800	C	-0.00929700	2.00095200	0.07562100
O	0.01144600	3.06536100	-0.17477400	O	-0.02126700	3.16057200	0.22876100
Mn	-0.00031000	0.13485600	0.17927400	Re	0.00164700	0.14387700	-0.18766500
C	0.00147800	-2.95354500	-0.29731700	C	0.00508000	-3.02616000	0.25222400
H	0.00502300	-3.97439600	0.12065500	H	0.00471100	-4.02850600	-0.21197900
O	0.00270700	-2.87114600	-1.56002000	O	0.00373900	-2.97583400	1.50349800
2Mn-OOCH				2Re-OOCH			

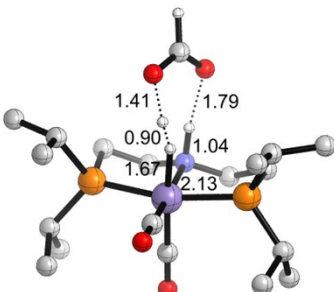
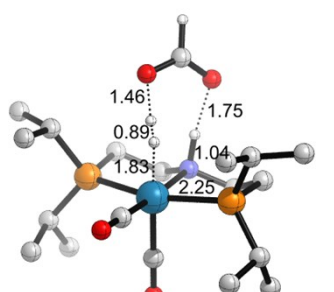


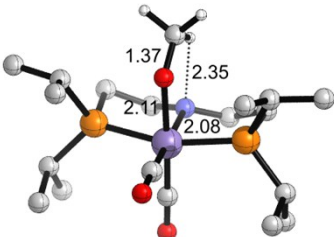
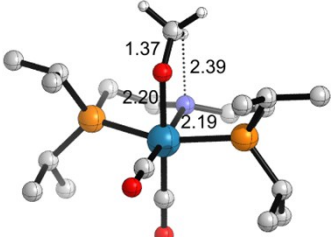
P	2.29116000	-0.01258900	-0.11378200
P	-2.29116500	-0.01255200	-0.11378900
C	2.43932700	-0.28054900	-1.95429200
C	-2.43935400	-0.28039800	-1.95431400
H	2.44215500	-1.36284900	-2.11027900
H	-2.44224800	-1.36268900	-2.11036000
H	3.36565400	0.11651400	-2.37266800
H	-3.36565500	0.11674700	-2.37266500
C	1.22125200	0.32138400	-2.63667800
C	-1.22123700	0.32149800	-2.63666000
H	1.21114000	0.04706500	-3.70078600
H	-1.21113500	0.04723000	-3.70078200
H	1.24318500	1.41350100	-2.58035300
H	-1.24309500	1.41361300	-2.58027800
N	-0.00001000	-0.15385000	-1.97256200
C	-3.16812000	-1.53852100	0.54767600
C	3.16813100	-1.53852100	0.54776700
H	-2.58039400	-2.33721000	0.08621600
H	2.58037200	-2.33723200	0.08638800
C	-3.45180500	1.41387700	0.28549600
C	3.45177000	1.41389300	0.28536900
C	-3.42212300	2.53678500	-0.75034700
C	3.42183700	2.53681600	-0.75044700
O	-0.00017600	0.40893000	3.06623300
H	4.45519000	0.97690800	0.27618900
H	-4.45519600	0.97681900	0.27646900
C	3.17502200	1.96925200	1.68279100
C	-3.17491400	1.96927200	1.68287400
H	3.18508000	1.19785800	2.45314400
H	-3.18483900	1.19789100	2.45324400
H	2.20341500	2.46447300	1.72384700
H	-2.20333000	2.46454800	1.72379700
H	3.93682300	2.71028500	1.94327000
H	-3.93672400	2.71026800	1.94343200
C	-3.03743000	-1.69470300	2.05969800
C	3.03749300	-1.69462000	2.05980100
H	-3.61779800	-0.94304600	2.60011500
H	3.61789700	-0.94295000	2.60016000
H	-1.99716600	-1.62878800	2.37691100
H	1.99724300	-1.62866900	2.37705000
H	-3.41995300	-2.67417200	2.36204800
H	3.42000700	-2.67408200	2.36218600
C	-4.61668600	-1.68790400	0.08726700
C	4.61667600	-1.68796800	0.08730600
H	-4.72866400	-1.58608300	-0.99451600
H	4.72861300	-1.58620500	-0.99448600
H	-5.27540400	-0.95961800	0.56714500
H	5.27543500	-0.95967700	0.56712000
H	-4.98649100	-2.68062200	0.36124900
H	4.98646700	-2.68068100	0.36132400
H	-0.00008300	-1.19251400	-2.00734200
H	-4.14157900	3.30947900	-0.46292000



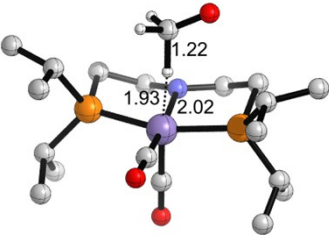
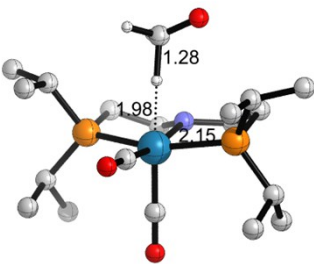
P	-2.37873200	-0.04887400	0.16798000
P	2.37874300	-0.04890300	0.16792600
C	-2.45817700	-0.43004700	1.99915800
C	2.45820000	-0.43014700	1.99908800
H	-2.47264000	-1.51990100	2.08933700
H	2.47260600	-1.52000800	2.08921900
H	-3.36917700	-0.05003100	2.46525100
H	3.36922700	-0.05020300	2.46518600
C	-1.22482000	0.11528100	2.70416500
C	1.22488300	0.11520800	2.70414400
H	-1.21298500	-0.22417200	3.74868000
H	1.21306600	-0.22427900	3.74864800
H	-1.23182200	1.20820900	2.71124800
H	1.23192800	1.20813600	2.71126600
N	0.00001200	-0.33064000	2.01572800
C	3.26619100	-1.54187500	-0.54813600
C	-3.26619700	-1.54187200	-0.54801400
H	2.65284400	-2.35814500	-0.15379200
H	-2.65289300	-2.35813300	-0.15358500
C	3.53562500	1.40573200	-0.10093300
C	-3.53561200	1.40575600	-0.10093400
C	3.40711200	2.47757000	0.98029300
C	-3.40695100	2.47773600	0.98013300
O	-0.00008900	0.59255500	-3.22399900
H	-4.54535100	0.98580900	-0.04580800
H	4.54536100	0.98575700	-0.04597500
C	-3.32703700	2.01497200	-1.48688300
C	3.32689900	2.01513900	-1.48677700
H	-3.43403400	1.28512700	-2.28968900
H	3.43378700	1.28540000	-2.28969300
H	-2.33265400	2.45604200	-1.57145300
H	2.33251300	2.45623800	-1.57116700
H	-4.06279200	2.80696100	-1.65551400
H	4.06264800	2.80713800	-1.65538900
C	3.18712400	-1.60822000	-2.07052800
C	-3.18707000	-1.60831700	-2.07039700
H	3.81932300	-0.85322100	-2.54354400
H	-3.81917700	-0.85328700	-2.54348900
H	2.16458200	-1.47714300	-2.42429700
H	-2.16449800	-1.47735100	-2.42412300
H	3.54025700	-2.58502500	-2.41408900
H	-3.54027700	-2.58511000	-2.41391800
C	4.69603700	-1.72929300	-0.04679000
C	-4.69606800	-1.72920900	-0.04671000
H	4.77028600	-1.69599600	1.04243900
H	-4.77037100	-1.69576500	1.04251000
H	5.37213300	-0.97477400	-0.45659500
H	-5.37213300	-0.97473500	-0.45665000
H	5.07347300	-2.70429300	-0.36922300
H	-5.07350100	-2.70424700	-0.36903300
H	-0.00002300	-1.37068000	1.99697900
H	4.12419900	3.27877800	0.77816900

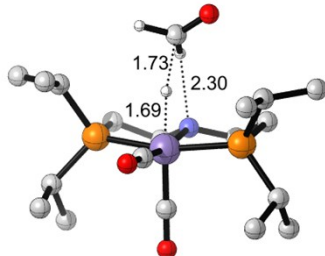
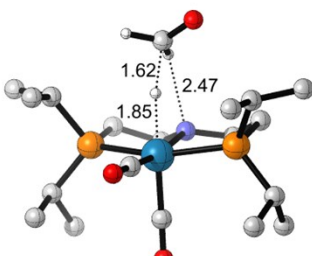
H 4.14126100 3.30957500 -0.46311500	H -4.12405600 3.27892400 0.77799200
H -2.44211700 3.01192700 -0.80456900	H 2.41301700 2.92632600 0.98682800
H 2.44177500 3.01186700 -0.80451800	H -2.41285000 2.92648100 0.98648300
H -3.69885000 2.19628100 -1.74968100	H 3.62460700 2.09643100 1.97981700
H 3.69844500 2.19635000 -1.74982700	H -3.62432300 2.09673500 1.97973700
O 0.00002600 -1.95035700 0.42440400	O 0.00001600 -2.05762800 -0.54747600
C -0.00000100 0.28940800 1.91761800	C -0.00002100 0.41659500 -2.07698500
C 0.00001800 1.87503200 0.00066200	C 0.00000800 1.99620200 0.05736200
O 0.00041300 3.03596200 -0.07942600	O 0.00003900 3.15677400 0.20793000
Mn 0.00000400 0.13466100 0.15056700	Re 0.00000400 0.13579900 -0.19278300
C -0.00000600 -2.92817300 -0.38035600	C -0.00005700 -3.05247500 0.24097700
H -0.00001800 -3.92128000 0.11427300	H -0.00002600 -4.03211200 -0.27561400
O -0.00007200 -2.89934200 -1.62201900	O -0.00012300 -3.04370600 1.48097800
1Mn-TS(HOCH₂OH-H-H)	
	
O 0.18178800 -3.21090900 -0.54928400	O 0.22218200 -3.26779400 -0.74337100
P -2.22722800 -0.23105400 -0.07640700	P -2.32974700 -0.16293100 -0.12514300
P 2.30983800 -0.02047100 -0.08147900	P 2.40864000 0.10402000 -0.12429300
C -2.40472000 0.35222800 -1.84107500	C -2.43643100 0.56301500 -1.84590300
C 2.46085000 0.46961300 -1.87707300	C 2.45530900 0.77443300 -1.86805000
H -2.44480500 1.44450600 -1.80418500	H -2.48995400 1.64789500 -1.71774400
H 2.42855500 1.56158400 -1.89737300	H 2.37792500 1.86041200 -1.76975500
H -3.32785300 0.00815600 -2.31043300	H -3.34220800 0.25307800 -2.37009300
H 3.39945600 0.14500600 -2.32812200	H 3.38936700 0.53884900 -2.38051400
C -1.18480000 -0.09004700 -2.63154300	C -1.19551700 0.20777800 -2.64995300
C 1.26019900 -0.07586300 -2.63362100	C 1.25371100 0.27304300 -2.65374300
H -1.18584000 0.37919300 -3.62557000	H -1.19634300 0.76271200 -3.59800400
H 1.22840900 0.34840000 -3.64710800	H 1.20222100 0.79366200 -3.61962100
H -1.19408900 -1.17318900 -2.78363900	H -1.18414000 -0.85813700 -2.89390000
H 1.31735500 -1.16341700 -2.73550800	H 1.32928600 -0.79852300 -2.85808100
N 0.03474800 0.26732600 -1.89900300	N 0.02124700 0.52396800 -1.88602100
C 3.01274600 1.50304400 0.76404100	C 3.10169400 1.56352300 0.83022000
C -3.10504800 1.14559500 0.84997700	C -3.21302100 1.15416900 0.87753600
H 2.32961100 2.26789100 0.37636400	H 2.37870100 2.33816900 0.54550400
H -2.49849500 2.01687000 0.57611200	H -2.58798100 2.03461400 0.68304800
C 3.58617800 -1.37582800 0.18002600	C 3.70628400 -1.24869000 -0.04899400
C -3.35863800 -1.72564400 0.07481000	C -3.45738400 -1.66331800 -0.12953000
C 3.62409700 -2.39478300 -0.95788500	C 3.66387600 -2.16981600 -1.26670600
C -3.29970300 -2.65560900 -1.13581500	C -3.30368100 -2.51201600 -1.39008400
O 0.08457700 -1.11416600 2.96620400	O 0.10604600 -1.34263600 3.08577700
H -4.37151700 -1.31392500 0.13594200	H -4.47537200 -1.25991400 -0.10837900
H 4.55208600 -0.86021800 0.20460000	H 4.66889500 -0.72611700 -0.04658600
C -3.06733200 -2.50243600 1.35863300	C -3.23435500 -2.51489000 1.11938100
C 3.37186200 -2.08141700 1.51855200	C 3.57657200 -2.05780500 1.24038400
H -3.09877100 -1.87439700 2.24920800	H -3.35305400 -1.94906300 2.04343300
H 3.33820200 -1.39042900 2.36120600	H 3.62191900 -1.43696700 2.13537800
H -2.08200500 -2.96977000 1.31813200	H -2.23153200 -2.94525200 1.12171600
H 2.43780800 -2.64608900 1.51719300	H 2.63073800 -2.60188300 1.26360200
H -3.80777700 -3.29800400 1.48548900	H -3.95425100 -3.33849200 1.13749000
H 4.18749600 -2.78801800 1.69937100	H 4.38767800 -2.78950900 1.30051900
C 2.88131900 1.47544200 2.28358400	C 3.04186300 1.38497100 2.34449300
C -3.03732700 1.00015000 2.36751900	C -3.18047900 0.89190600 2.38105800
1Re-TS(HOCH₂OH-H-H)	
	

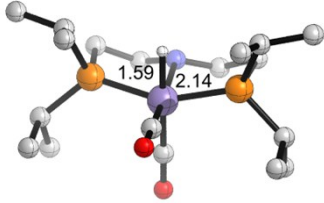
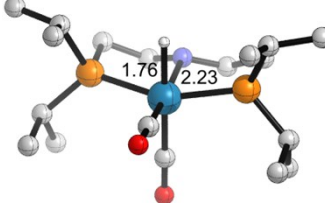
H	3.57480600	0.76597700	2.74175500	H	3.79720100	0.68077200	2.70142700
H	-3.68392000	0.19725500	2.73056400	H	-3.86719200	0.09254400	2.67002900
H	1.87080000	1.21799800	2.60197900	H	2.06497000	1.03228900	2.67750600
H	-2.02342400	0.80646400	2.71851700	H	-2.18213100	0.62599400	2.73080800
H	3.11820800	2.46330700	2.69025000	H	3.23858800	2.34281900	2.83498000
H	-3.38036800	1.92711500	2.83604400	H	-3.49262400	1.79469900	2.91332300
C	4.43618900	1.85932400	0.34068800	C	4.49195500	2.00413400	0.37811500
C	-4.53912600	1.40014600	0.38932000	C	-4.63158800	1.45772800	0.40102900
H	4.55527900	1.90055900	-0.74401700	H	4.55391100	2.16229900	-0.70046300
H	-4.61985500	1.52312100	-0.69261700	H	-4.68210800	1.66882900	-0.66905100
H	5.17014900	1.15251800	0.73708800	H	5.26146300	1.28132300	0.66221800
H	-5.21682900	0.59735500	0.69230600	H	-5.32079200	0.63770700	0.62006400
H	4.69975200	2.84621900	0.73322300	H	4.75035600	2.95191000	0.85963200
H	-4.90822700	2.32262700	0.84681100	H	-5.00725800	2.34273800	0.92217600
H	-0.07159600	1.18747700	0.79996000	H	-0.08880200	1.29904600	1.00620100
H	0.05065200	1.30479200	-1.74371200	H	0.02292500	1.55490500	-1.62400300
H	4.40832900	-3.13088700	-0.75688900	H	4.45274400	-2.92259600	-1.17818100
H	2.68299800	-2.93953400	-1.04429300	H	2.71389900	-2.70194300	-1.33498600
H	3.84916500	-1.94034400	-1.92424600	H	3.82992100	-1.63657400	-2.20442400
H	-4.00011000	-3.48344700	-0.98962200	H	-3.99282400	-3.36021400	-1.34084700
H	-3.58083500	-2.15670300	-2.06498100	H	-3.53723100	-1.95954100	-2.30198500
H	-2.30743700	-3.09074000	-1.26340000	H	-2.29526500	-2.91883900	-1.47991300
H	0.04463800	1.78630300	0.07450200	H	0.03197200	1.85047200	0.18031900
O	0.32446400	2.76515500	-0.77361600	O	0.24509500	2.87791500	-0.70296800
C	-0.47285200	3.85779600	-0.87301000	C	-0.64748500	3.89233000	-0.77639000
H	0.12214100	4.74143800	-1.16495900	H	-0.16052100	4.83169600	-1.09998800
H	-1.28984900	3.74992000	-1.60961800	H	-1.48857500	3.70444800	-1.47243800
C	0.13193500	-2.07666000	-0.30752400	C	0.16031500	-2.15380100	-0.41302200
C	0.07064500	-0.81480700	1.84883300	C	0.08647700	-0.96926400	1.98736900
Mn	0.05043400	-0.37481000	0.13750500	O	-1.32959600	4.14839200	0.46957000
O	-1.17936900	4.17340300	0.34366600	H	-0.63650400	4.29230700	1.12295100
H	-0.50605500	4.29955500	1.02098500	Re	0.05535100	-0.35397800	0.18140000
1Mn-TS(HCOOH-H-H)				1Re-TS(HCOOH-H-H)			
							
O	-0.04118900	2.95932700	-1.10378000	O	0.07280200	-3.01820200	-1.19941700
P	2.26142800	0.06174900	-0.03833200	P	-2.36228000	-0.00127800	-0.09140600
P	-2.29121800	0.05435900	-0.02960300	P	2.39661800	0.04174800	-0.07860500
C	2.39703700	-0.89449500	-1.63271000	C	-2.42531400	1.04171700	-1.64014300
C	-2.47400900	-0.76516200	-1.69480900	C	2.48494900	0.95815800	-1.70532800
H	2.37316400	-1.95284100	-1.35891500	H	-2.41504600	2.08209300	-1.30420100
H	-2.50684300	-1.84302700	-1.51666900	H	2.50354300	2.02453200	-1.46503100
H	3.33339300	-0.71279600	-2.16310300	H	-3.34424500	0.88814700	-2.20909600
H	-3.39244200	-0.48163400	-2.21028200	H	3.39225100	0.72609100	-2.26519800
C	1.19542800	-0.56966400	-2.50292300	C	-1.20406800	0.77661800	-2.50698300
C	-1.24341400	-0.44672600	-2.52590100	C	1.24247600	0.66927400	-2.53299400
H	1.17553700	-1.22691900	-3.38237500	H	-1.18468100	1.48157000	-3.34807200
H	-1.23909200	-1.05528800	-3.43964000	H	1.22875200	1.31957800	-3.41693800
H	1.24186400	0.46186800	-2.86190100	H	-1.23196800	-0.23450500	-2.92022000
H	-1.22422100	0.60485100	-2.82362000	H	1.22294700	-0.36799900	-2.87602200
N	-0.04142800	-0.73222300	-1.72131600	N	0.03530800	0.91589300	-1.71617800
C	-3.08441600	-1.23025400	1.09154700	C	3.22701600	1.27241000	1.07324600

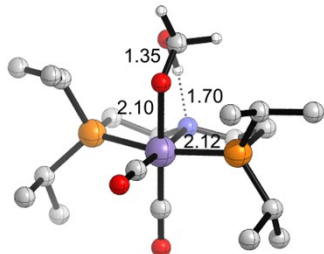
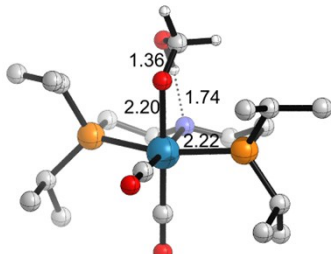
C 3.14973500 -1.08156900 1.16067100	C -3.29424200 1.07917200 1.12793100
H -2.44252400 -2.09630500 0.89554900	H 2.56656900 2.13928500 0.95626800
H 2.51282000 -1.97054100 1.12081000	H -2.66840300 1.97740000 1.13253200
C -3.49046300 1.50422700 -0.03633600	C 3.59150400 -1.40013400 -0.22359600
C 3.41913100 1.53498800 -0.22349100	C -3.48937700 -1.47034300 -0.41348100
C -3.51355100 2.26509100 -1.36134100	C 3.52416800 -2.09557800 -1.58215900
C 3.39974100 2.15955100 -1.61755600	C -3.35237600 -2.03717600 -1.82505000
O -0.00025500 1.57773800 2.77101100	O -0.00274300 -1.73268900 2.89391300
H 4.42143000 1.12920300 -0.05137300	H -4.50529500 -1.07692700 -0.30293100
H -4.47979500 1.06027200 0.11516100	H 4.58852600 -0.96080800 -0.11375200
C 3.13516300 2.59542600 0.84080500	C -3.26984700 -2.56617100 0.62887900
C -3.19999800 2.46045200 1.12030600	C 3.36634900 -2.40650100 0.90411400
H 3.13107900 2.18924300 1.85241500	H -3.37444700 -2.20326500 1.65141600
H -3.17210700 1.95962800 2.08835800	H 3.41939800 -1.95230500 1.89373100
H 2.16873100 3.07238200 0.67172400	H -2.27403900 -3.00115900 0.53302700
H -2.24100900 2.96216000 0.98049600	H 2.38794700 -2.88052400 0.81128400
H 3.90161200 3.37519700 0.79805500	H -4.00145500 -3.36630700 0.48190500
H -3.97499500 3.23139900 1.16621500	H 4.12701300 -3.19127100 0.85536400
C -2.97231700 -0.89462600 2.57594100	C 3.18631000 0.84739400 2.53846100
C 3.14723100 -0.57017900 2.59910800	C -3.30657500 0.51040000 2.54445400
H -3.63292500 -0.07022500 2.85475200	H 3.88880500 0.03581300 2.74187100
H 3.82293100 0.27865100 2.73120000	H -3.98914300 -0.33796200 2.63709600
H -1.95401800 -0.62906500 2.86094400	H 2.19078000 0.52178300 2.84245800
H 2.15236100 -0.27075700 2.92957400	H -2.31509700 0.18902300 2.86557100
H -3.26973100 -1.76182200 3.17250900	H 3.47342500 1.68943500 3.17457900
H 3.49291900 -1.36364900 3.26790000	H -3.65025800 1.27883200 3.24265400
C -4.51721200 -1.60096200 0.71530500	C 4.63628900 1.68082000 0.65095800
C 4.55753900 -1.48141100 0.72319600	C -4.69850800 1.47173800 0.67422700
H -4.62246400 -1.86065900 -0.33987500	H 4.68687100 2.00722300 -0.38960700
H 4.58738300 -1.87742200 -0.29379100	H -4.71301500 1.90281200 -0.32893900
H -5.21845800 -0.79305000 0.93926500	H 5.35253100 0.86682800 0.78862500
H 5.26122600 -0.64693900 0.78426900	H -5.38850100 0.62392900 0.69105300
H -4.83571500 -2.47039400 1.29799800	H 4.97786400 2.51495500 1.27074600
H 4.93445100 -2.26522600 1.38695800	H -5.10277300 2.22566100 1.35604600
H -0.16188900 -1.07185000 1.05800400	H 0.18944800 1.18949200 1.24707200
H -0.11946900 -1.74026500 -1.48345000	H 0.10823900 1.91903100 -1.43549900
H -4.24679300 3.07470000 -1.29807900	H 4.25457300 -2.90967900 -1.60580900
H -2.54768500 2.72046700 -1.58368900	H 2.54268000 -2.53651000 -1.76118100
H -3.80124900 1.63601700 -2.20526500	H 3.76064500 -1.42672200 -2.41140900
H 4.11830100 2.98397300 -1.65317500	H -4.05165700 -2.86951800 -1.94830200
H 3.68192000 1.45287900 -2.39992900	H -3.58600200 -1.30327800 -2.59856800
H 2.42103300 2.57478900 -1.86202200	H -2.35052800 -2.42846300 -2.00729800
H 0.21177100 -1.81528400 0.72013200	H -0.27161200 1.83749800 0.83831100
O 0.63102300 -3.15591400 0.67278700	O -0.79670500 3.19856200 0.73344200
C -0.02590300 1.89580800 -0.63814500	C 0.04405400 -1.96859400 -0.69598900
C -0.00630500 1.07795300 1.72826900	C 0.00567400 -1.19071100 1.86822000
Mn -0.01810100 0.31656700 0.13364000	Re 0.02032700 -0.28914300 0.18764900
C 0.12955200 -3.87775700 -0.24671200	C -0.24440000 3.95804400 -0.11865600
H 0.25157600 -4.96803000 -0.09481700	H -0.38240900 5.04289100 0.05838900
O -0.45714300 -3.48591200 -1.26431900	O 0.41495900 3.60826500 -1.11154600
1Mn-OCH₃⁻	1Re-OCH₃⁻
	
O -0.03633100 2.94805800 -0.78912500	O 0.00024800 -3.09002500 -0.77943200

P	-2.23895500	-0.04877100	0.18583400	P	2.34324700	0.05741000	0.26116800
P	2.24653400	-0.01855900	0.21228300	P	-2.34328300	0.05755800	0.26089600
C	-2.39607300	0.20414900	2.02450200	C	2.43145300	-0.11496500	2.11906500
C	2.41652600	0.35899200	2.03014700	C	-2.43120900	-0.11332200	2.11892200
H	-2.33209200	-0.78955400	2.47595000	H	2.42648900	0.90267300	2.51918500
H	2.43149100	-0.60409800	2.54725700	H	-2.42537400	0.90466700	2.51814500
H	-3.35119000	0.65351400	2.31405100	H	3.35249900	-0.60617500	2.44805800
H	3.34356100	0.89033900	2.26751400	H	-3.35256300	-0.60355000	2.44852700
C	-1.19473400	1.03051300	2.47422300	C	1.18237500	-0.84525800	2.60751500
C	1.16693600	1.12794500	2.45107500	C	-1.18261000	-0.84411000	2.60781900
H	-1.15019200	1.00724900	3.58265600	H	1.13946200	-0.74780400	3.71091200
H	1.12350400	1.14338400	3.55931700	H	-1.13966400	-0.74601500	3.71116500
H	-1.36967600	2.10084900	2.21761500	H	1.29958700	-1.93506100	2.41573000
H	1.27596700	2.19659700	2.15351600	H	-1.30051800	-1.93396100	2.41673000
N	0.00518900	0.48710500	1.90714000	N	0.00007300	-0.29057700	2.00600100
C	3.05524400	-1.71905000	0.10136000	C	-3.16490900	1.73368700	0.00202400
C	-3.04514200	-1.73746800	-0.03318000	C	3.16478500	1.73384100	0.00355300
H	2.55622800	-2.22876500	0.93015900	H	-2.62610700	2.33390400	0.74087400
H	-2.48023500	-2.31430000	0.70313900	H	2.62678300	2.33326300	0.74364900
C	3.51739800	1.13278900	-0.57943900	C	-3.59279900	-1.19828200	-0.37431600
C	-3.50551600	1.15451300	-0.53726400	C	3.59286500	-1.19769400	-0.37524300
C	3.34253100	2.58903800	-0.15238500	C	-3.35224600	-2.59001800	0.20694600
C	-3.40088800	2.55983500	0.05327300	C	3.35273500	-2.58995400	0.20494000
O	0.03904300	-0.46057500	-3.01241900	O	0.00066600	0.36410000	-3.21927900
H	-4.49022700	0.75369700	-0.27210600	H	4.57381400	-0.84942100	-0.03196900
H	4.49411000	0.79368200	-0.21640900	H	-4.57377400	-0.84994200	-0.03117100
C	-3.39200200	1.21273800	-2.05971100	C	3.58620800	-1.24444200	-1.90147200
C	3.49319600	1.01953100	-2.10208300	C	-3.58636200	-1.24630600	-1.90051000
H	-3.53913200	0.23768100	-2.52658400	H	3.87067400	-0.28951500	-2.34685400
H	3.71730000	0.00861600	-2.44692300	H	-3.87141000	-0.29191200	-2.34664900
H	-2.40629000	1.57398300	-2.35973700	H	2.59154100	-1.49929500	-2.27341800
H	2.51150300	1.29082900	-2.49602000	H	-2.59162600	-1.50097100	-2.27240100
H	-4.14294300	1.89777900	-2.47057300	H	4.29099400	-2.00360900	-2.25927900
H	4.23403500	1.69552800	-2.54486900	H	-4.29080900	-2.00614400	-2.25756100
C	2.66740900	-2.47846000	-1.16330700	C	-2.84960800	2.34517300	-1.35897900
C	-2.75333000	-2.37628900	-1.38605200	C	2.84828100	2.34684800	-1.35649500
H	3.05750400	-2.01168800	-2.07175300	H	-3.29267300	1.78301100	-2.18515100
H	-3.23817000	-1.85150500	-2.21398100	H	3.29061700	1.78554300	-2.18363800
H	1.57860100	-2.53172600	-1.21884800	H	-1.76837900	2.38820500	-1.49319700
H	-1.67680400	-2.39710200	-1.55077000	H	1.76690500	2.39000100	-1.48970400
H	3.06864100	-3.49841500	-1.12108300	H	-3.24750000	3.36595200	-1.40607900
H	-3.12285400	-3.40879100	-1.39467700	H	3.24616600	3.36766800	-1.40284300
C	4.55914600	-1.74134100	0.36041600	C	-4.65417700	1.77507300	0.33233600
C	-4.52742600	-1.79722400	0.32566200	C	4.65433800	1.77490100	0.33265300
H	4.83392800	-1.19855300	1.26958500	H	-4.87659400	1.34267900	1.31214700
H	-4.74151100	-1.33458800	1.29317100	H	4.87759500	1.34141600	1.31179400
H	5.12307200	-1.31066500	-0.47234500	H	-5.25032100	1.24192100	-0.41416300
H	-5.15108800	-1.30631600	-0.42773700	H	5.24985200	1.24260300	-0.41495200
H	4.90152000	-2.77588900	0.47807700	H	-5.00650500	2.81272600	0.34266300
H	-4.85541300	-2.84165700	0.38050600	H	5.00664400	2.81255300	0.34384100
H	0.18468700	-1.81719400	2.34066500	H	0.00076300	2.08573300	2.23322100
C	0.00873000	-2.53856100	1.52286800	C	0.00006100	2.75569500	1.35623800
H	4.14892300	3.19586500	-0.58138200	H	-4.12662200	-3.27638100	-0.15519100
H	2.39464900	2.99925700	-0.50094000	H	-2.38348100	-2.98713400	-0.09771800
H	3.37852000	2.71067800	0.93194400	H	-3.38993000	-2.59504300	1.29808500
H	-4.18266300	3.19699800	-0.37746200	H	4.12736800	-3.27577300	-0.15767300
H	-3.53073700	2.56520500	1.13703400	H	3.39036500	-2.59581100	1.29608100
H	-2.43757400	3.01882900	-0.17152500	H	2.38411500	-2.98716600	-0.10003900
O	-0.05625000	-1.95347600	0.28718900	O	-0.00158400	2.08636000	0.15708900
H	-0.92572200	-3.08894400	1.79899200	H	0.88055500	3.43039600	1.46515500

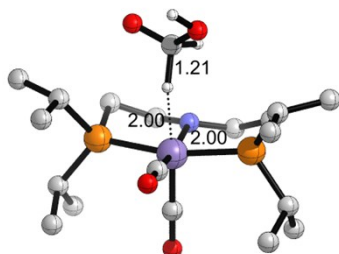
C -0.01054900 1.80682600 -0.52022200 Mn 0.00377000 0.11405000 -0.13740100 C 0.02256900 -0.27986900 -1.86029300 H 0.80666100 -3.31552200 1.58514900	C 0.00029400 -1.93477700 -0.53330200 Re 0.00009300 -0.09205600 -0.17035100 C 0.00039600 0.22308300 -2.05619600 H -0.87974700 3.43097000 1.46704400
1Mn-HCH₂O⁻ 	1Re-HCH₂O⁻ 
N 0.05294500 -0.20861600 1.89227900 P 2.28510600 0.07048900 0.19629400 P -2.22340500 -0.02837200 0.14138600 H -0.16580900 1.74808800 0.11823700 C -0.12841000 2.86333600 0.61936000 C 2.45126600 0.00558400 2.04661100 C -2.33519700 0.19613400 1.97639200 H 2.42594200 1.04498900 2.38502900 H -2.21705800 1.27743600 2.11487200 H 3.38910900 -0.44576700 2.38182300 H -3.29575100 -0.12121300 2.39316400 C 1.21191800 -0.70307300 2.57987100 C -1.15282400 -0.52111300 2.61060800 H 1.13480600 -0.49858200 3.66417400 H -1.06645400 -0.18837700 3.66267800 H 1.34857100 -1.80452900 2.50065900 H -1.36076500 -1.61206600 2.66793600 C -3.13446300 1.48315800 -0.47845800 C 3.10183100 1.72690100 -0.18418600 H -2.49071100 2.28774700 -0.06567600 H 2.41035600 2.41354100 0.31593400 C -3.36645600 -1.47273800 -0.27540200 C 3.52493600 -1.19102000 -0.46670700 H -4.38062500 -1.06795100 -0.18039400 H 4.51186400 -0.72522900 -0.36521700 C 0.06804400 0.17659100 -1.85407400 O 0.09635300 0.34585900 -3.00847300 C 3.27223200 -1.48686500 -1.94509200 C -3.16424400 -1.94382400 -1.71552000 H 3.26020500 -0.58671000 -2.55997400 H -3.25836000 -1.13193800 -2.43714600 H 2.31166400 -1.98619700 -2.07979600 H -2.17566000 -2.38717300 -1.84405500 H 4.05408100 -2.14998200 -2.33279100 H -3.90912400 -2.70732800 -1.96911300 C 3.53143800 -2.49296300 0.33365300 C -3.23546000 -2.64736900 0.69110500 H 2.55950600 -2.98705800 0.29783900 H -2.23112700 -3.07344600 0.66678100 H 3.79434500 -2.33814600 1.38137300 H -3.45683500 -2.36129600 1.72080500 H 4.26840600 -3.18214900 -0.09426800 H -3.93774000 -3.43993600 0.40661200 C -3.18316000 1.62788400 -1.99592400 C 3.11185500 2.08748000 -1.66672900 H -3.90736600 0.94677700 -2.45647100 H 3.84759300 1.49695400 -2.22063000	N 0.03707600 -0.05640000 1.96907600 P 2.37301700 0.10770800 0.25944200 P -2.32976200 -0.00476900 0.20982100 H -0.16984800 1.81856400 0.02455000 C -0.16391100 2.98830000 0.54608500 C 2.45239700 0.18263300 2.12030800 C -2.37063300 0.33657000 2.03538100 H 2.42690900 1.24528400 2.37795400 H -2.26456500 1.42581900 2.10054300 H 3.37767600 -0.24470200 2.51755800 H -3.31620400 0.03858400 2.49861500 C 1.20320200 -0.48282600 2.69130500 C -1.17003400 -0.31950400 2.70699700 H 1.12180400 -0.19493100 3.75595900 H -1.08642400 0.09125100 3.73094400 H 1.34156900 -1.58606900 2.69470600 H -1.36491900 -1.40507700 2.84313600 C -3.25268100 1.47467500 -0.46501200 C 3.19532200 1.74258100 -0.19377300 H -2.61205300 2.29289100 -0.08576600 H 2.51199900 2.44548600 0.29671500 C -3.46014300 -1.48492200 -0.06691400 C 3.62500000 -1.21122800 -0.23063000 H -4.47601700 -1.11414800 0.11317800 H 4.61346000 -0.78676600 -0.01967300 C 0.06234000 0.15730100 -2.06315400 O 0.08771200 0.33212600 -3.22118100 C 3.52639600 -1.53680300 -1.71987300 C -3.36476000 -1.99164800 -1.50509800 H 3.69419200 -0.66518400 -2.35315100 H -3.60550400 -1.21947600 -2.23616500 H 2.53755000 -1.93136600 -1.95969200 H -2.35694700 -2.35002200 -1.72163900 H 4.27072900 -2.29522900 -1.98716900 H -4.06031600 -2.82543100 -1.65494500 C 3.46099500 -2.48396500 0.59845900 C -3.18141200 -2.61889700 0.91615800 H 2.47615000 -2.92826000 0.44743800 H -2.15720600 -2.98308900 0.81702400 H 3.59290400 -2.30599800 1.66716800 H -3.33420800 -2.31358200 1.95278400 H 4.20972600 -3.22177100 0.28909600 H -3.85455400 -3.45939800 0.71170500 C -3.28281200 1.56416800 -1.98725300 C 3.17175000 2.05528000 -1.68673900 H -4.01258900 0.87822500 -2.42987700

H -2.21213900 1.45797000 -2.46055700	H 3.91168900 1.46567200 -2.23494800
H 2.13547000 1.94122000 -2.12825400	H -2.30788800 1.35758300 -2.42887000
H -3.49455000 2.64706400 -2.24999600	H 2.19094300 1.86482400 -2.12256900
H 3.38456900 3.14109800 -1.78937800	H -3.57220600 2.57820100 -2.28322400
C -4.52418000 1.66576100 0.12674200	H 3.41449700 3.11081000 -1.84892200
C 4.48722400 1.91422400 0.43087200	C -4.64738100 1.66426900 0.12569200
H -4.50695600 1.62655500 1.21737200	C 4.59071300 1.94176400 0.39290800
H 4.50224600 1.69570100 1.50044000	H -4.63837100 1.65470900 1.21750600
H -5.24338400 0.92105500 -0.23373500	H 4.62411400 1.74194000 1.46616600
H 5.23628600 1.28091800 -0.05406700	H -5.35381100 0.90085500 -0.21904600
H -4.91242200 2.65123500 -0.15298500	H 5.32808600 1.29702400 -0.09433800
H 4.81352700 2.95220400 0.30205900	H -5.04485500 2.63651900 -0.18486400
H 0.56194700 2.63871700 1.46810800	H 4.91743400 2.97612300 0.23948900
H 0.44874300 3.40100400 -0.17925000	H 0.51010700 2.75015200 1.40069100
O -1.29244000 3.35329500 0.92733800	H 0.41729900 3.48717900 -0.26985700
C 0.10237700 -1.86587000 -0.38905900	O -1.33106100 3.45074500 0.81626400
O 0.13239600 -3.02200800 -0.56736800	C 0.10858700 -1.98889700 -0.49283800
Mn 0.04818500 -0.15588500 -0.12398500	O 0.13968700 -3.14211500 -0.72299300
	Re 0.04004000 -0.13914200 -0.17545900
1Mn-TS(HCH₂O)	1Re-TS(HCH₂O)
	
N 0.05401200 -0.02263600 1.95535900	N 0.03574100 0.05276900 2.00138600
P 2.26800000 0.08076200 0.18180500	P 2.36612400 0.11891300 0.24743900
P -2.19390000 -0.02518200 0.12863500	P -2.31749200 -0.00436800 0.20323000
H -0.09385900 1.53175500 -0.12822100	H -0.11669000 1.70666900 -0.12440900
C -0.13790300 2.97128600 0.83493600	C -0.16592600 3.09479800 0.71411500
C 2.46036300 0.08838600 2.03578000	C 2.45693000 0.23057200 2.10863800
C -2.35566300 0.20967400 1.96536500	C -2.39066600 0.29681500 2.03995500
H 2.48064100 1.13844500 2.34208300	H 2.44937500 1.29721800 2.35213000
H -2.30520200 1.29068800 2.12630000	H -2.34391400 1.38405700 2.15396100
H 3.38696200 -0.38345100 2.37419300	H 3.37791900 -0.20287400 2.50910200
H -3.30529700 -0.15739800 2.36535100	H -3.32406200 -0.05878800 2.48659100
C 1.20873200 -0.56573900 2.60877700	C 1.20346200 -0.41386900 2.69434700
C -1.14700000 -0.45134200 2.61494100	C -1.16387100 -0.32771000 2.69719000
H 1.17616900 -0.36718400 3.69887400	H 1.15109300 -0.14688600 3.76787600
H -1.12741900 -0.17223100 3.68798000	H -1.12597300 0.01609100 3.74954300
H 1.29815500 -1.67264700 2.51641800	H 1.31655000 -1.52087500 2.67094200
H -1.28429500 -1.55638500 2.60542900	H -1.30019800 -1.43011000 2.75416000
C -3.14012300 1.46235800 -0.52620600	C -3.25812900 1.47738600 -0.45886000
C 3.12360300 1.70784200 -0.25620800	C 3.21078200 1.73442400 -0.24063900
H -2.52338600 2.28237300 -0.14291100	H -2.64232300 2.29668000 -0.06624100
H 2.52909300 2.40535000 0.34247700	H 2.57937500 2.45033100 0.29698300
C -3.34675400 -1.46970800 -0.28436600	C -3.46073500 -1.47321900 -0.10150000
C 3.51053900 -1.21750900 -0.41307700	C 3.62264400 -1.21157600 -0.20907000
H -4.36100500 -1.05653300 -0.24400200	H -4.47813000 -1.09371000 0.04853000
H 4.50240900 -0.76930800 -0.28896400	H 4.60987100 -0.78410600 0.00033300
C 0.06826700 0.01774600 -1.88204800	C 0.05687200 0.01186500 -2.08179200
O 0.08995500 0.12933300 -3.04531100	O 0.07615500 0.10322600 -3.25015900
C 3.29758600 -1.53809800 -1.89184000	C 3.53212500 -1.56051400 -1.69327500
C -3.09040600 -1.99122100 -1.69864100	C -3.32758400 -1.98291500 -1.53578500
H 2.31612400 -1.98831000 -2.04997200	H 2.53819600 -1.94155200 -1.93495000
H -3.14260900 -1.20469300 -2.45195300	H -3.53887200 -1.21028000 -2.27558900
H 4.05679800 -2.24964700 -2.23685800	

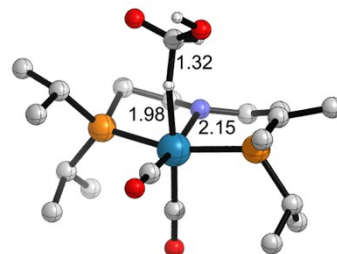
H -2.10209900 -2.44762500 -1.76900400 H 3.35488400 -0.65311900 -2.52696000 H -3.83308600 -2.75530000 -1.95763300 C 3.47285500 -2.50310500 0.41200000 C -3.26862100 -2.61800500 0.71945600 H 2.50260800 -2.99533300 0.34192700 H -2.26970300 -3.05558900 0.74688500 H 3.68656300 -2.32787000 1.46782000 H -3.52810900 -2.30345100 1.73189100 H 4.22796800 -3.20204800 0.03346200 H -3.96891600 -3.40984600 0.42775100 C -3.16236200 1.57047700 -2.04803100 C 2.95853900 2.11832100 -1.71546400 H -3.84792000 0.84719100 -2.50085200 H 3.56681200 1.50147000 -2.38260700 H -2.17353000 1.42335500 -2.48206000 H 1.91870400 2.04042400 -2.03284100 H -3.50890000 2.56837400 -2.33881100 H 3.28004700 3.15701400 -1.85259600 C -4.54388300 1.63289000 0.05057700 C 4.57732200 1.82763200 0.19548900 H -4.54997800 1.59794400 1.14177300 H 4.71479900 1.52755400 1.23710400 H -5.24040900 0.87302100 -0.31898800 H 5.24506200 1.21969900 -0.42168400 H -4.94519200 2.60842200 -0.24575500 H 4.91478600 2.86630900 0.10319800 H 0.07454000 2.25111300 1.64409300 H 0.74411700 3.34109900 0.26993800 O -1.19954600 3.60331500 0.77217800 C 0.09351600 -1.90205400 -0.21030500 O 0.10561400 -3.06819500 -0.32419700 Mn 0.04817000 -0.15333900 -0.13858200	H 4.26630300 -2.33477200 -1.94319300 H -2.31607000 -2.34837400 -1.72119100 H 3.71934600 -0.70149900 -2.33891400 H -4.02519900 -2.81124800 -1.70551500 C 3.45864700 -2.47123800 0.63925500 C -3.22544400 -2.61223600 0.88745600 H 2.47934400 -2.92615100 0.48676800 H -2.20794400 -2.99845900 0.80975100 H 3.57804700 -2.27444800 1.70624900 H -3.39400600 -2.30567900 1.92134000 H 4.21708300 -3.20783800 0.35049000 H -3.91212500 -3.43798700 0.66798900 C -3.24896100 1.59083100 -1.98019100 C 3.09305900 2.06240800 -1.72536100 H -3.94308000 0.88760600 -2.45069400 H 3.75928400 1.44363600 -2.33229300 H -2.25406100 1.41767800 -2.39081900 H 2.07305300 1.91630000 -2.08186800 H -3.56092900 2.59917700 -2.27236200 H 3.37128400 3.10733700 -1.90153000 C -4.66957100 1.63710200 0.10042700 C 4.64399800 1.89472300 0.25970500 H -4.69133800 1.58654500 1.19133900 H 4.74110600 1.66345600 1.32326300 H -5.35651300 0.87894600 -0.28978100 H 5.33691200 1.25154100 -0.29032200 H -5.07043000 2.61491500 -0.18778800 H 4.98068000 2.92721400 0.11380700 H 0.11058900 2.49098100 1.59622500 H 0.69251200 3.46825800 0.11488100 O -1.25702300 3.68461000 0.64767100 C 0.10264200 -2.03030900 -0.32821900 O 0.12460100 -3.19450900 -0.49170300 Re 0.03870400 -0.13582900 -0.17999200
2Mn⁻  P -2.16308400 0.07989000 -0.31820000 P 2.16306800 0.07977500 -0.31821900 C -2.38859500 -0.85373300 -1.92024100 C 2.38856200 -0.85410000 -1.92012200 H -2.36360700 -0.11619400 -2.72750800 H 2.36379600 -0.11668300 -2.72750600 H -3.34413000 -1.38539700 -1.96622900 H 3.34401200 -1.38593300 -1.96592000 C -1.18090700 -1.77335100 -2.05564700 C 1.18072700 -1.77354200 -2.05551100 H -1.15725100 -2.17784100 -3.08945900 H 1.15706200 -2.17811200 -3.08929000 H -1.32689900 -2.66234900 -1.39591500 H 1.32654900 -2.66251200 -1.39570200 N -0.00004700 -1.02331800 -1.76881000 C 2.82076100 1.78034200 -0.82770200 C -2.82077200 1.78053200 -0.82744300 H 2.19028900 1.95428100 -1.70704700	2Re⁻  P -2.30322900 0.06710400 -0.38126700 P 2.30322400 0.06710100 -0.38126300 C -2.41113600 -0.90371300 -1.97474700 C 2.41113100 -0.90372100 -1.97474000 H -2.37232200 -0.17234500 -2.78728900 H 2.37232700 -0.17235600 -2.78728600 H -3.34901700 -1.46158100 -2.05726600 H 3.34901000 -1.46159400 -2.05725100 C -1.18276600 -1.80482300 -2.06852400 C 1.18275800 -1.80482600 -2.06852000 H -1.15022900 -2.23768300 -3.08960700 H 1.15022100 -2.23768500 -3.08960300 H -1.32004300 -2.67385700 -1.38298000 H 1.32003000 -2.67386100 -1.38297600 N -0.00000400 -1.04544400 -1.79969000 C 3.04290800 1.71644000 -0.93094300 C -3.04291300 1.71644500 -0.93094400 H 2.39349400 1.92232100 -1.78910600

H -2.19030800 1.95457400 -1.70677300	H -2.39351700 1.92230700 -1.78912500
C 3.55860200 -0.61911300 0.75447500	C 3.64185900 -0.70389100 0.70433300
C -3.55858100 -0.61913100 0.75446100	C -3.64185400 -0.70389300 0.70433700
C 3.45497800 -2.13731100 0.88159300	C 3.46778000 -2.21696000 0.81120300
C -3.45511200 -2.13736700 0.88123600	C -3.46775600 -2.21695900 0.81122000
H -4.49788800 -0.38268400 0.24046400	H -4.60122400 -0.49961100 0.21429900
H 4.49786800 -0.38287900 0.24030200	H 4.60122300 -0.49959600 0.21429100
C -3.57534000 0.02024000 2.14083300	C -3.64136400 -0.07550900 2.09584900
C 3.57561400 0.02056100 2.14070100	C 3.64137300 -0.07551300 2.09584800
H -3.77090100 1.09325600 2.10395800	H -3.87604200 0.98989700 2.07358400
H 3.77142000 1.09352600 2.10356500	H 3.87605800 0.98989200 2.07358600
H -2.61541000 -0.12213800 2.64223700	H -2.65943600 -0.18647400 2.56158000
H 2.61570000 -0.12149500 2.64222800	H 2.65944600 -0.18647600 2.56158000
H -4.35361200 -0.43837300 2.76237000	H -4.38302200 -0.56807700 2.73525800
H 4.35383800 -0.43808300 2.76227600	H 4.38302900 -0.56808700 2.73525600
C 2.50537600 2.89141300 0.16729200	C 2.82626100 2.84719200 0.06818600
C -2.50536000 2.89148100 0.16768000	C -2.82622500 2.84720700 0.06816500
H 3.11748200 2.82400300 1.07027300	H 3.47151300 2.75083100 0.94529800
H -3.11751100 2.82400400 1.07062600	H -3.47147100 2.75087400 0.94528600
H 1.45690700 2.85073900 0.46235300	H 1.78920900 2.86405900 0.40458700
H -1.45690700 2.85073800 0.46278500	H -1.78916900 2.86405600 0.40455500
H 2.70122200 3.87069600 -0.28584800	H 3.05627900 3.81150900 -0.40009000
H -2.70114100 3.87082300 -0.28536000	H -3.05622700 3.81152200 -0.40012200
C 4.28354500 1.81388300 -1.26214700	C 4.49011500 1.65179200 -1.41079700
C -4.28355800 1.81415700 -1.26187800	C -4.49013400 1.65181000 -1.41075900
H 4.51923000 1.02580200 -1.98209700	H 4.65204400 0.84641900 -2.13196700
H -4.51927000 1.02615500 -1.98190500	H -4.65209300 0.84642900 -2.13191400
H 4.95968500 1.70299200 -0.40919100	H 5.18387200 1.50256300 -0.57813100
H -4.95969700 1.70320400 -0.40893000	H -5.18387100 1.50260100 -0.57807300
H 4.51820900 2.77519800 -1.73453300	H 4.77109700 2.59308400 -1.89732900
H -4.51819800 2.77552600 -1.73416600	H -4.77111600 2.59309900 -1.89729500
H -0.00001900 1.27318200 -0.64520900	H -0.00000100 1.48090900 -0.84331400
H 4.30387600 -2.52028100 1.46085200	H 4.26781000 -2.63795700 1.43145400
H 2.53822200 -2.42888900 1.39543200	H 2.51375300 -2.47055500 1.27555400
H 3.46113700 -2.63767900 -0.08882900	H 3.50650100 -2.71032500 -0.16198900
H -4.30391200 -2.52035000 1.46063200	H -4.26777200 -2.63795800 1.43148800
H -3.46158600 -2.63753000 -0.08928900	H -3.50648400 -2.71033600 -0.16196600
H -2.53826600 -2.42916300 1.39479200	H -2.51371800 -2.47053500 1.27556100
Mn -0.00000600 -0.10175300 0.16073400	Re -0.00000400 0.02819600 0.15430400
C 0.00002500 0.83869400 1.63269900	C -0.00001100 1.13112300 1.70514100
C -0.00007000 -1.63663800 1.03909200	C -0.00001500 -1.55514100 1.25388500
O 0.00040900 1.47337000 2.61830200	O 0.00005200 1.81418100 2.66140300
O -0.00024300 -2.61014000 1.69106600	O -0.00002900 -2.46386500 1.99925300
1Mn-OCH₂OH⁻	1Re-OCH₂OH⁻
	
O -0.13569400 -3.08434700 -0.01794700	O -0.11508600 -3.21160800 0.10697100
P 2.25122600 -0.06596100 0.12530000	P 2.35013900 -0.01796400 0.18126500
P -2.26939600 0.05967400 0.13330300	P -2.36304800 0.10304100 0.20153100
C 2.45154400 -0.07625400 1.98082100	C 2.47703200 0.16324400 2.03712400
C -2.38771800 0.37373400 1.96579700	C -2.41029100 0.54020400 2.01688600
H 2.59171800 0.96452300 2.27997600	H 2.60912300 1.23021600 2.22974600
H -2.29323000 1.45539500 2.09898000	H -2.34833000 1.63128000 2.06877200
H 3.32375300 -0.64995100 2.30548700	H 3.34128500 -0.36840400 2.44419300

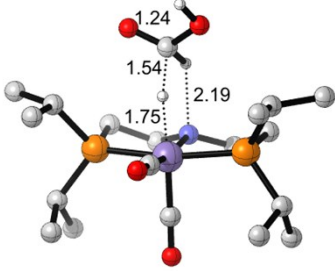
H	-3.34354900	0.05850400	2.39549300	H	-3.34117800	0.22969000	2.50114800
C	1.15231400	-0.60551900	2.58328400	C	1.17129900	-0.30857400	2.67416300
C	-1.19906300	-0.31590500	2.62767500	C	-1.18658300	-0.06094600	2.70380700
H	1.15889400	-0.39843100	3.67099200	H	1.17599800	-0.00302400	3.73764700
H	-1.16055500	-0.00986300	3.69155700	H	-1.14427200	0.32842600	3.73884300
H	1.12286900	-1.71079400	2.49158600	H	1.14071400	-1.41609200	2.67820500
H	-1.37512300	-1.41147100	2.64326700	H	-1.32756000	-1.15587400	2.80224400
N	0.02315600	0.03389500	1.94823100	N	0.02852500	0.26193900	1.98968700
C	-3.11007700	1.58617300	-0.58088200	C	-3.23469200	1.58175200	-0.57530600
C	3.11438400	1.53964800	-0.33963900	C	3.21581900	1.54416600	-0.40486200
H	-2.57184400	2.37267100	-0.04472600	H	-2.70748200	2.40502200	-0.08343700
H	2.59466600	2.22040400	0.34293400	H	2.66755300	2.28487900	0.18742700
C	-3.52640900	-1.32002000	-0.16906600	C	-3.59212800	-1.31255100	0.02440900
C	3.44797600	-1.41529900	-0.43769700	C	3.53412600	-1.42532700	-0.22151400
C	-3.42326300	-2.47106400	0.83008800	C	-3.38558500	-2.40964800	1.06690200
C	3.25705200	-2.73883800	0.30125900	C	3.28958300	-2.66122900	0.64202000
O	-0.01988600	-0.41682300	-3.07845400	O	-0.04674800	-0.61345900	-3.23253300
H	4.44634200	-1.03709000	-0.19041300	H	4.53508300	-1.04185800	0.00773500
H	-4.51014500	-0.85663500	-0.03800600	H	-4.58065700	-0.87070800	0.19138300
C	3.37065800	-1.63964800	-1.94629500	C	3.46995500	-1.79137200	-1.70249000
C	-3.42079700	-1.84599500	-1.59964800	C	-3.54104700	-1.89642900	-1.38583000
H	3.58858700	-0.73385400	-2.51363100	H	3.73673200	-0.95480300	-2.34984400
H	-3.56829300	-1.06139000	-2.34332100	H	-3.78152800	-1.15651200	-2.15109700
H	2.37482500	-1.97842900	-2.23884900	H	2.46260300	-2.11161200	-1.97586500
H	-2.43904400	-2.28826500	-1.77901000	H	-2.54468500	-2.28551600	-1.60389000
H	4.09104200	-2.40742800	-2.25190100	H	4.16042900	-2.61489700	-1.91743200
H	-4.17691400	-2.61997300	-1.77523900	H	-4.25837300	-2.71962800	-1.47874700
C	-2.81545300	1.79901300	-2.06156500	C	-2.95218800	1.71832000	-2.06775600
C	2.79655000	2.00244300	-1.75794800	C	2.94672500	1.86119500	-1.87202300
H	-3.27025500	1.03368600	-2.69656400	H	-3.40661000	0.91579600	-2.65466800
H	3.23157500	1.35327300	-2.52328900	H	3.41779500	1.14571000	-2.55176600
H	-1.73777500	1.80604900	-2.22134900	H	-1.87623700	1.71884500	-2.24185400
H	1.71304700	2.04495800	-1.88439800	H	1.87036700	1.87647000	-2.04920000
H	-3.21688600	2.76785600	-2.38159600	H	-3.36266100	2.66585400	-2.43577600
H	3.20469400	3.00803000	-1.91590100	H	3.34975300	2.85222600	-2.11228900
C	-4.59686300	1.71980300	-0.26254700	C	-4.72099300	1.70232300	-0.25081700
C	4.60910700	1.57862500	-0.03675800	C	4.69820000	1.62096400	-0.05340800
H	-4.81341700	1.55947600	0.79730800	H	-4.92467400	1.60237200	0.81903900
H	4.83817600	1.24412700	0.97906400	H	4.89006100	1.39101500	0.99843200
H	-5.20520600	1.01844900	-0.84153700	H	-5.31516800	0.95118500	-0.77943800
H	5.18691800	0.96331100	-0.73381400	H	5.29977800	0.93981200	-0.66347800
H	-4.94109300	2.72808500	-0.51894700	H	-5.09232100	2.68392300	-0.56557700
H	4.97912700	2.60564800	-0.13397800	H	5.07206200	2.63393800	-0.24015300
H	-1.10659600	3.08540400	0.91438400	H	-1.12410100	3.15706900	0.71429300
C	-0.05961400	2.87534100	0.56172000	C	-0.06737900	3.00587600	0.37372700
H	-4.20979500	-3.20581800	0.62089000	H	-4.14961100	-3.18444300	0.93440900
H	-2.46376300	-2.98351000	0.75729400	H	-2.40954200	-2.88395400	0.96123100
H	-3.55161400	-2.13670600	1.86114800	H	-3.47326700	-2.03267000	2.08771200
H	4.03881700	-3.44401400	-0.00498600	H	4.04211300	-3.42350100	0.40902600
H	3.32340800	-2.62506800	1.38487100	H	3.36118000	-2.44460800	1.70967300
H	2.29245300	-3.19220500	0.07335700	H	2.30679600	-3.09321400	0.45236900
O	-0.01757800	1.91043800	-0.38518100	O	0.04072800	2.00178000	-0.53124300
C	-0.07431900	-1.91437300	-0.05597300	C	-0.06884300	-2.03600200	0.01152800
Mn	-0.02207500	-0.17991300	-0.15727200	Re	-0.01952200	-0.16864100	-0.18673800
C	-0.02172900	-0.28725800	-1.92198400	C	-0.03608400	-0.41908100	-2.07922800
H	0.31315000	3.84012400	0.15891300	H	0.24784700	3.96634000	-0.07640400
O	0.72064500	2.61938600	1.72391500	O	0.72692600	2.85359300	1.54422900
H	0.43781100	1.67891500	1.95656900	H	0.45094200	1.94578700	1.86963700
1Mn-HCH(OH)O⁻				1Re-HCH(OH)O⁻			

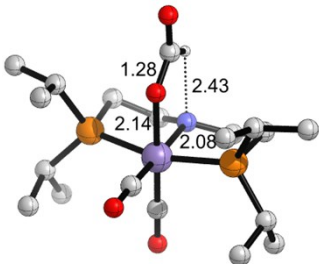
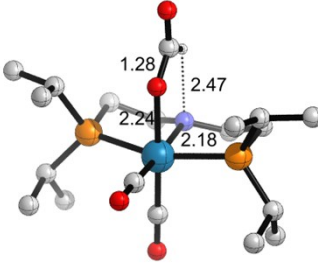


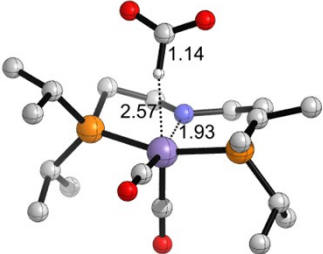
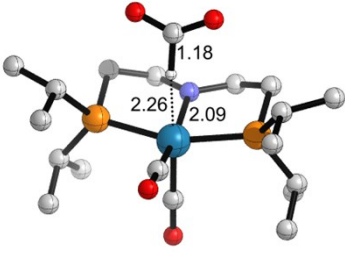
N	-0.01120800	-0.21055400	1.87995500
P	2.25807700	-0.10612900	0.12761100
P	-2.27595600	-0.07634900	0.17197700
H	0.13215500	1.73735600	0.09911400
C	0.14292800	2.77186100	0.73493400
C	2.38739400	0.16066900	1.95677200
C	-2.41423600	0.03267700	2.02062400
H	2.29768400	1.24533800	2.07588100
H	-2.37804600	1.10041100	2.25413200
H	3.34219400	-0.17079900	2.37537500
H	-3.35132300	-0.37465800	2.41011700
C	1.19142300	-0.51375900	2.61332100
C	-1.17733600	-0.63126800	2.61013800
H	1.10737400	-0.14102900	3.65132500
H	-1.09403600	-0.33288300	3.67165000
H	1.37824300	-1.60477300	2.71058000
H	-1.31509300	-1.73393400	2.62772400
C	-3.19164000	1.47455700	-0.37443500
C	3.17317800	1.38355100	-0.54512900
H	-2.50404700	2.26335000	-0.05179900
H	2.52032400	2.19681400	-0.17743700
C	-3.44983400	-1.46726100	-0.33702400
C	3.40064500	-1.56078300	-0.25486400
H	-4.45566900	-1.03610500	-0.27285600
H	4.41417200	-1.15020500	-0.17892700
C	-0.04118500	0.07053200	-1.85508600
O	-0.06903400	0.23172200	-3.00976500
C	3.19329100	-2.07994200	-1.67791700
C	-3.20209700	-1.90924900	-1.77996400
H	3.27281100	-1.29159400	-2.42660900
H	-3.22237300	-1.07812300	-2.48468600
H	2.21002600	-2.53979800	-1.78492300
H	-2.23151300	-2.39733600	-1.87505000
H	3.94591200	-2.84217500	-1.91142700
H	-3.97031300	-2.62899100	-2.08562600
C	3.28040300	-2.70501200	0.74931100
C	-3.39347800	-2.67464000	0.59776200
H	2.27861200	-3.13722300	0.74288500
H	-2.40243700	-3.13074000	0.59915500
H	3.50589600	-2.38621100	1.76836500
H	-3.65068400	-2.41792200	1.62673500
H	3.98553900	-3.50218300	0.48601400
H	-4.10603000	-3.43504100	0.25789000
C	-3.32694600	1.60929500	-1.88883400
C	3.24258400	1.45851300	-2.06714700
H	-4.07998700	0.92644700	-2.29440200
H	3.97669300	0.76031000	-2.48348300
H	-2.38252800	1.42918600	-2.40228200
H	2.27938700	1.26248800	-2.53791500
H	-3.64574900	2.62759600	-2.13432900
H	3.55478100	2.46574500	-2.36437300
C	-4.54108800	1.68722600	0.30805900



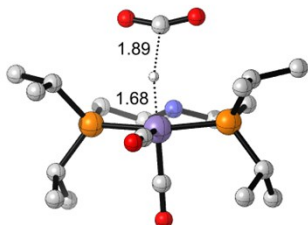
N	-0.00674500	-0.03076700	1.96124100
P	2.35770500	-0.05877400	0.20158200
P	-2.36491000	-0.03683600	0.23033800
H	0.10771800	1.77036600	0.00701000
C	0.15455500	2.89116400	0.69338300
C	2.41546700	0.29327700	2.02710800
C	-2.43116800	0.19824100	2.07704200
H	2.35317900	1.38339000	2.09829000
H	-2.41304900	1.28052800	2.23539000
H	3.35094600	-0.03663800	2.48884300
H	-3.35198400	-0.19570100	2.51703200
C	1.19419200	-0.32143900	2.70277000
C	-1.18007300	-0.40885400	2.70389000
H	1.12153900	0.09863100	3.72365100
H	-1.10784700	-0.04243000	3.74511100
H	1.35678900	-1.41085800	2.84626200
H	-1.30518800	-1.50954300	2.78874200
C	-3.31777500	1.46910500	-0.36903700
C	3.30496500	1.39730900	-0.49845400
H	-2.66211200	2.27525800	-0.02230600
H	2.65806000	2.22398100	-0.16384400
C	-3.51813700	-1.48844400	-0.11372500
C	3.48406600	-1.54771200	-0.05308200
H	-4.53169600	-1.10674000	0.05636600
H	4.50106000	-1.17239400	0.11111300
C	-0.02792100	0.07852000	-2.06961900
O	-0.04614200	0.25067800	-3.22775100
C	3.38153900	-2.08890400	-1.47839700
C	-3.40328300	-1.96047900	-1.56255500
H	3.60637900	-1.33223200	-2.23012500
H	-3.61114300	-1.16679100	-2.28018500
H	2.37736300	-2.46580600	-1.67754100
H	-2.39968500	-2.33574200	-1.76728100
H	4.08646400	-2.91726900	-1.61396300
H	-4.11369200	-2.77460400	-1.74613500
C	3.21703200	-2.66102800	0.95712500
C	-3.28139700	-2.65622800	0.84183500
H	2.19489500	-3.03372900	0.87264600
H	-2.26885800	-3.04957100	0.74136000
H	3.37585500	-2.33355300	1.98606100
H	-3.43640500	-2.37800700	1.88570400
H	3.89367900	-3.50185200	0.76620000
H	-3.97788500	-3.46912800	0.60703300
C	-3.38753600	1.58895800	-1.88870300
C	3.36269400	1.43572300	-2.02251900
H	-4.12110600	0.90201800	-2.32081300
H	4.09903500	0.73384900	-2.42686200
H	-2.42030400	1.39788200	-2.35385200
H	2.39523200	1.21558900	-2.47431200
H	-3.69461600	2.60415500	-2.16143300
H	3.66045400	2.43819500	-2.34816500
C	-4.69656700	1.64552300	0.26205400

C 4.55427800 1.59871800 0.06928300	C 4.68985100 1.60075200 0.11033000
H -4.46815500 1.65893600 1.39678700	H -4.66532200 1.59882900 1.35273300
H 4.52167900 1.61870100 1.15994800	H 4.66258500 1.62935800 1.20155200
H -5.28234900 0.94291300 -0.00099400	H -5.40794700 0.89131600 -0.08906100
H 5.27672500 0.83487100 -0.24027100	H 5.39675400 0.82125300 -0.19419600
H -4.93888600 2.67015400 0.03308800	H -5.10538700 2.62434400 -0.01163200
H 4.94870100 2.56684800 -0.25834600	H 5.10040800 2.55832900 -0.22792400
H -0.37758400 2.44128000 1.66009600	H -0.20539800 2.46477500 1.64912900
O 1.31186700 3.28761000 0.85372800	O 1.29078600 3.43992400 0.62695700
O -0.81123900 3.62424500 0.02940300	O -0.93016300 3.64566400 0.13003500
H -0.22035000 4.24364700 -0.41584400	H -0.47222400 4.26208700 -0.45529200
C -0.03545400 -1.95698400 -0.35668000	C -0.02986900 -2.05332600 -0.46025300
O -0.04267600 -3.11855300 -0.50104300	O -0.03200300 -3.21261600 -0.66250000
Mn -0.01573600 -0.24568000 -0.11984500	Re -0.00953200 -0.19672200 -0.17882500
Mn-TS(HCH(OH)O)	
	
N 0.01417100 0.03389200 -1.91640800	N -0.00699600 0.04313000 1.96741700
P -2.24532600 -0.06981100 -0.11436100	P 2.35501200 -0.04806900 0.19775100
P 2.25896800 -0.06324700 -0.13924700	P -2.36124200 -0.03305200 0.22108900
H -0.07207600 1.55250000 0.13490700	H 0.08457300 1.72606700 -0.07274100
C -0.14642400 2.82619000 -0.71909900	C 0.15353600 2.92208300 0.68455600
C -2.39790400 0.28058500 -1.93214100	C 2.41952300 0.32588400 2.01996000
C 2.42600500 0.15877100 -1.97886700	C -2.43434000 0.23825300 2.06350100
H -2.34411700 1.36971000 -2.01677400	H 2.36979400 1.41686900 2.08414300
H 2.43129400 1.23945200 -2.14867400	H -2.42594200 1.32342300 2.20213100
H -3.34526700 -0.05851600 -2.36100500	H 3.35186700 -0.00887000 2.48445200
H 3.35338200 -0.25545100 -2.38377400	H -3.35254600 -0.15502400 2.50945100
C -1.18543100 -0.33590100 -2.61898100	C 1.19216900 -0.27168900 2.70100200
C 1.17663200 -0.43184500 -2.62061000	C -1.17978500 -0.34870100 2.70323800
H -1.15171500 0.02791900 -3.66509600	H 1.13355800 0.14295500 3.72556300
H 1.14401500 -0.11523900 -3.68187300	H -1.12139400 0.02177300 3.74450800
H -1.32432100 -1.43667000 -2.69896000	H 1.33914400 -1.36473200 2.83596400
H 1.26409000 -1.54086000 -2.65081100	H -1.29109200 -1.45111800 2.79012500
C 3.24245600 1.40879800 0.50602800	C -3.32394600 1.45502900 -0.40836900
C -3.21155200 1.35074500 0.64818100	C 3.31248400 1.39308800 -0.52390600
H 2.61080700 2.23772000 0.17491800	H -2.68529500 2.26960900 -0.05131100
H -2.56825600 2.19625500 0.37787600	H 2.67460500 2.22751900 -0.19962300
C 3.39760000 -1.51572000 0.28860700	C -3.51235200 -1.49367700 -0.09669700
C -3.38054300 -1.55275100 0.20185400	C 3.48354200 -1.53987100 -0.03944200
H 4.41191500 -1.10072400 0.28678600	H -4.52713000 -1.10864900 0.05719400
H -4.39589500 -1.13959700 0.20405900	H 4.50185700 -1.15938000 0.10282000
C 0.02509500 -0.06920300 1.89032000	C -0.02272700 -0.00263500 -2.08233900
O 0.04246400 0.01217300 3.05594500	O -0.03763100 0.12006900 -3.24736300
C -3.11224900 -2.18016400 1.57052600	C 3.36254400 -2.11012100 -1.45197500
C 3.10125000 -2.05801400 1.68748600	C -3.38710500 -1.99716500 -1.53403400
H -3.15054900 -1.45212700 2.38092000	H 3.57343200 -1.36809600 -2.22220800
H 3.11543000 -1.28087000 2.45195600	H -3.58858800 -1.21882400 -2.27029700
H -2.12819900 -2.64917900 1.59616500	H 2.35654800 -2.49323900 -1.62864400
H 2.11884400 -2.53014900 1.72012800	H -2.38207500 -2.37701000 -1.72313400
H -3.85918500 -2.95546100 1.77914500	H 4.06814200 -2.93898800 -1.58126000
H 3.84712600 -2.81374200 1.96095900	H -4.09685800 -2.81452400 -1.70584100
C -3.31447300 -2.62153000 -0.88736000	C 3.23556100 -2.63433400 0.99608300

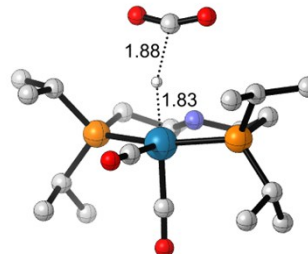
C 3.35670300 -2.65076000 -0.73329200 H -2.31778400 -3.05938000 -0.95642600 H 2.36184400 -3.09251200 -0.79950700 H -3.58185900 -2.22993700 -1.87035000 H 3.64999100 -2.32313300 -1.73221200 H -4.01516700 -3.43111100 -0.65055500 H 4.05043700 -3.44316600 -0.42831000 C 3.31282500 1.47739600 2.02907700 C -3.31156300 1.29035400 2.16972900 H 3.99689200 0.72888200 2.44064300 H -4.02997800 0.53501500 2.50423800 H 2.33412200 1.33615200 2.48847600 H -2.34960700 1.07944200 2.63756100 H 3.68869700 2.45960700 2.33735400 H -3.66161000 2.25620900 2.55109100 C 4.62940300 1.57937600 -0.10972700 C -4.58410800 1.59505700 0.02519500 H 4.60326300 1.57489100 -1.20124500 H -4.52981600 1.71491300 -1.05829300 H 5.32538600 0.79900400 0.21449200 H -5.29286600 0.78928300 0.24507400 H 5.05723900 2.53866800 0.20338600 H -5.01151500 2.51831300 0.43250200 H 0.11448700 2.19447600 -1.58609300 O -1.25035900 3.38314800 -0.58463900 O 0.97915700 3.54534700 -0.27431300 H 0.59410900 4.23351200 0.28482600 C 0.01732500 -1.94192000 0.13644500 O 0.01291100 -3.11355200 0.16140900 Mn 0.00931600 -0.19956700 0.14056200	C -3.28503600 -2.64078400 0.88570200 H 2.21520100 -3.01550500 0.93190600 H -2.27351400 -3.03973300 0.80023600 H 3.40508800 -2.28594000 2.01646300 H -3.44551900 -2.33919200 1.92226600 H 3.91552100 -3.47440000 0.81334200 H -3.98312700 -3.45628900 0.66464400 C -3.36218200 1.56322900 -1.92992400 C 3.36000000 1.41021800 -2.04881800 H -4.07135100 0.85846300 -2.37377800 H 4.08354800 0.69233500 -2.44775200 H -2.38071300 1.38638900 -2.37059800 H 2.38589500 1.19569800 -2.48912300 H -3.68383300 2.56975800 -2.21872100 H 3.66899000 2.40360100 -2.39165100 C -4.71691000 1.62043300 0.19377100 C 4.70265200 1.59461900 0.07354400 H -4.70724200 1.57287800 1.28497300 H 4.68349200 1.63129400 1.16482000 H -5.41496000 0.86087500 -0.17201500 H 5.40266600 0.80864300 -0.22948600 H -5.12860400 2.59608100 -0.08744800 H 5.11696000 2.54682200 -0.27543400 H -0.13081900 2.40610900 1.61807000 O 1.26588200 3.47882300 0.54619500 O -0.97388100 3.63759900 0.20088300 H -0.58005000 4.27466000 -0.40926900 C -0.02429900 -2.06966700 -0.36897400 O -0.02427000 -3.23567000 -0.52663900 Re -0.00798100 -0.19252200 -0.18257500
1Mn-OOCH⁻  O -0.00087800 -3.11025900 0.27457200 P -2.25604900 -0.03670800 -0.16963100 P 2.25626400 -0.03699700 -0.17109700 C -2.41202400 -0.03785500 -2.02447900 C 2.41293900 -0.04247400 -2.02593700 H -2.39245700 1.01102400 -2.33246800 H 2.39608100 1.00564700 -2.33658200 H -3.34953400 -0.47892100 -2.37529700 H 3.34955300 -0.48668100 -2.37519300 C -1.18019200 -0.74144100 -2.58374400 C 1.17953300 -0.74454200 -2.58375500 H -1.14000800 -0.55832100 -3.67615900 H 1.13910500 -0.56271500 -3.67636600 H -1.30950600 -1.84341900 -2.48176200 H 1.30685900 -1.84663200 -2.48044700 N 0.00035200 -0.23523400 -1.94232900 C 3.08869300 1.59654200 0.26820100 C -3.08918300 1.59545200 0.27300000 H 2.53592600 2.28739900 -0.37426100 H -2.53295700 2.28867100 -0.36383400	1Re-OOCH⁻  O 0.00114700 -3.23446000 -0.38429900 P 2.35253200 0.00214000 0.23529300 P -2.35246200 0.00103200 0.23737000 C 2.43213100 0.12220100 2.09546800 C -2.43287700 0.11264200 2.09817100 H 2.42356100 1.19015000 2.33064200 H -2.42978100 1.17940400 2.33869700 H 3.35286100 -0.30667700 2.50182300 H -3.35156700 -0.32277500 2.50217800 C 1.18304700 -0.52551800 2.68681800 C -1.18072200 -0.53208700 2.68650900 H 1.13757300 -0.26063600 3.76125300 H -1.13533900 -0.27023800 3.76167300 H 1.29961800 -1.63161700 2.66333300 H -1.29311100 -1.63854800 2.65968900 N -0.00001600 -0.07034700 2.00619200 C -3.19305700 1.61032000 -0.26677100 C 3.19328400 1.60903100 -0.27536000 H -2.63079200 2.33224100 0.33308300 H 2.62460500 2.33400100 0.31458500

C	3.48359600	-1.34896100	0.40726500
C	-3.48243900	-1.35043400	0.40682400
C	3.39347800	-2.64856400	-0.39151400
C	-3.39569800	-2.64680900	-0.39754800
O	0.00283700	-0.13811300	3.06825500
H	-4.47706800	-0.92183600	0.24326200
H	4.47791100	-0.92162300	0.23855600
C	-3.31319000	-1.64222100	1.89711000
C	3.31921900	-1.63447300	1.89926500
H	-3.41525300	-0.74805000	2.51335300
H	3.42511100	-0.73798300	2.51150100
H	-2.32838000	-2.06768300	2.09927100
H	2.33441800	-2.05742500	2.10671800
H	-4.06751200	-2.36556300	2.22740100
H	4.07349900	-2.35775400	2.22976800
C	2.82937700	2.04504200	1.70216100
C	-2.83614200	2.03761600	1.71001800
H	3.32229000	1.40120200	2.43583400
H	-3.33467900	1.39219700	2.43852800
H	1.75873200	2.06234100	1.90240500
H	-1.76659500	2.05151700	1.91613700
H	3.21535400	3.06025000	1.84472300
H	-3.22023200	3.05325000	1.85456900
C	4.56735500	1.68095200	-0.10112600
C	-4.56621100	1.68222400	-0.10228200
H	4.76195000	1.34762500	-1.12406900
H	-4.75656000	1.35352000	-1.12749200
H	5.19133000	1.08644900	0.57286900
H	-5.19350300	1.08517000	0.56637700
H	4.90908900	2.71871400	-0.02265100
H	-4.90771000	2.71983200	-0.02076800
H	0.01135800	2.19797400	-1.89979600
C	0.00198600	2.71410200	-0.91655700
H	4.15833500	-3.34850300	-0.03537700
H	2.42245500	-3.12908900	-0.26911100
H	3.55997800	-2.49340400	-1.45881700
H	-4.15907900	-3.34819800	-0.04109400
H	-3.56657600	-2.48733800	-1.46352200
H	-2.42418100	-3.12782000	-0.28094400
O	-0.00282400	1.92636300	0.09068100
C	-0.00010800	-1.94132900	0.21498300
Mn	0.00024000	-0.20881100	0.13594200
C	0.00162200	-0.11747000	1.90421100
O	-0.00349700	3.94782600	-0.87265200
1Mn-HCOO⁻			
			
N	0.00008500	-0.05964100	-1.81470600
P	2.26883100	-0.07663400	-0.12730900
P	-2.26868500	-0.07665700	-0.12719500
H	-0.00064000	2.16890600	0.23485800
C	-0.00057500	3.16215500	-0.33467500
C	-2.38637300	0.42010500	-1.90713600
C	2.38663100	0.41940800	-1.90743900
C	-3.57634000	-1.35476600	-0.21038700
C	3.57510500	-1.35648900	-0.20741800
C	-3.35527400	-2.62415500	0.61031500
C	3.35731400	-2.62030400	0.62273200
O	-0.00217800	-0.15005300	-3.25318800
H	4.56688100	-0.95707300	0.03272900
H	-4.56717700	-0.95715400	0.03648800
C	3.51529400	-1.68104800	-1.69841600
C	-3.52240700	-1.66870600	-1.70381700
H	3.76148300	-0.82099500	-2.32266600
H	-3.77407000	-0.80489600	-2.32073300
H	2.51472500	-2.01633400	-1.97812100
H	-2.52216400	-1.99909000	-1.99051900
H	4.22374300	-2.48210000	-1.93705200
H	-4.22967100	-2.47004000	-1.94497900
C	-2.95708800	1.98665600	-1.72554500
C	2.96743200	1.97407000	-1.73855200
H	-3.46625900	1.31075000	-2.41750500
H	3.48788900	1.29748600	-2.42146800
H	-1.89115400	1.98462900	-1.95099800
H	1.90368900	1.96312200	-1.97370900
H	-3.33964300	2.99632600	-1.90958200
H	3.34434700	2.98524400	-1.92580500
C	-4.66545100	1.70453200	0.12348300
C	4.66268400	1.70902200	0.12455900
H	-4.83834900	1.43240200	1.16827300
H	4.82859300	1.44552600	1.17265000
H	-5.29260600	1.06209800	-0.50159500
H	5.29552200	1.06286700	-0.49092300
H	-5.02090900	2.73157000	-0.01214300
H	5.01726000	2.73561800	-0.01662800
H	-0.02292500	2.39019700	1.81674700
C	-0.00572800	2.87425800	0.81797600
H	-4.11265400	-3.36870200	0.33991200
H	-2.37527900	-3.06021700	0.41417200
H	-3.43717500	-2.44469600	1.68390800
H	4.11245600	-3.36739400	0.35310300
H	3.44507700	-2.43397400	1.69467800
H	2.37585700	-3.05660900	0.43435400
O	0.00551000	2.05058900	-0.16621200
C	0.00011100	-2.06016200	-0.28612000
Re	-0.00021100	-0.19112900	-0.17007600
C	-0.00131000	-0.13368700	-2.08389300
O	0.00212800	4.10152100	0.72924500
1Re-HCOO⁻			
			
N	0.00000200	0.07643400	1.90393600
P	-2.36812900	-0.01453700	0.20482500
P	2.36812600	-0.01454300	0.20482400
H	0.00001100	2.01358400	-0.16241000
C	0.00001600	3.09780500	0.30674300
C	2.41084900	0.51294900	1.98467700
C	-2.41084400	0.51296200	1.98467500

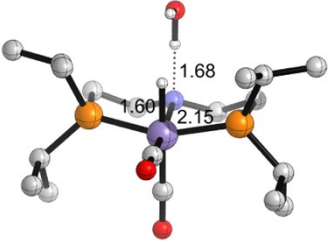
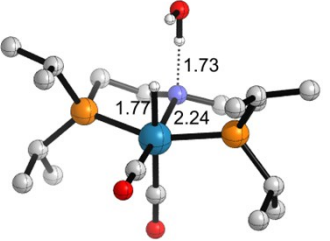
H	-2.29362300	1.51014500	-1.89736600	H	2.33752000	1.60375400	1.94709700
H	2.29404100	1.50946300	-1.89805900	H	-2.33750500	1.60376600	1.94708600
H	-3.33954200	0.14706100	-2.36862900	H	3.34629300	0.23731400	2.48068200
H	3.33974000	0.14603900	-2.36885500	H	-3.34629000	0.23733900	2.48068600
C	-1.18922000	-0.16467900	-2.63621000	C	1.19103300	-0.03298700	2.71513800
C	1.18930500	-0.16536500	-2.63624000	C	-1.19103000	-0.03297500	2.71513900
H	-1.04678600	0.39507600	-3.57510400	H	1.06461500	0.54946400	3.64392600
H	1.04700300	0.39404700	-3.57535700	H	-1.06460700	0.54948300	3.64392300
H	-1.39299400	-1.20897500	-2.94076400	H	1.37909100	-1.07415700	3.04416200
H	1.39278100	-1.20984300	-2.94036300	H	-1.37908900	-1.07414100	3.04417200
C	3.08206800	1.40633600	0.69108200	C	-3.27505400	1.41221000	-0.60780600
C	-3.08213200	1.40590600	0.69171400	C	3.27505600	1.41219900	-0.60781000
H	2.41600100	2.21515300	0.34692500	H	-2.61608300	2.24386800	-0.31516800
H	-2.41640300	2.21496300	0.34744600	H	2.61609000	2.24386200	-0.31517100
C	3.48704200	-1.49645000	0.08424600	C	-3.52167000	-1.49569300	0.09968500
C	-3.48693000	-1.49660000	0.08335300	C	3.52165700	-1.49570600	0.09968400
H	4.48295100	-1.04843300	-0.00722100	H	-4.52453300	-1.10240700	0.30346800
H	-4.48277300	-1.04852800	-0.00853500	H	4.52452600	-1.10242400	0.30344500
C	0.00027200	-0.22943600	1.84449300	C	-0.00000100	0.00619000	-2.05790600
O	0.00047500	-0.19878600	3.00913600	O	0.00002100	0.16164300	-3.21690400
C	-3.36041400	-2.13697800	1.46498900	C	3.50688900	-2.12354000	-1.29271600
C	3.35973700	-2.13646400	1.46598000	C	-3.50693600	-2.12350900	-1.29272500
H	-3.49290300	-1.41625200	2.27241100	H	3.80089200	-1.41911400	-2.07100800
H	3.49159500	-1.41551200	2.27330100	H	-3.80093400	-1.41906700	-2.07100400
H	-2.37948800	-2.59849900	1.59067000	H	2.51144100	-2.49627100	-1.53922200
H	2.37878500	-2.59806400	1.59114700	H	-2.51149900	-2.49625900	-1.53924900
H	-4.11736900	-2.92001600	1.58630500	H	4.20179600	-2.97004400	-1.32674200
H	4.11671600	-2.91937100	1.58798300	H	-4.20186300	-2.96999700	-1.32675300
C	-3.33533400	-2.55220000	-1.01025200	C	3.18951600	-2.54228300	1.16093900
C	3.33596700	-2.55233000	-1.00916500	C	-3.18952500	-2.54229000	1.16091800
H	-2.34215500	-3.00409700	-0.99042500	H	2.17493800	-2.92396900	1.03275500
H	2.34274200	-3.00414700	-0.98972500	H	-2.17494800	-2.92397600	1.03272000
H	-3.50200700	-2.14097500	-2.00748500	H	3.27899600	-2.14616600	2.17398000
H	3.50318100	-2.14138300	-2.00642400	H	-3.27899800	-2.14619200	2.17396700
H	-4.06659100	-3.35346900	-0.85489500	H	3.87793700	-3.38999500	1.07178200
H	4.06707800	-3.35361600	-0.85321900	H	-3.87794700	-3.39000000	1.07174900
C	3.07940200	1.39898900	2.21623200	C	-3.31752300	1.36001100	-2.13172400
C	-3.07892700	1.39841200	2.21685900	C	3.31752000	1.36000100	-2.13172700
H	3.80531700	0.69040500	2.62772700	H	-4.05603800	0.64134000	-2.49954800
H	-3.80440700	0.68951700	2.62857900	H	4.05602700	0.64132300	-2.49955200
H	2.10059100	1.16358000	2.63075100	H	-2.34972200	1.10693700	-2.56287300
H	-2.09987300	1.16333900	2.63098500	H	2.34971500	1.10693700	-2.56287400
H	3.35958200	2.39347800	2.57871900	H	-3.60461600	2.34349100	-2.51794500
H	-3.35934800	2.39276500	2.57953600	H	3.60462200	2.34347900	-2.51794700
C	4.48221000	1.70689300	0.15903300	C	-4.66395700	1.67481900	-0.03014700
C	-4.48251300	1.70618600	0.16013900	C	4.66396500	1.67479800	-0.03015700
H	4.51235600	1.75885900	-0.93082400	H	-4.65260100	1.76726200	1.05771800
H	-4.51306300	1.75799600	-0.92971700	H	4.65261600	1.76724200	1.05770800
H	5.21947100	0.96731000	0.48939900	H	-5.37809100	0.88980700	-0.30037100
H	-5.21954200	0.96654000	0.49087700	H	5.37809200	0.88978200	-0.30038500
H	4.80870000	2.68143500	0.53621100	H	-5.05258100	2.61702600	-0.43044400
H	-4.80900400	2.68073400	0.53729900	H	5.05259300	2.61700200	-0.43045600
O	1.13200100	3.61136200	-0.59836100	O	-1.13328700	3.55395700	0.50456600
O	-1.13313200	3.61189700	-0.59760500	O	1.13332400	3.55397800	0.50449200
C	-0.00002400	-2.10833200	0.23922100	C	-0.00000200	-2.07814600	-0.48758800
O	-0.00014000	-3.27697600	0.28448600	O	-0.00000500	-3.24277300	-0.65906300
Mn	0.00009300	-0.39208400	0.08255000	Re	0.00000000	-0.24832100	-0.16136900
Mn-TS(HCO₂)				Re-TS(HCO₂)			

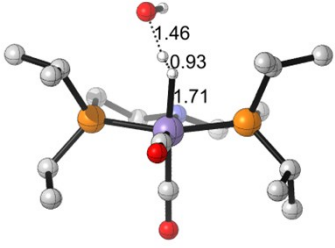
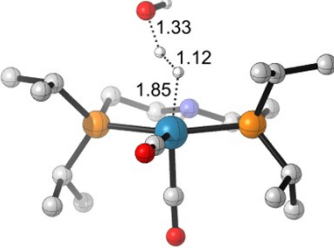


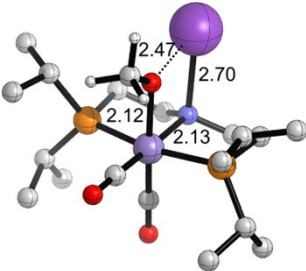
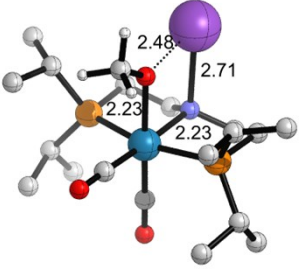
N	0.00003500	0.49945600	-1.84692800
P	2.23881400	0.00175100	-0.08737400
P	-2.23882300	0.00177300	-0.08747000
H	-0.00018500	1.44365200	0.54874600
C	0.00003600	3.11371600	-0.34381600
C	-2.41926900	0.61023400	-1.83537100
C	2.41935100	0.61003800	-1.83533200
H	-2.41812100	1.70018400	-1.77316600
H	2.41831700	1.69999100	-1.77322800
H	-3.34889700	0.28816400	-2.31263200
H	3.34895500	0.28782600	-2.31253800
C	-1.17519100	0.15968300	-2.59328500
C	1.17524900	0.15955500	-2.59324400
H	-1.17262900	0.65785300	-3.58501500
H	1.17275000	0.65768700	-3.58499300
H	-1.25806700	-0.93051100	-2.81725400
H	1.25803800	-0.93065600	-2.81717000
C	3.21197900	1.29004000	0.89088400
C	-3.21189000	1.29002400	0.89093100
H	2.57186800	2.16438500	0.76482200
H	-2.57177300	2.16435800	0.76483200
C	3.38329600	-1.50665000	0.03345300
C	-3.38333700	-1.50660500	0.03318800
H	4.39409500	-1.09890900	0.15031800
H	-4.39415400	-1.09885400	0.14984900
C	-0.00014500	-0.47804000	1.87990400
O	-0.00028700	-0.66165900	3.03495800
C	-3.06004900	-2.35292200	1.26536700
C	3.05980000	-2.35302900	1.26553300
H	-3.04238900	-1.76933700	2.18590300
H	3.04218200	-1.76952700	2.18612300
H	-2.08429900	-2.82847700	1.16213100
H	2.08399000	-2.82843200	1.16220600
H	-3.80984600	-3.14469400	1.38193500
H	3.80947900	-3.14492000	1.38206100
C	-3.37767900	-2.38504800	-1.21682000
C	3.37781400	-2.38504300	-1.21659400
H	-2.38788300	-2.80203100	-1.40659100
H	2.38787200	-2.80141200	-1.40695800
H	-3.69286100	-1.84251700	-2.10966900
H	3.69385400	-1.84266700	-2.10923700
H	-4.06929900	-3.22456300	-1.07765100
H	4.06882400	-3.22499700	-1.07705900
C	3.29760900	0.98402800	2.38363500
C	-3.29736900	0.98398500	2.38368600
H	3.99350800	0.16560300	2.59104500
H	-3.99334200	0.16563800	2.59115900
H	2.32520200	0.72121900	2.80156600
H	-2.32494400	0.72105500	2.80149200
H	3.66828200	1.86379100	2.92218100
H	-3.66786800	1.86377800	2.92230300
C	4.58985300	1.62456900	0.32399900
C	-4.58982600	1.62461100	0.32422400



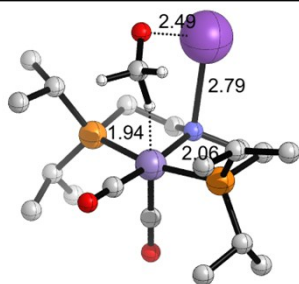
N	-0.00000100	0.43505000	-1.92380400
P	2.34967300	0.02088600	-0.17774300
P	-2.34967500	0.02088800	-0.17774500
H	0.00000700	1.62287500	0.48776900
C	0.00000600	3.31009300	-0.33527600
C	-2.43260100	0.59820100	-1.94731800
C	2.43259900	0.59819800	-1.94731700
H	-2.42021100	1.69013700	-1.90216800
H	2.42021000	1.69013500	-1.90216600
H	-3.35134900	0.28183100	-2.45023200
H	3.35134800	0.28182800	-2.45023100
C	-1.17969400	0.11993700	-2.67716700
C	1.17969300	0.11993500	-2.67716700
H	-1.15320000	0.61554200	-3.66863000
H	1.15320000	0.61554100	-3.66863000
H	-1.27985100	-0.96805300	-2.89719200
H	1.27984800	-0.96805500	-2.89719100
C	3.32871800	1.36409700	0.70807100
C	-3.32872100	1.36409900	0.70806800
H	2.72450700	2.23708600	0.45194200
H	-2.72452100	2.23709100	0.45192100
C	3.49132600	-1.48166300	-0.10307300
C	-3.49132800	-1.48166100	-0.10308100
H	4.51057000	-1.08446700	-0.17218700
H	-4.51057100	-1.08446700	-0.17220800
C	-0.00000200	-0.40959700	2.08657800
O	-0.00000200	-0.54304400	3.25169500
C	-3.33795600	-2.22352800	1.22390600
C	3.33794100	-2.22353500	1.22390900
H	-3.54231200	-1.58802100	2.08608600
H	3.54227500	-1.58802800	2.08609400
H	-2.32268800	-2.60751800	1.33284400
H	2.32267500	-2.60753600	1.33282900
H	-4.02996200	-3.07290500	1.26036600
H	4.02995500	-3.07290500	1.26037800
C	-3.27866300	-2.44216000	-1.27121000
C	3.27867600	-2.44215800	-1.27120800
H	-2.26731200	-2.85022600	-1.26943000
H	2.26732500	-2.85022300	-1.26944200
H	-3.45085900	-1.96596200	-2.23805400
H	3.45088400	-1.96595700	-2.23804800
H	-3.97662500	-3.28308500	-1.18479000
H	3.97663700	-3.28308300	-1.18478200
C	3.31422200	1.23085900	2.22780700
C	-3.31420500	1.23087900	2.22780500
H	3.98363800	0.43888500	2.57541800
H	-3.98360700	0.43890300	2.57543500
H	2.31128100	1.01900200	2.59946300
H	-2.31125600	1.01903800	2.59945000
H	3.65627400	2.16560000	2.68611400
H	-3.65626000	2.16562300	2.68610600
C	4.74422300	1.58850000	0.18178100

H 4.54549200 1.90236300 -0.73067700	C -4.74423500 1.58848500 0.18179300
H -4.54569600 1.90178800 -0.73062400	H 4.76920400 1.70510000 -0.90411800
H 5.29120800 0.79020100 0.42527100	H -4.76923100 1.70506800 -0.90410800
H -5.29137500 0.79049100 0.42618500	H 5.41570300 0.76714000 0.45008300
H 5.02087300 2.47210000 0.86957700	H -5.41570600 0.76712500 0.45011700
H -5.02046000 2.47257200 0.86943500	H 5.16435000 2.50116000 0.61948600
O 1.15052800 3.34773900 -0.42261500	H -5.16436200 2.50115000 0.61948900
O -1.15041800 3.34790300 -0.42270100	O 1.15166400 3.53341900 -0.41859400
C 0.00002900 -1.88945600 -0.26253600	O -1.15165200 3.53342400 -0.41859200
O 0.00001100 -3.03957900 -0.48755000	C 0.00000000 -2.07184400 -0.03450400
Mn -0.00004200 -0.18714500 0.15331700	O 0.00000500 -3.24717900 -0.08943600
	Re -0.00000100 -0.18044200 0.19395000
2Mn...H₂O	2Re...H₂O
	
O -0.00246500 -3.16011600 0.26548900	O -0.00219500 -3.15407400 0.77307600
P 2.18637300 0.13616100 0.11274800	P 2.31647500 0.21809100 0.12949200
P -2.18587500 0.13835400 0.11149400	P -2.31640300 0.21865800 0.12834300
C 2.40899600 0.43588000 1.94192800	C 2.42769300 0.90188500 1.86535700
C -2.40679800 0.44715200 1.93927300	C -2.42772600 0.90434300 1.86325500
H 2.41475300 1.51895500 2.08983100	H 2.41847900 1.99142300 1.77389100
H -2.40630200 1.53086400 2.08259000	H -2.41624600 1.99376200 1.77032100
H 3.34868900 0.02912000 2.32572700	H 3.35318600 0.60662200 2.36775700
H -3.34876900 0.04727600 2.32481600	H -3.35408200 0.61165800 2.36555100
C 1.18473500 -0.14780600 2.63490200	C 1.18700200 0.46550900 2.63749400
C -1.18587400 -0.14056200 2.63464900	C -1.18817900 0.46703100 2.63671900
H 1.17442100 0.19425800 3.68846600	H 1.16677300 1.01137200 3.60024200
H -1.17491200 0.20379100 3.68747100	H -1.16822700 1.01346200 3.59914500
H 1.27042800 -1.25317200 2.67453900	H 1.27044200 -0.60941200 2.89630900
H -1.27682700 -1.24543100 2.67672200	H -1.27277100 -0.60764500 2.89608700
N 0.00087300 0.29001500 1.94007800	N -0.00011800 0.75189700 1.86696300
C -2.89496600 1.74703000 -0.58559200	C -3.07989000 1.63899600 -0.85254200
C 2.89512100 1.74783900 -0.57717700	C 3.07998800 1.63966400 -0.84987100
H -2.28955300 2.46563700 -0.02207400	H -2.44985900 2.46113900 -0.49530000
H 2.29148100 2.46405800 -0.00863200	H 2.45218100 2.46196800 -0.48909400
C -3.53262200 -1.13503100 -0.26910100	C -3.62654100 -1.13860600 0.09026800
C 3.53166400 -1.13642900 -0.27494900	C 3.62747300 -1.13835500 0.09159200
C -3.44594600 -2.34928800 0.65325200	C -3.45838800 -2.11534700 1.25177700
C 3.44199700 -2.35665700 0.63927000	C 3.45432000 -2.11938000 1.24867000
O 0.00080900 -0.59276800 -3.03460100	O 0.00058400 -1.17168800 -3.08349600
H 4.49148000 -0.64140900 -0.08721900	H 4.59579100 -0.63741800 0.20578700
H -4.49200500 -0.63747100 -0.08610200	H -4.59576700 -0.63797300 0.19807300
C 3.47552000 -1.57397600 -1.73674700	C 3.60050100 -1.88449300 -1.24025500
C -3.47441600 -1.58193200 -1.72804800	C -3.59310100 -1.88987500 -1.23857800
H 3.63050900 -0.74439300 -2.42843900	H 3.81858300 -1.23381100 -2.08852100
H -3.62851300 -0.75667900 -2.42513800	H -3.80443300 -1.24207600 -2.09074800
H 2.50421100 -2.01630900 -1.96797900	H 2.61586700 -2.32598300 -1.40938800
H -2.50268900 -2.02550400 -1.95515200	H -2.60838300 -2.33406400 -1.39990900
H 4.24756600 -2.32565400 -1.93879300	H 4.34261600 -2.69103300 -1.23776000
H -4.24608800 -2.33494300 -1.92651400	H -4.33694400 -2.69483000 -1.23744800
C -2.59634200 1.96824900 -2.06410600	C -2.86310600 1.52711100 -2.35726100
C 2.59341400 1.97670800 -2.05391200	C 2.85919900 1.53216500 -2.35431200
H -3.19095700 1.31420600 -2.70732100	H -3.49674700 0.75863900 -2.80796000
H 3.18738000 1.32680300 -2.70191300	H 3.48882400 0.76256500 -2.80862000

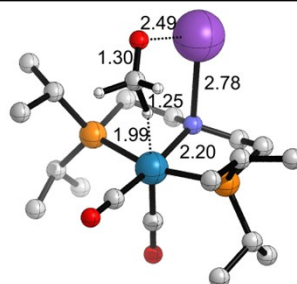
H -1.54239600 1.78692500 -2.27459800	H -1.82238300 1.28696500 -2.57666800
H 1.53912400 1.79532900 -2.26304500	H 1.81705700 1.29616400 -2.57146900
H -2.83253200 3.00138400 -2.34483000	H -3.11008700 2.47793500 -2.84337000
H 2.82785400 3.01162000 -2.32948200	H 3.10829400 2.48335400 -2.83866700
C -4.36513400 2.00502800 -0.26671800	C -4.53296000 1.95554300 -0.51019500
C 4.36619500 2.00305900 -0.25999700	C 4.53438600 1.95294200 -0.51023000
H -4.59256500 1.85044100 0.79100700	H -4.69568000 2.04261500 0.56704000
H 4.59520100 1.84429000 0.79677800	H 4.70013100 2.03620600 0.56686500
H -5.02531900 1.35862900 -0.85270700	H -5.21419400 1.19081000 -0.89494000
H 5.02477900 1.35815200 -0.84944900	H 5.21338400 1.18838500 -0.89926200
H -4.62834900 3.04025800 -0.51237100	H -4.82848700 2.90743700 -0.96556000
H 4.63007900 3.03891800 -0.50221100	H 4.83022900 2.90587200 -0.96321700
H -0.00164700 1.31963400 -0.44143300	H 0.00032600 1.45284700 -0.78233500
H -4.26665700 -3.04142300 0.43032100	H -4.24533300 -2.87717800 1.20931600
H -2.50792800 -2.88767900 0.51386600	H -2.49572200 -2.62575400 1.20163600
H -3.52061000 -2.07754400 1.70803500	H -3.52719100 -1.62265500 2.22359200
H 4.26328600 -3.04750900 0.41449800	H 4.24169600 -2.88083000 1.20715100
H 3.51328800 -2.09189300 1.69605100	H 3.51844900 -1.63009100 2.22253600
H 2.50428300 -2.89388500 0.49362300	H 2.49202600 -2.62985400 1.19238200
H 0.00376500 1.97123300 1.90915900	H 0.00051000 2.45268400 1.52638000
O 0.00487000 2.99246300 1.82280900	O 0.00062500 3.41978800 1.22592900
C -0.00127600 -1.99294000 0.16113500	C -0.00095700 -2.01891400 0.47023300
C 0.00089400 -0.46391500 -1.87139500	C 0.00033500 -0.80636200 -1.96843200
Mn -0.00001500 -0.25239900 -0.13666000	Re 0.00006000 -0.20281400 -0.16485400
H 0.00215100 3.08015400 0.86466300	H 0.00050800 3.28792100 0.27180200
Mn-TS(H⁺ transfer, H₂ formation)	
	
O -0.05076500 -3.02252600 -0.21220000	O 0.08138200 3.06837900 -0.52270300
P 2.20751600 0.11217300 0.13305600	P -2.34035400 -0.11512400 0.20928400
P -2.26054200 0.12392000 0.19269500	P 2.37763700 -0.13008800 0.26137400
C 2.31311500 0.27530800 1.97659800	C -2.36532400 -0.52773700 2.02255900
C -2.44609400 -0.02847600 2.03942500	C 2.46537100 -0.15069900 2.11578800
H 2.14261300 1.33993500 2.16856200	H -2.24342300 -1.60842700 2.03225600
H -2.45250200 0.99622700 2.43657300	H 2.54772300 -1.20061600 2.41329000
H 3.29095800 -0.02137300 2.37257300	H -3.31716400 -0.25888500 2.50112600
H -3.38434600 -0.51476500 2.32764800	H 3.35743100 0.37289100 2.49459400
C 1.16582900 -0.51064500 2.59434600	C -1.16799400 0.11853400 2.71068300
C -1.20031000 -0.73675900 2.56109600	C 1.17112600 0.41228800 2.67788900
H 1.10135900 -0.24578900 3.66419800	H -1.11896100 -0.28118500 3.73549400
H -1.14742400 -0.58124800 3.65748000	H 1.12590300 0.19413300 3.75374700
H 1.40187700 -1.60428000 2.57497100	H -1.34743200 1.20814700 2.82470900
H -1.32028800 -1.83732600 2.42461000	H 1.19527900 1.53136700 2.60426600
N -0.05016400 -0.16185700 1.92966600	N 0.04286200 -0.16995500 1.99855400
C -2.97691100 1.84644500 -0.09366200	C 3.23399600 -1.76083400 -0.15331700
C 3.04172000 1.69746200 -0.43211300	C -3.35914100 -1.52600600 -0.49999900
H -2.25971900 2.44432800 0.48222800	H 2.57445400 -2.45660900 0.38224700
H 2.33470600 2.42229600 0.00733100	H -2.80326400 -2.37319400 -0.05659600
C -3.55639300 -1.04084900 -0.53183100	C 3.59324000 1.20230100 -0.28954300
C 3.41644000 -1.25318000 -0.36590700	C -3.43486500 1.40216400 0.01389900
C -3.57468100 -2.40131300 0.16788200	C 3.43754300 2.49392100 0.52126700
C 3.44781100 -2.42463900 0.60681300	C -3.14207800 2.50600900 1.03128900
O -0.05597800 0.03641800 -3.09699800	O 0.06417600 -0.17023300 -3.26007600
H 4.40940700 -0.77746800 -0.35571000	H -4.45412700 1.04150700 0.19376600
Re-TS(H⁺ transfer, H₂ formation)	
	

H -4.52954800 -0.56403500 -0.38069000	H 4.58679800 0.79911200 -0.10440400
C 3.13224500 -1.74524400 -1.78336100	C -3.36204600 1.95172200 -1.41397300
C -3.33292500 -1.24386200 -2.02995900	C 3.44283400 1.49560800 -1.78174600
H 3.08538400 -0.92941900 -2.50512000	H -3.56479600 1.19735400 -2.16736800
H -3.30006800 -0.30462400 -2.58563300	H 3.55632400 0.60265300 -2.40585300
H 2.17938700 -2.27343000 -1.81817200	H -2.37277400 2.36409900 -1.61763200
H -2.39348100 -1.76122200 -2.21582300	H 2.45215500 1.91422300 -1.99073800
H 3.91521800 -2.43709100 -2.10212400	H -4.09125100 2.75930600 -1.54182000
H -4.14342300 -1.85166000 -2.45157100	H 4.18990300 2.22835300 -2.09663300
C -2.90543400 2.31012800 -1.54220300	C 3.16756500 -2.12676700 -1.62932700
C 3.06945300 1.87227000 -1.94615700	C -3.28577100 -1.66146500 -2.01058500
H -3.64942400 1.80567500 -2.16832200	H 3.87759600 -1.54176300 -2.23057800
H 3.80331900 1.20618700 -2.42518800	H -3.91051300 -0.91926100 -2.52127100
H -1.92209200 2.13088100 -1.97568900	H 2.16754200 -1.98114000 -2.03075000
H 2.09846700 1.68384000 -2.40170800	H -2.26012200 -1.56400200 -2.37926800
H -3.11027000 3.38512000 -1.60294300	H 3.43223600 -3.18576600 -1.76407800
H 3.36225400 2.89989100 -2.19720200	H -3.64631700 -2.65320900 -2.30755500
C -4.37058300 2.07033500 0.48633400	C 4.64638900 -1.89838800 0.40140900
C 4.41805400 1.93837200 0.17831600	C -4.80545200 -1.58341100 -0.00536000
H -4.44339700 1.77098600 1.53208600	H 4.70369900 -1.64506600 1.45919700
H 4.38500600 1.90748000 1.27028500	H -4.86705400 -1.52985400 1.08715800
H -5.13363100 1.51338000 -0.07330100	H 5.36165800 -1.25462100 -0.14044600
H 5.16926000 1.21555800 -0.16740800	H -5.42600500 -0.78609400 -0.42192000
H -4.64012200 3.13064700 0.42216000	H 4.99559400 -2.92499900 0.28669100
H 4.77839200 2.93438200 -0.10388800	H -5.25770200 -2.54002100 -0.30290500
H -0.17120800 1.60316300 -0.26644500	H 0.37188200 -1.80483700 -0.24559700
H -4.33293000 -3.04371000 -0.29263800	H 4.18217500 3.22057700 0.17193800
H -2.61384000 -2.90801900 0.08104600	H 2.45623400 2.93189600 0.38777100
H -3.81029600 -2.31882000 1.23454000	H 3.59582300 2.34053800 1.58867500
H 4.19484300 -3.15718500 0.27809000	H -3.84237900 3.34289800 0.88113400
H 3.70603100 -2.11910300 1.62563700	H -3.25964100 2.15697300 2.06064000
H 2.48513700 -2.93102000 0.65347500	H -2.13682600 2.89765000 0.92526800
H 0.19725600 1.90454700 0.53471500	H -0.34669100 -2.23337700 0.49433500
O 0.75479200 3.03898300 1.26072800	O -0.84007500 -3.36232300 1.00555100
C -0.04058500 -1.85383800 -0.19582400	C 0.03633100 1.90325400 -0.33865000
C -0.05025400 0.01260900 -1.92849400	C 0.04375200 -0.10017900 -2.09015300
Mn -0.04036300 -0.10382900 -0.17663700	Re 0.03727000 0.00932700 -0.19177200
H 0.38537800 2.94664200 2.18333200	H -0.45518400 -3.38088400 1.90530600
1Mn-OCH₃⁻...K⁺	
	
N 0.00000200 -0.58756000 -1.80763400	N -0.00004200 0.70079700 -1.84455900
P 2.27804100 0.08853800 -0.08453700	P -2.36925500 -0.03855400 -0.15399100
P -2.27794400 0.08860800 -0.08442600	P 2.36922200 -0.03843400 -0.15401300
C -0.00037200 -2.08856800 2.16670900	C -0.00001300 2.15138600 2.24474500
C 2.43072700 -0.64292500 -1.79351900	C -2.45224600 0.73408700 -1.85484200
C -2.43073400 -0.64281600 -1.79341600	C 2.45218000 0.73441800 -1.85476500
H 2.46948800 -1.73046600 -1.66307200	H -2.50594100 1.81801800 -1.69782300
H -2.46956200 -1.73035600 -1.66297900	H 2.50573200 1.81833500 -1.69759500
H 3.35263900 -0.35630600 -2.30368800	H -3.35497600 0.45409000 -2.40205900
H -3.35264600 -0.35613400 -2.30355200	H 3.35494800 0.45459800 -2.40201000
C 1.18153300 -0.25784700 -2.57462500	C -1.18350700 0.38233000 -2.62296400
C -1.18155000 -0.25779600 -2.57456900	C 1.18349900 0.38260100 -2.62295800
1Re-OCH₃⁻...K⁺	
	

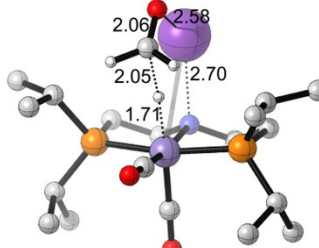
H	1.19042500	-0.78843600	-3.54874300	H	-1.18739700	0.93667900	-3.58234500
H	-1.19050800	-0.78837900	-3.54869000	H	1.18734700	0.93708700	-3.58226200
H	1.23984500	0.81628100	-2.83729700	H	-1.22228300	-0.68600300	-2.90560300
H	-1.23982800	0.81633600	-2.83723800	H	1.22244100	-0.68568500	-2.90575900
C	-3.23875600	-1.14295700	0.96824000	C	3.32968600	1.20044000	0.88823200
C	3.23883300	-1.14303000	0.96812900	C	-3.32977600	1.20038500	0.88812200
H	-2.52338200	-1.97048900	1.02716800	H	2.61247100	2.02818800	0.93938000
H	2.52355600	-1.97065600	1.02686900	H	-2.61262800	2.02819700	0.93915300
C	-3.41699600	1.59677000	-0.09210000	C	3.50119500	-1.54245000	-0.22051900
C	3.41723400	1.59660400	-0.09222800	C	-3.50110600	-1.54267100	-0.22031000
H	-4.42192700	1.19713800	0.08751700	H	4.51718900	-1.14588900	-0.10807500
H	4.42216800	1.19681600	0.08702800	H	-4.51713600	-1.14620400	-0.10786400
C	0.00007600	0.87509200	1.80381500	C	0.00011800	-0.94119300	1.95027000
O	0.00004700	1.33539100	2.87034300	O	0.00016300	-1.39967500	3.02280200
C	3.06694700	2.55474700	1.04765900	C	-3.21243100	-2.49543900	0.94043300
C	-3.06623800	2.55513500	1.04745400	C	3.21266500	-2.49536500	0.94013900
H	3.02738700	2.06353500	2.01954500	H	-3.25187000	-2.00582400	1.91301400
H	-3.02641800	2.06414700	2.01943900	H	3.25202200	-2.00583300	1.91276500
H	2.09777100	3.02461200	0.87673400	H	-2.22284100	-2.94132500	0.83639700
H	-2.09705700	3.02484500	0.87610800	H	2.22314400	-2.94139100	0.83605800
H	3.81745800	3.34979400	1.10480400	H	-3.94931000	-3.30497400	0.94184500
H	-3.81663500	3.35028600	1.10465300	H	3.94966600	-3.30479000	0.94148200
C	3.44466800	2.35422900	-1.41933500	C	-3.42698700	-2.29733800	-1.54703800
C	-3.44467000	2.35410100	-1.41936300	C	3.42710700	-2.29699200	-1.54731800
H	2.46431500	2.76151700	-1.66985200	H	-2.42531200	-2.69083400	-1.72543100
H	-2.46432200	2.76119000	-1.67023400	H	2.42545800	-2.69054100	-1.72574100
H	3.78331800	1.73700400	-2.25291600	H	-3.71455300	-1.68253300	-2.40156900
H	-3.78362100	1.73673100	-2.25271300	H	3.71462000	-1.68208000	-2.40179000
H	4.13748900	3.19788000	-1.33734000	H	-4.11229600	-3.15011500	-1.51431900
H	-4.13734600	3.19787400	-1.33738300	H	4.11247500	-3.14972600	-1.51469400
C	-3.48543900	-0.62863500	2.38538500	C	3.56448700	0.69911800	2.31167700
C	3.48525400	-0.62879100	2.38535100	C	-3.56446900	0.69921700	2.31164000
H	-4.25386400	0.14915600	2.39719200	H	4.34486800	-0.06587800	2.33901700
H	4.25354100	0.14913500	2.39732000	H	-4.34475400	-0.06587300	2.33910300
H	-2.58236600	-0.22193100	2.84183700	H	2.65941500	0.27965800	2.75305500
H	2.58205400	-0.22228100	2.84172800	H	-2.65932400	0.27993400	2.75303300
H	-3.84254100	-1.44440000	3.02160900	H	3.89854100	1.52384300	2.94869500
H	3.84241300	-1.44455200	3.02154900	H	-3.89859800	1.52398300	2.94856600
C	-4.54488700	-1.64121800	0.35300500	C	4.63622300	1.69415900	0.27105600
C	4.54512000	-1.64105000	0.35303300	C	-4.63637600	1.69390600	0.27093100
H	-4.40770600	-2.09427600	-0.63069300	H	4.50232200	2.12591100	-0.72280100
H	4.40813900	-2.09406500	-0.63071300	H	-4.50253600	2.12563400	-0.72294600
H	-5.27624700	-0.83492300	0.24678400	H	5.37141300	0.88909400	0.18630500
H	5.27637100	-0.83463500	0.24696000	H	-5.37146000	0.88874100	0.18621300
H	-4.99761100	-2.39763000	1.00289600	H	5.08174600	2.46584900	0.90765300
H	4.99787300	-2.39743700	1.00293400	H	-5.08200100	2.46556400	0.90749400
H	-0.87867400	-1.70477900	2.71410200	H	0.87970900	1.74895100	2.77260200
C	0.00005000	1.85769800	-0.49813800	C	0.00007500	-2.00111500	-0.48409600
O	-0.00076600	2.94214800	-0.92850700	O	0.00007900	-3.10992800	-0.86923000
Mn	0.00004200	0.24096100	0.15415600	Re	0.00004600	-0.23867400	0.17438000
K	-0.00009500	-3.21455200	-1.18984500	K	-0.00032500	3.31792900	-1.13112300
O	-0.00013500	-1.77572400	0.81956100	O	-0.00013100	1.87376300	0.88501600
H	-0.00042300	-3.18611400	2.32887100	H	-0.00002600	3.24321800	2.42763700
H	0.87774700	-1.70480900	2.71441100	H	-0.87962600	1.74890100	2.77275500
1Mn-HCH₂O⁻...K⁺				1Re-HCH₂O⁻...K⁺			

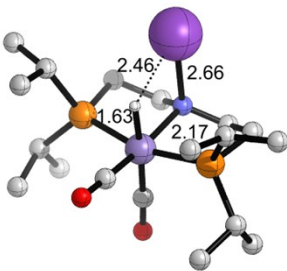
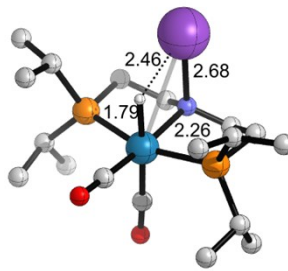


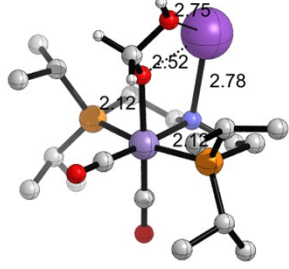
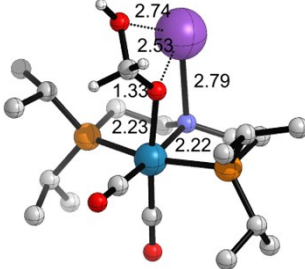
N	0.02652300	0.69387300	-1.64034800
P	-2.22832000	-0.26954400	-0.06553700
P	2.32687600	-0.05927300	-0.04551800
H	0.00270200	1.33072400	1.03489500
C	-0.27720000	2.26372400	1.73856500
C	-2.41838400	0.65496100	-1.66995900
C	2.46099100	0.88748000	-1.64470300
H	-2.54767000	1.70370900	-1.38412400
H	2.48061400	1.94800600	-1.36877400
H	-3.30860100	0.36416400	-2.23077600
H	3.38247300	0.68286000	-2.19319200
C	-1.14063400	0.46615300	-2.47311700
C	1.21616300	0.57679700	-2.46235400
H	-1.15293300	1.16129400	-3.33951600
H	1.17294300	1.26937100	-3.32867800
H	-1.14311900	-0.54203900	-2.92754200
H	1.32096400	-0.42798800	-2.91330800
C	3.19302800	1.11631400	1.14553300
C	-3.21756700	0.81280800	1.11004600
H	2.52749800	1.98593700	1.11075200
H	-2.61197100	1.73016500	1.13783000
C	3.53507200	-1.49914000	-0.19351500
C	-3.28047600	-1.82536700	-0.23563800
H	4.52240600	-1.06661000	-0.00129300
H	-4.30598800	-1.49100100	-0.04553800
C	0.08297500	-1.08909500	1.73923600
O	0.09442300	-1.57476200	2.79204700
C	-2.90702300	-2.86131400	0.82550500
C	3.25541100	-2.56045700	0.87142200
H	-2.90856200	-2.45123100	1.83539000
H	3.21611900	-2.14921700	1.88026400
H	-1.91558800	-3.27522200	0.63795900
H	2.30604700	-3.06309500	0.68354600
H	-3.62276800	-3.68904800	0.79987500
H	4.04379200	-3.31926700	0.85057400
C	-3.24178700	-2.45219200	-1.62840900
C	3.56490500	-2.13427200	-1.58319500
H	-2.23839200	-2.78737500	-1.89336800
H	2.59999500	-2.56521500	-1.85203200
H	-3.59386400	-1.77257600	-2.40618800
H	3.85546200	-1.42819100	-2.36280900
H	-3.89416900	-3.33094200	-1.64617600
H	4.29852200	-2.94641900	-1.59126700
C	3.20717100	0.61421800	2.58654900
C	-3.29909900	0.24000000	2.52346600
H	3.90769300	-0.21449400	2.71500700
H	-3.98977300	-0.60652200	2.57696000
H	2.22241900	0.28310000	2.91626800
H	-2.32890100	-0.08756700	2.89804600
H	3.53143600	1.41699800	3.25547800
H	-3.67485900	1.00719100	3.20673600



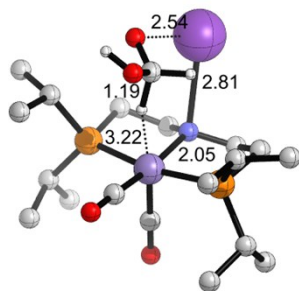
O	0.18761100	-3.18188500	-0.96815200
P	-2.33306400	-0.19502100	-0.13495100
P	2.40451500	0.01300700	-0.11203500
C	-2.45162000	0.73195800	-1.75250000
C	2.45930800	0.97764400	-1.71169800
H	-2.58954700	1.78364900	-1.47952900
H	2.47431100	2.03624200	-1.42693500
H	-3.32711400	0.44215100	-2.33715400
H	3.36987200	0.79028900	-2.28485500
C	-1.15934400	0.54296700	-2.53720800
C	1.20585400	0.66513100	-2.51937100
H	-1.17310600	1.22593300	-3.41166500
H	1.16645900	1.35105900	-3.38997500
H	-1.14785700	-0.47324600	-2.97147500
H	1.30340400	-0.34552300	-2.95636100
N	0.00794900	0.79226600	-1.70647600
C	3.28265300	1.20123100	1.05557900
C	-3.31640700	0.92579000	1.00815600
H	2.61012900	2.06636600	1.01662000
H	-2.69200400	1.82928800	1.02439600
C	3.61342700	-1.40986100	-0.33772900
C	-3.40029900	-1.72989900	-0.34385200
C	3.50094500	-2.07036400	-1.71085500
C	-3.23863800	-2.38836200	-1.71275300
O	0.07671300	-1.54508000	3.00185800
H	-4.43326400	-1.37640300	-0.25268900
H	4.60943400	-0.96162900	-0.25545300
C	-3.12600900	-2.74190300	0.76852800
C	3.44617700	-2.45016500	0.76969700
H	-3.23731300	-2.31561000	1.76525800
H	3.53666400	-2.02374900	1.76877500
H	-2.11349100	-3.13948800	0.69058100
H	2.47058500	-2.93342000	0.70463400
H	-3.82448000	-3.58007500	0.68261600
H	4.21311300	-3.22383000	0.66571000
C	3.31014600	0.71343600	2.50135500
C	-3.40571600	0.38663100	2.43435000
H	4.04078400	-0.08687700	2.63953000
H	-4.12994600	-0.42881600	2.51010700
H	2.33647200	0.34579000	2.82646300
H	-2.44437400	0.02367100	2.79988600
H	3.60076200	1.53340300	3.16480200
H	-3.74112800	1.18124400	3.10696700
C	4.66861900	1.64666600	0.59445100
C	-4.70141400	1.30501000	0.48691000
H	4.67428800	2.01807100	-0.43268600
H	-4.67623500	1.72952700	-0.51893100
H	5.39650900	0.83439600	0.66182200
H	-5.38219900	0.44947200	0.47394400
H	5.03193000	2.45372700	1.23826300
H	-5.14505900	2.05745900	1.14597200

C 4.58693900 1.56043800 0.70623900	H -0.03441500 1.42157700 1.05486200
C -4.61194800 1.17893800 0.60335300	C -0.28277100 2.39655300 1.79661000
H 4.60700700 1.94479500 -0.31571500	H 4.23460700 -2.87919800 -1.78186100
H -4.59758000 1.63628700 -0.38794200	H 2.51508800 -2.51038300 -1.86493900
H 5.31265800 0.74602400 0.77246300	H 3.70166100 -1.37744700 -2.52981600
H -5.28068400 0.31413000 0.56593300	H -3.89021600 -3.26573600 -1.76986900
H 4.94402800 2.35835300 1.36490400	H -3.51389700 -1.72615100 -2.53538700
H -5.06431000 1.90406500 1.28683800	H -2.21594300 -2.73172500 -1.87366600
H 0.73236900 2.53636800 2.12117200	O -0.83330000 3.39708700 1.16996600
O -0.94244300 3.22085900 1.12068500	C 0.13378300 -2.08963500 -0.55174600
C 0.14293600 -1.94633100 -0.62981800	Re 0.05011700 -0.35782200 0.16275800
O 0.19592800 -2.99532000 -1.13212400	C 0.06742600 -1.10027100 1.92622400
Mn 0.06657600 -0.37990900 0.11597400	H -0.88433600 1.88418500 2.56965900
K -0.27500400 3.44644500 -1.26330100	K -0.28423200 3.52391900 -1.25326700
H -0.80284500 1.75266500 2.56886400	H 0.73917200 2.55200100 2.20342600
Mn-TS(HCH₂O⁻...K⁺)	
	
O 0.00699900 -3.22933700 0.21457300	O 0.07291000 -3.30361600 0.43285900
P 2.26268300 -0.16297200 0.10490300	P 2.37835300 -0.06747400 0.15411400
P -2.24482100 -0.18853400 0.10535300	P -2.34146000 -0.14767300 0.15733000
C 2.43850800 0.17777100 1.93043100	C 2.46522000 0.49671900 1.93463000
C -2.42950200 0.09173500 1.94188800	C -2.44287100 0.38461900 1.94973900
H 2.48826600 1.26672600 2.05499900	H 2.51264200 1.59235900 1.91195100
H -2.51442000 1.17364300 2.09840700	H -2.52187500 1.47778200 1.93675000
H 3.35840400 -0.22516000 2.35545000	H 3.36964700 0.15690500 2.44045000
H -3.33400200 -0.35168100 2.35736800	H -3.33747200 0.01145400 2.45174300
C 1.19357500 -0.37129700 2.60982700	C 1.20284100 0.03589100 2.65903000
C -1.16247200 -0.42487500 2.60829700	C -1.16522000 -0.03912500 2.65953100
H 1.20000000 -0.07191500 3.67992700	H 1.19693700 0.48988100 3.66963600
H -1.17984100 -0.14745100 3.68036400	H -1.16701600 0.38826600 3.67827400
H 1.25112800 -1.47733100 2.61703400	H 1.27453800 -1.05568500 2.83081800
H -1.18356000 -1.53183300 2.59311000	H -1.19124900 -1.13602600 2.80292800
N 0.00310700 0.11329500 1.94359200	N 0.00718400 0.39879400 1.92319400
C -3.21499800 1.26500700 -0.60993700	C -3.34218900 1.20588500 -0.69511200
C 3.21340100 1.28940000 -0.64166500	C 3.30687100 1.32753400 -0.71913500
H -2.54668100 2.11337100 -0.42409300	H -2.66255400 2.05980700 -0.64388400
H 2.54614200 2.13014300 -0.42037600	H 2.62303600 2.16840100 -0.54922500
C -3.38270500 -1.63785600 -0.31553900	C -3.45150300 -1.66946200 -0.01387200
C 3.42295100 -1.61607200 -0.24122700	C 3.55594000 -1.53182100 0.02639800
C -3.48601000 -2.68485400 0.79246700	C -3.41458700 -2.57413500 1.21836500
C 3.44095700 -2.66638600 0.86548500	C 3.49134900 -2.45740800 1.24055300
O 0.00543700 -0.49507500 -3.06443700	O 0.02521000 -0.89116600 -3.20895800
H 4.42545600 -1.18036900 -0.30943200	H 4.56088400 -1.09832400 -0.02417800
H -4.37852800 -1.19869900 -0.45655500	H -4.46769800 -1.27946900 -0.12096400
C 3.08352400 -2.27155200 -1.58255700	C 3.29781900 -2.32429700 -1.25688600
C -2.96176400 -2.29993200 -1.62893700	C -3.09287100 -2.46330900 -1.26415900
H 3.08249700 -1.56808900 -2.41212100	H 3.38600800 -1.71631600 -2.15755600
H -2.76368900 -1.58028700 -2.42572700	H -3.07397600 -1.85658900 -2.17055400
H 2.10072800 -2.74296700 -1.54657600	H 2.30209500 -2.76172200 -1.24739700
H -2.05786200 -2.89611200 -1.49148200	H -2.10970900 -2.92850300 -1.16166600
H 3.82169600 -3.05117100 -1.80809400	H 4.02750000 -3.14039400 -1.33676500
H -3.75529700 -2.97063500 -1.97620200	H -3.82947200 -3.25956300 -1.41426400
C -3.40487500 1.13753500 -2.11971400	C -3.59939300 0.88072800 -2.16459000

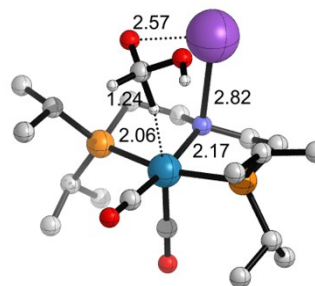
C 3.35119300 1.18473600 -2.15864200 H -4.13429900 0.35789000 -2.35931100 H 4.09986800 0.44270100 -2.43451400 H -2.47509400 0.88910000 -2.63748900 H 2.41375600 0.91361900 -2.64573500 H -3.78556400 2.07439700 -2.53254300 H 3.68131600 2.14240100 -2.57180300 C -4.55213800 1.54772500 0.07490000 C 4.57108700 1.57330600 -0.00244700 H -4.44302000 1.78601000 1.13320200 H 4.50841700 1.72801800 1.07581600 H -5.23901100 0.69979500 -0.00750300 H 5.28091300 0.76113400 -0.17962400 H -5.04124100 2.40194800 -0.40428300 H 5.00821300 2.47535800 -0.44193700 H 0.00414700 1.32628200 -0.56938600 C -0.06094800 2.87232200 -1.52532700 H -4.10714000 -3.51811300 0.44647900 H -2.50673800 -3.09642300 1.04638300 H -3.94388000 -2.29606500 1.70181900 H 4.14187500 -3.46190500 0.59437600 H 3.76550300 -2.26262400 1.82740700 H 2.45875500 -3.12922000 1.00127800 O -0.08274400 3.85164500 -0.75204600 C 0.01157700 -2.06947900 0.10427500 Mn 0.00901100 -0.33079300 -0.14877200 C 0.00868000 -0.45906500 -1.90115400 H 0.87985500 2.51414400 -1.99315200 K -0.02984200 2.78933100 1.59648000 H -0.99282100 2.46656100 -1.97555300	C 3.40345700 1.10629100 -2.22624600 H -4.35436000 0.10131800 -2.27140200 H 4.11443100 0.31054300 -2.46173100 H -2.69542200 0.54590500 -2.67922700 H 2.44309600 0.84054200 -2.66205200 H -3.97231000 1.77058100 -2.68368400 H 3.77093100 2.01528400 -2.71514800 C -4.64805800 1.57855300 0.00706800 C 4.66671600 1.67500500 -0.12093700 H -4.48817700 1.99512300 1.00028200 H 4.61797600 1.90334200 0.94746100 H -5.32052500 0.72206200 0.10496400 H 5.38804000 0.86441200 -0.25450400 H -5.18020300 2.33341800 -0.58477200 H 5.07968400 2.55729100 -0.62598900 H 0.01068700 1.47923800 -0.71674400 C -0.17332000 2.81189000 -1.67774100 H -4.04105500 -3.45377000 1.03357800 H -2.40683300 -2.93449900 1.41763100 H -3.79327500 -2.08440600 2.11703900 H 4.19327700 -3.28523100 1.09864000 H 3.76309600 -1.95638600 2.17013700 H 2.49772100 -2.88763700 1.35927300 O -0.37690700 3.82546000 -0.94819300 C 0.05493600 -2.15250000 0.22477100 Re 0.02340200 -0.29885400 -0.19573900 C 0.02413400 -0.67818100 -2.06085700 H 0.83080400 2.61848500 -2.13840400 K -0.06810400 3.06734000 1.46589700 H -1.02000900 2.27966000 -2.18601800
2Mn...K⁺ 	2Re...K⁺ 
O -0.00013500 -2.96543300 -0.90525600 P -2.22456200 0.03940600 -0.05741200 P 2.22461800 0.03952700 -0.05760900 C -2.43463200 0.77676000 -1.76326300 C 2.43464000 0.77688200 -1.76348200 H -2.52515500 1.86446100 -1.64587700 H 2.52517900 1.86458400 -1.64614300 H -3.34623800 0.44299000 -2.26342100 H 3.34620400 0.44303700 -2.26366400 C -1.17844800 0.43548400 -2.55349300 C 1.17840700 0.43557900 -2.55361700 H -1.20238100 0.97801700 -3.51943600 H 1.20223200 0.97811300 -3.51956700 H -1.21241500 -0.63935500 -2.82011500 H 1.21241700 -0.63925400 -2.82026900 N 0.00001200 0.77289600 -1.78687000 C 3.09506200 1.35564100 0.99348800 C -3.09516700 1.35538100 0.99371000 H 2.51522500 2.24830900 0.72105500 H -2.51481300 2.24798200 0.72217500	O -0.00002300 -3.03437800 -1.05798400 P -2.34320300 0.09715400 -0.10244600 P 2.34318500 0.09715000 -0.10247100 C -2.45599900 0.98002800 -1.75211200 C 2.45596900 0.97998500 -1.75215700 H -2.54807800 2.05370600 -1.54254400 H 2.54805700 2.05366500 -1.54260400 H -3.35022600 0.69863200 -2.31296500 H 3.35018500 0.69857800 -2.31302100 C -1.18191100 0.70271800 -2.54338700 C 1.18186100 0.70268500 -2.54340500 H -1.19403400 1.32402300 -3.45990900 H 1.19398100 1.32397600 -3.45993700 H -1.20922100 -0.34623200 -2.89556500 H 1.20914400 -0.34627100 -2.89556700 N -0.00001500 0.97299000 -1.74748400 C 3.23925300 1.33056300 1.01854900 C -3.23925300 1.33056300 1.01861200 H 2.65958200 2.24143500 0.81511900 H -2.65969700 2.24147300 0.81502300

C 3.44245200 -1.40389000 -0.01535500 C -3.44210800 -1.40427200 -0.01487000 C 3.41484400 -2.24970400 -1.28785800 C -3.41537700 -2.24944500 -1.28782600 O 0.00018800 -1.19251500 2.88972300 H -4.43893700 -0.95985700 0.07139100 H 4.43924000 -0.95917000 0.06983400 C -3.18834200 -2.28763800 1.20644900 C 3.18990300 -2.28668600 1.20662300 H -3.22167800 -1.73435300 2.14569100 H 3.22432700 -1.73298500 2.14558500 H -2.20861600 -2.76362900 1.14239400 H 2.21004100 -2.76257500 1.14382800 H -3.94378200 -3.07823000 1.25767500 H 3.94528700 -3.07735800 1.25741100 C 2.91347100 1.15211900 2.49376900 C -2.91465600 1.15094500 2.49400300 H 3.49874000 0.30429800 2.85623100 H -3.50063300 0.30322600 2.85556600 H 1.86754300 0.97657000 2.74563000 H -1.86899500 0.97471900 2.74650300 H 3.25855200 2.03612600 3.04069200 H -3.25964400 2.03481700 3.04120100 C 4.55583400 1.62200000 0.63804300 C -4.55560600 1.62249600 0.63746000 H 4.71012300 1.75642700 -0.43518800 H -4.70910600 1.75781000 -0.43577000 H 5.20247200 0.80625200 0.96947100 H -5.20277800 0.80673200 0.96780100 H 4.90823900 2.52869200 1.14122700 H -4.90804000 2.52891900 1.14110900 H -0.00002100 1.20441900 0.91932100 H 4.15158700 -3.05480600 -1.20046400 H 2.44048100 -2.71329200 -1.44286600 H 3.66607000 -1.67635500 -2.18177300 H -4.15152200 -3.05505000 -1.20003500 H -3.66794500 -1.67578800 -2.18116400 H -2.44090000 -2.71237100 -1.44411900 C 0.00000700 -1.85486300 -0.54872000 C 0.00014100 -0.82857800 1.78447700 Mn 0.00005200 -0.22775800 0.13558700 K -0.00029300 3.14747100 -0.58269200	C 3.55162900 -1.34036600 -0.25121300 C -3.55163500 -1.34036200 -0.25129900 C 3.39687000 -2.10275500 -1.56596500 C -3.39676500 -2.10270200 -1.56606500 O 0.00002400 -1.48892400 2.97482900 H -4.55292900 -0.89731300 -0.23154900 H 4.55291900 -0.89730700 -0.23140300 C -3.40257100 -2.29220300 0.93434100 C 3.40250600 -2.29214600 0.93447100 H -3.56733000 -1.80099300 1.89403200 H 3.56707400 -1.80085500 1.89415600 H -2.40179700 -2.72684400 0.95561200 H 2.40177700 -2.72689000 0.95563100 H -4.12645800 -3.10865200 0.84901900 H 4.12649400 -3.10852100 0.84929800 C 3.07084700 1.02221100 2.50238500 C -3.07059700 1.02239000 2.50245500 H 3.66076000 0.15355100 2.80210300 H -3.66037500 0.15370700 2.80235900 H 2.02597000 0.82553600 2.74410000 H -2.02566300 0.82584500 2.74403600 H 3.41590300 1.86844900 3.10584600 H -3.41564800 1.86866100 3.10587100 C 4.69643700 1.60533800 0.65703100 C -4.69651100 1.60519000 0.65727000 H 4.83360300 1.81837800 -0.40606000 H -4.83384600 1.81810300 -0.40582500 H 5.33726400 0.75885400 0.91455600 H -5.33724000 0.75869000 0.91498300 H 5.06958800 2.46762500 1.21944600 H -5.06964600 2.46751200 1.21964200 H -0.00004200 1.34299900 1.07241300 H 4.13261100 -2.91247200 -1.60090900 H 2.40832000 -2.55332600 -1.65476900 H 3.56563600 -1.47283600 -2.44118700 H -4.13255900 -2.91236600 -1.60114000 H -3.56537300 -1.47273100 -2.44127900 H -2.40823000 -2.55332900 -1.65476500 C -0.00003100 -1.94139600 -0.64275000 C 0.00001300 -1.01311900 1.90983600 K -0.00000700 3.30212500 -0.41268200 Re -0.00000800 -0.20727500 0.18174000
1Mn-OCH₂OH...K⁺  N -0.03159200 0.15895300 -1.89586000 P -2.34876600 -0.10901900 -0.09509700 P 2.21370900 -0.37296600 -0.09684500 C 0.24712200 2.53315800 1.46182500 C -2.45970200 0.39061400 -1.88589900 C 2.39885600 -0.00355300 -1.91607800 H -2.41514300 1.48516900 -1.89620400 H 2.55926500 1.07721100 -2.00038000	1Re-OCH₂OH...K⁺  N 0.02894900 0.30617300 -1.93830500 P -2.30883500 -0.31822400 -0.17108900 P 2.43274000 -0.04236800 -0.16367800 C -0.31481400 2.62262500 1.52763800 C -2.42104200 0.13755700 -1.98142800 C 2.47771000 0.51737000 -1.94463700 H -2.58590800 1.22088600 -2.01754200 H 2.44902500 1.61246200 -1.91469100

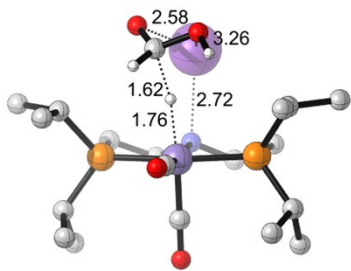
H	-3.40134400	0.10118100	-2.35759700	H	-3.28024000	-0.31985000	-2.47635600
H	3.27333000	-0.48033900	-2.36307200	H	3.40196200	0.23481200	-2.45393800
C	-1.24684200	-0.18359100	-2.60457200	C	-1.10907400	-0.22017400	-2.67040900
C	1.09994700	-0.39819500	-2.60598100	C	1.24460200	-0.01390700	-2.66588400
H	-1.22876200	0.20779900	-3.64198000	H	-1.13452800	0.18178000	-3.70265200
H	1.13099100	-0.04019200	-3.65512200	H	1.21989600	0.42064200	-3.68468700
H	-1.38214500	-1.27726500	-2.71740600	H	-1.05845700	-1.31865400	-2.78951700
H	1.05892100	-1.50221700	-2.68566300	H	1.36239900	-1.10304300	-2.82004900
C	3.30014000	0.95668100	0.68496100	C	3.28599300	1.38712500	0.70752300
C	-3.20158200	1.33148800	0.76290400	C	-3.40655100	0.99530700	0.62042300
H	2.69863700	1.86229500	0.55158800	H	2.54930400	2.17998700	0.53855100
H	-2.46677400	2.12322000	0.58601600	H	-2.80177200	1.90207000	0.50465600
C	3.23120700	-1.93851200	0.20215600	C	3.64371100	-1.47496800	-0.04023600
C	-3.57126300	-1.53047600	0.11753400	C	-3.32326700	-1.89524100	0.02521000
H	4.26312400	-1.58784900	0.31563200	H	4.63781600	-1.01391400	-0.02136000
H	-4.55245900	-1.05275800	0.21619000	H	-4.36598400	-1.56083100	0.07034800
C	-0.08509800	-0.64308600	1.90721500	C	0.07517700	-0.68293100	2.06735000
O	-0.09268000	-0.86045300	3.04832600	O	0.07694700	-0.91574400	3.21050800
C	-3.28240200	-2.31131800	1.40103500	C	-2.98220300	-2.60861700	1.33392100
C	2.81309600	-2.62859300	1.50161400	C	3.43598900	-2.25413000	1.25892500
H	-3.21501500	-1.67110300	2.28074200	H	-3.06552900	-1.96001400	2.20564200
H	2.80487200	-1.95422900	2.35775700	H	3.48101300	-1.62088500	2.14485000
H	-2.34343000	-2.86032700	1.32033800	H	-1.96414900	-2.99750000	1.30974800
H	1.81506000	-3.05849500	1.41196100	H	2.46617500	-2.75288700	1.25916200
H	-4.08018300	-3.03990600	1.57784700	H	-3.66287800	-3.45376000	1.47802800
H	3.50819800	-3.44440000	1.72487000	H	4.21066600	-3.02143800	1.35530200
C	-3.63190200	-2.48284200	-1.07603100	C	-3.18549500	-2.85932100	-1.15231500
C	3.20391400	-2.93744700	-0.95431600	C	3.57925600	-2.42013800	-1.23910100
H	-2.67517500	-2.97940500	-1.24297800	H	-2.15773200	-3.20470000	-1.26866500
H	2.19603100	-3.30766600	-1.14466700	H	2.59960400	-2.89272600	-1.32188800
H	-3.92409900	-1.98186200	-2.00032000	H	-3.51313700	-2.42290300	-2.09731600
H	3.59780000	-2.52074400	-1.88251500	H	3.80230600	-1.91998000	-2.18307000
H	-4.37497600	-3.26221300	-0.87871900	H	-3.80778100	-3.74084300	-0.96871300
H	3.82585900	-3.80083500	-0.69709900	H	4.31772900	-3.21753300	-1.10955300
C	3.48987100	0.74068100	2.18557400	C	3.39580700	1.18012300	2.21571900
C	-3.32158500	1.13644700	2.27188100	C	-3.60318500	0.75791600	2.11660300
H	4.16859200	-0.09274300	2.38519000	H	4.16934100	0.44997500	2.46712400
H	-4.07678900	0.38662300	2.52239600	H	-4.29789200	-0.06565200	2.30017300
H	2.54854700	0.53935600	2.69895800	H	2.45291700	0.84293200	2.64778700
H	-2.37598900	0.83205800	2.72134800	H	-2.66502800	0.52764200	2.62433300
H	3.93449900	1.63287500	2.63759100	H	3.67356200	2.12106600	2.70117000
H	-3.63211100	2.07362300	2.74477600	H	-4.03131400	1.65009900	2.58428300
C	4.65279500	1.16594000	0.00597000	C	4.62844800	1.79457800	0.10674800
C	-4.54404900	1.73391700	0.15778400	C	-4.75223900	1.21491300	-0.06840000
H	4.56374900	1.39142700	-1.05839400	H	4.57022700	1.98807700	-0.96646200
H	-4.48288400	1.92811900	-0.91489100	H	-4.65317200	1.44477600	-1.13109000
H	5.29948300	0.28997000	0.10669000	H	5.39384700	1.03028500	0.26708200
H	-5.30908100	0.96831200	0.31486600	H	-5.40257500	0.34095100	0.02353900
H	5.17712200	2.00472500	0.47576000	H	4.98911800	2.71033700	0.58679300
H	-4.90810500	2.64877600	0.63724900	H	-5.27745000	2.05334200	0.40089400
H	-0.57932900	3.00614800	2.03544400	H	-1.00383300	2.08503500	2.19935000
O	1.00567400	3.67718000	0.85939400	O	-1.09129200	3.73623800	0.91164200
H	1.23462200	4.29461600	1.56230300	H	-1.38435400	4.32788100	1.61268700
C	-0.15999300	-2.04351800	-0.18750400	C	0.14742500	-2.15915200	-0.15073400
O	-0.23798700	-3.18314000	-0.42234200	O	0.21823500	-3.31460800	-0.34283100
Mn	-0.07120500	-0.34178700	0.16564900	Re	0.06584700	-0.31659100	0.19259600
K	0.37465600	2.90598600	-1.70699200	K	-0.37011300	3.04899300	-1.64601200
O	-0.15665600	1.75798300	0.46864000	O	0.17539800	1.88371900	0.53572400
H	0.93175500	2.04975800	2.18071500	H	0.46741100	3.11070800	2.14338500
1Mn-HCH(OH)O⁻...K⁺				1Re-HCH(OH)O⁻...K⁺			



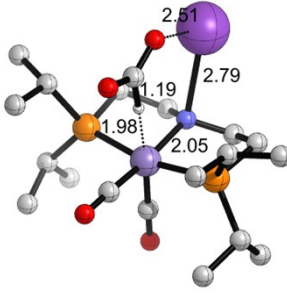
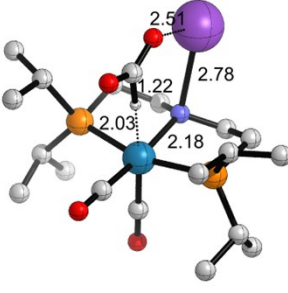
N	-0.01553100	0.49580800	-1.70923300
P	-2.22173100	-0.41561300	-0.04809900
P	2.33086900	-0.10958100	-0.08980200
H	-0.19716500	1.33176100	0.89154600
C	-0.11227900	2.50708900	1.03989900
C	-2.46016300	0.37305300	-1.71940300
C	2.40959500	0.78713600	-1.72107600
H	-2.63263100	1.43242200	-1.50590900
H	2.36835800	1.85373100	-1.47203900
H	-3.33869200	0.00221500	-2.25066100
H	3.33907700	0.61587700	-2.26809400
C	-1.17739000	0.17548000	-2.51748100
C	1.17881900	0.38961800	-2.52415300
H	-1.21820200	0.81149800	-3.43079800
H	1.11112100	1.04221800	-3.42229800
H	-1.14878800	-0.85708400	-2.91162300
H	1.32396800	-0.62654900	-2.93541900
C	3.23526000	1.08228400	1.05646200
C	-3.18461700	0.75508400	1.05600200
H	2.55237300	1.93662000	1.08351500
H	-2.61964700	1.68976300	0.91588300
C	3.53767200	-1.55177800	-0.23389400
C	-3.24980600	-1.99484000	-0.07693400
H	4.52511000	-1.10624000	-0.07383800
H	-4.28069600	-1.65916700	0.07772200
C	0.12378300	-1.00783100	1.78883300
O	0.16830900	-1.41351200	2.87263000
C	-2.86513300	-2.92128600	1.07726300
C	3.29584100	-2.59147200	0.86180400
H	-2.88539100	-2.42026600	2.04528100
H	3.26141300	-2.15546400	1.85993500
H	-1.86295700	-3.32833000	0.93658500
H	2.35747200	-3.12213100	0.70011600
H	-3.56259700	-3.76359300	1.12269800
H	4.10198500	-3.33172300	0.84827900
C	-3.19599000	-2.74638700	-1.40630700
C	3.54412000	-2.21866600	-1.60870800
H	-2.18730400	-3.09058400	-1.63670100
H	2.57962400	-2.66984800	-1.84432900
H	-3.55401700	-2.14561000	-2.24419100
H	3.80604100	-1.52668000	-2.41084600
H	-3.83681400	-3.63171900	-1.34579900
H	4.28893000	-3.02066900	-1.61546900
C	3.36195500	0.56589900	2.48729800
C	-3.12234600	0.38909000	2.53657400
H	4.09211900	-0.24405400	2.56053000
H	-3.72094200	-0.49649400	2.76726300
H	2.40927100	0.21627200	2.88391400
H	-2.10183700	0.21154200	2.87569600
H	3.70844400	1.37528800	3.13599300
H	-3.52869200	1.21360100	3.13059600



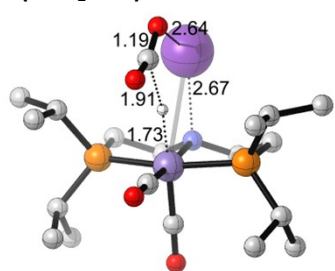
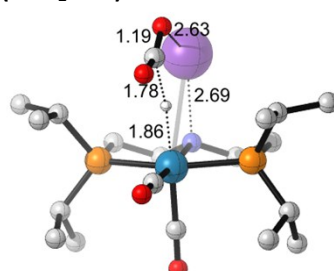
O	0.00990000	-3.36370000	0.40011300
P	2.39191000	-0.18130100	0.15450500
P	-2.37308500	-0.24532700	0.15521700
C	2.43093500	0.73496900	1.77498800
C	-2.48940200	0.42728700	1.89543400
H	2.42515800	1.79267200	1.49142300
H	-2.67590900	1.50307400	1.79866700
H	3.34321600	0.54266900	2.34485200
H	-3.33701300	0.01350700	2.44516200
C	1.18626100	0.39473200	2.58258300
C	-1.17207100	0.17245600	2.61786300
H	1.14441300	1.06593700	3.46452100
H	-1.16646600	0.76097100	3.55710600
H	1.29112500	-0.61976100	3.00633000
H	-1.13980300	-0.88314000	2.94297900
N	-0.02820700	0.51728900	1.78911100
C	-3.39492500	1.03279400	-0.77924700
C	3.41991300	0.95199200	-0.93381600
H	-2.81704500	1.94282900	-0.58152400
H	2.85522500	1.88790100	-0.84174800
C	-3.45330600	-1.78620200	0.13145200
C	3.46466600	-1.70371500	0.41132300
C	-3.28052900	-2.65913000	1.37361600
C	3.18885900	-2.42066100	1.73116600
O	-0.02201400	-1.02492200	-3.19666400
H	4.48752200	-1.31407700	0.44796900
H	-4.48319800	-1.41431000	0.12104700
C	3.35509100	-2.67345000	-0.76538100
C	-3.21402400	-2.60455700	-1.13823000
H	3.56392300	-2.19714400	-1.72330400
H	-3.27502900	-2.00630500	-2.04757600
H	2.35913900	-3.11334600	-0.82222900
H	-2.22983400	-3.07324400	-1.11934800
H	4.07319500	-3.48925400	-0.63611500
H	-3.96315000	-3.39903300	-1.20952500
C	-3.39888500	0.80739800	-2.28918100
C	3.43529600	0.54931400	-2.40610100
H	-4.03129200	-0.03892200	-2.56633200
H	4.08181800	-0.31275800	-2.58844700
H	-2.39754200	0.61372000	-2.67765500
H	2.43945000	0.30878500	-2.77926500
H	-3.80435300	1.68686100	-2.79998700
H	3.82706000	1.37666700	-3.00555700
C	-4.81281500	1.24057300	-0.25096000
C	4.83550300	1.20132400	-0.41660900
H	-4.84320500	1.40595200	0.82819200
H	4.85755700	1.46852900	0.64214300
H	-5.45813100	0.38852000	-0.47771800
H	5.48638300	0.33475300	-0.56254100
H	-5.26256500	2.11602100	-0.72993900
H	5.28156500	2.03400000	-0.96884000

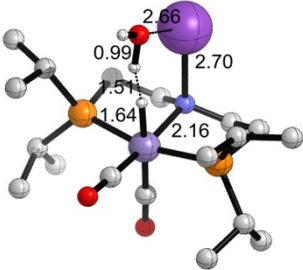
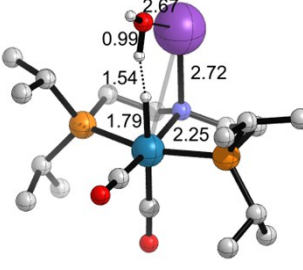
C 4.58409100 1.56740400 0.52791100	H 0.13525400 1.57117400 -0.81631400
C -4.62796600 0.99169300 0.61559900	C 0.41667500 2.70674200 -1.23562000
H 4.51999900 1.98655100 -0.47841900	H -3.91957800 -3.54287400 1.28327800
H -4.71117300 1.26585200 -0.43860300	H -2.25408400 -3.01041300 1.48073700
H 5.32953000 0.76793700 0.51192500	H -3.56815700 -2.14479800 2.29218400
H -5.26208200 0.11694000 0.78651400	H 3.85911300 -3.28131400 1.82091300
H 4.97268700 2.35143300 1.18521300	H 3.36325900 -1.78030500 2.59762600
H -5.05461000 1.81407400 1.19827700	H 2.16685800 -2.79789600 1.78025000
H 0.86060500 2.73984600 0.53824500	O 1.26212100 3.31097200 -0.50160100
O -1.15170800 3.15074300 0.58870400	C 0.00180100 -2.21290900 0.18654200
O 0.15024000 2.67287900 2.43187200	Re 0.00041800 -0.38060200 -0.18684000
H -0.67127900 3.05321100 2.76494100	C -0.00651500 -0.79461500 -2.05510400
C 0.16831700 -2.06707800 -0.49446500	H 0.68884600 2.47689000 -2.28379800
O 0.22861300 -3.15295300 -0.91068800	O -0.89191300 3.36368900 -1.23066700
Mn 0.06486800 -0.44359000 0.10765600	H -1.41901000 2.98540200 -1.94345700
K -0.53204600 3.25791300 -1.86975700	K -0.30215400 3.31532800 1.54218400
Mn-TS(HCH(OH)O⁻...K⁺)	
	
O 0.01007500 -3.24899900 0.11105800	O 0.01539800 -3.37600700 0.11468700
P 2.28243700 -0.26510500 0.10344900	P 2.38417000 -0.20154800 0.17206300
P -2.26779800 -0.29535700 0.10765000	P -2.36410600 -0.24646000 0.16965700
C 2.42809600 0.11416800 1.91896200	C 2.44272200 0.38668600 1.94079600
C -2.45211100 -0.05646600 1.94724200	C -2.47619900 0.16267900 1.99061200
H 2.46478000 1.20640300 1.99831100	H 2.47133100 1.48073200 1.88831700
H -2.58544800 1.01919200 2.11524500	H -2.63372200 1.24601100 2.06100800
H 3.34775400 -0.27030600 2.36503500	H 3.34966100 0.06571000 2.45853700
H -3.33741000 -0.54517300 2.35798800	H -3.33758800 -0.30495500 2.47177800
C 1.18309000 -0.42521600 2.60429500	C 1.18722500 -0.07927600 2.66587400
C -1.16458300 -0.53769800 2.59846600	C -1.16817900 -0.23221100 2.66542200
H 1.18598900 -0.09948400 3.66356600	H 1.17492600 0.37345200 3.67673100
H -1.17804600 -0.25591800 3.67000200	H -1.17516900 0.15889000 3.70148600
H 1.24922600 -1.52972900 2.64442000	H 1.25923200 -1.16909000 2.83852000
H -1.15720000 -1.64531500 2.59371400	H -1.14279000 -1.33329500 2.77043200
N -0.01407400 0.02589000 1.92356200	N -0.01872400 0.26771400 1.93220200
C -3.31361800 1.13368000 -0.54853300	C -3.40651900 1.14680500 -0.56316300
C 3.31713400 1.11215800 -0.65692500	C 3.41031200 1.10808300 -0.69935000
H -2.71649700 2.00417800 -0.25693900	H -2.83771900 2.02558800 -0.23796000
H 2.71445500 1.99935100 -0.44100000	H 2.81082600 2.00681500 -0.52072200
C -3.35079300 -1.78467800 -0.32671900	C -3.45105500 -1.76688000 -0.07410900
C 3.37130900 -1.78214200 -0.18945900	C 3.46774500 -1.74054700 0.11889700
C -3.36204100 -2.88308700 0.73577100	C -3.30169700 -2.80303500 1.03889200
C 3.34410100 -2.80734900 0.94293300	C 3.27137500 -2.66468100 1.31908600
O -0.00651300 -0.41387300 -3.08178000	O -0.01151000 -0.66772500 -3.25830900
H 4.38931700 -1.38299700 -0.24927500	H 4.49429400 -1.36010300 0.15229300
H -4.36757900 -1.38453100 -0.39952000	H -4.47982900 -1.39282500 -0.04824800
C 3.04336000 -2.45305900 -1.52454800	C 3.27482100 -2.50967300 -1.18815300
C -2.96755200 -2.36572400 -1.68864700	C -3.19705400 -2.40692300 -1.43898700
H 3.04542500 -1.75415300 -2.36111400	H 3.43078000 -1.88835800 -2.06989000
H -2.94387900 -1.61522100 -2.47910200	H -3.31369000 -1.70489600 -2.26510500
H 2.06397700 -2.93044300 -1.49488600	H 2.27007000 -2.92776000 -1.25138600
H -1.98462800 -2.83553100 -1.65282700	H -2.18796000 -2.81572200 -1.49635500
H 3.78501800 -3.22967000 -1.73745800	H 3.98718100 -3.33943100 -1.23425200

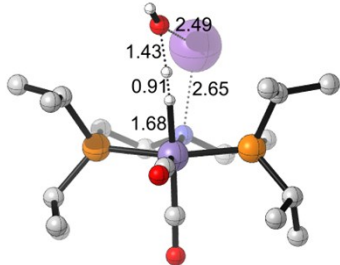
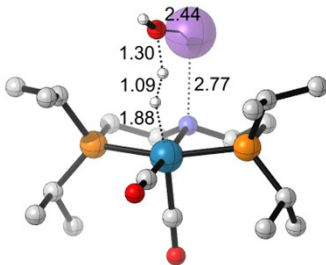
H -3.69323000 -3.13232200 -1.97827800	H -3.90308100 -3.22809800 -1.59680900
C -3.41400100 1.13230700 -2.07327700	C -3.41467000 1.13941600 -2.09049200
C 3.45303400 0.98974500 -2.17389600	C 3.49439800 0.89999300 -2.21024200
H -4.09727200 0.35530900 -2.42419000	H -4.07242500 0.35985300 -2.48089300
H 4.15210700 0.19647000 -2.45149800	H 4.19901900 0.10625200 -2.47076200
H -2.45075300 0.95134900 -2.55737000	H -2.42042100 0.95858400 -2.50687800
H 2.50088000 0.78199500 -2.66479800	H 2.52683300 0.64732400 -2.64682600
H -3.81041000 2.08835000 -2.43027500	H -3.79257700 2.09227100 -2.47613500
H 3.84665400 1.92382700 -2.58619500	H 3.85187500 1.81694100 -2.68836800
C -4.69908100 1.27561300 0.07893300	C -4.82303200 1.27099500 -0.00649900
C 4.68778200 1.31157800 -0.01165700	C 4.79672300 1.33618800 -0.10030400
H -4.66487000 1.32231500 1.16895600	H -4.84639500 1.27744700 1.08532700
H 4.62756200 1.45763400 1.06839000	H 4.76593900 1.51943900 0.97584000
H -5.35892600 0.44985500 -0.19832800	H -5.46530200 0.45698300 -0.35046600
H 5.36156800 0.47151000 -0.20100100	H 5.46795800 0.49225800 -0.28086300
H -5.17493200 2.19587200 -0.27516300	H -5.28007100 2.20396500 -0.35159800
H 5.16230600 2.20276700 -0.43444400	H 5.25492700 2.21409100 -0.56622100
H 0.08652700 1.38835900 -0.46781500	H 0.12318600 1.52306700 -0.59006700
C 0.38244600 2.85707600 -1.08086400	C 0.38768000 2.91761800 -1.15088500
H -4.02085600 -3.69295800 0.40675900	H -3.97050600 -3.64520000 0.83584900
H -2.37121600 -3.31140600 0.88757600	H -2.28726600 -3.19800600 1.08990300
H -3.73691800 -2.53371400 1.69909600	H -3.56809200 -2.40821000 2.02078200
H 4.03072100 -3.62569000 0.70327400	H 3.94876200 -3.51974100 1.22919400
H 3.66242100 -2.38658600 1.89814500	H 3.49296000 -2.17268000 2.26775100
H 2.35294900 -3.24245100 1.07258700	H 2.25537000 -3.05800200 1.36358200
O 1.05376700 3.50480000 -0.26871800	O 1.17359100 3.52604900 -0.41079400
C 0.00276100 -2.08759800 0.02388900	C 0.00188100 -2.20964000 0.03097300
Mn 0.00116700 -0.34676100 -0.16106600	Re 0.00284500 -0.33078100 -0.20149600
C -0.00049700 -0.41427400 -1.91779900	C -0.00117300 -0.55889500 -2.09681500
H 0.82577400 2.40322800 -1.97545600	H 0.69525500 2.52414700 -2.12883900
O -0.92021800 3.29459800 -1.28919900	O -0.92934200 3.41221900 -1.16698100
H -1.33296800 2.71570000 -1.94216100	H -1.44577400 2.87211600 -1.77807500
K -0.21329000 2.74201300 1.84322900	K -0.26369500 3.00856100 1.70906700
1Mn-OOCH...K⁺	1Re-OOCH...K⁺
O -0.00051900 -3.17940600 -0.59430100	O -0.00004900 -3.32068800 -0.47810000
P -2.28203100 -0.23337100 -0.09666300	P -2.37356400 -0.17008500 -0.16339900
P 2.28176000 -0.23385800 -0.09673800	P 2.37356500 -0.17010500 -0.16360600
C -2.44037600 0.28212300 -1.88073300	C -2.45817000 0.42100300 -1.93416600
C 2.44020000 0.28159000 -1.88081100	C 2.45806500 0.42066900 -1.93447400
H -2.51082500 1.37581200 -1.87907700	H -2.53191300 1.51376000 -1.88686000
H 2.51095600 1.37524900 -1.87923600	H 2.53179200 1.51343400 -1.88737200
H -3.34886600 -0.09201500 -2.35690500	H -3.35232200 0.06794300 -2.45244900
H 3.34859700 -0.09282400 -2.35694600	H 3.35213900 0.06747300 -2.45279000
C -1.17754600 -0.16115100 -2.60585800	C -1.18137400 0.01156400 -2.65888000
C 1.17725300 -0.16145400 -2.60587100	C 1.18115600 0.01120600 -2.65894800
H -1.18384400 0.26858900 -3.62763800	H -1.18045200 0.48366800 -3.66092400
H 1.18360300 0.26818300 -3.62769400	H 1.18019300 0.48299000 -3.66113600
H -1.22065500 -1.25698200 -2.76009400	H -1.21584600 -1.07667200 -2.85334100
H 1.22013900 -1.25730600 -2.76002500	H 1.21532400 -1.07710100 -2.85303900
N -0.00008700 0.25552100 -1.87084600	N -0.00004300 0.39689900 -1.90529800
	C 3.30945300 1.19764500 0.72976400

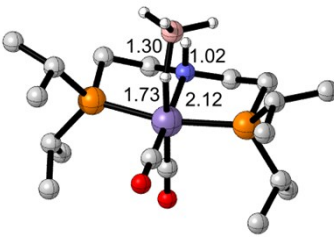
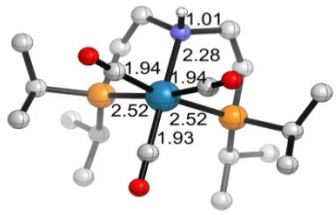
C 3.20936300 1.15125400 0.78067100	C -3.30941900 1.19749600 0.73027000
C -3.20913100 1.15207200 0.78074500	H 2.65758200 2.05797800 0.54157900
H 2.56306000 2.01070100 0.57567400	H -2.65747300 2.05783100 0.54236100
H -2.56255500 2.01126900 0.57556100	C 3.50769300 -1.66614200 -0.06082100
C 3.41992200 -1.72249400 0.11693300	C -3.50766100 -1.66614600 -0.06077200
C -3.42058400 -1.72167100 0.11715700	C 3.39458000 -2.58641800 -1.27542500
C 3.44264200 -2.66243100 -1.08802300	C -3.39466100 -2.58619600 -1.27555400
C -3.44366600 -2.66158100 -1.08781300	O 0.00016600 -1.09203900 3.17189800
O -0.00016600 -1.08667300 2.99876700	H -4.52430100 -1.25878600 -0.03470100
H -4.42504000 -1.30085000 0.23341300	H 4.52433100 -1.25876500 -0.03494500
H 4.42450400 -1.30194400 0.23308300	C -3.25712200 -2.45199400 1.22633000
C -3.07147300 -2.49841600 1.38757300	C 3.25731300 -2.45176200 1.22644000
C 3.07074200 -2.49915300 1.38738400	H -3.33754400 -1.83602900 2.12200800
H -3.03009800 -1.86580600 2.27438200	H 3.33815000 -1.83570100 2.12201600
H 3.02969400 -1.86655000 2.27421300	H -2.26122300 -2.89632900 1.22062400
H -2.10369600 -2.99203800 1.29039700	H 2.26128800 -2.89582400 1.22105800
H 2.10279300 -2.99246100 1.29032900	H -3.98806800 -3.26218200 1.30999800
H -3.82419200 -3.27316500 1.56420900	H 3.98806100 -3.26213800 1.31001500
H 3.82323300 -3.27415000 1.56390100	C 3.36554900 0.98872500 2.24085700
C 3.25882600 0.96469200 2.29482400	C -3.36560400 0.98817100 2.24130400
C -3.25838000 0.96566600 2.29491700	H 4.08375100 0.21023200 2.50909600
H 3.94970700 0.16596300 2.57607000	H -4.08380400 0.20958800 2.50928900
H -3.94928400 0.16703000 2.57637600	H 2.39410700 0.70934800 2.65051800
H 2.27940900 0.72801600 2.71155600	H -2.39417800 0.70872500 2.65095700
H -2.27890600 0.72894700 2.71149100	H 3.68928600 1.91041900 2.73333800
H 3.61447100 1.88257300 2.77226900	H -3.68939900 1.90972600 2.73400800
H -3.61386500 1.88362700 2.77233300	C 4.69399600 1.50400600 0.16326800
C 4.59979800 1.44740500 0.22217400	C -4.69392100 1.50406000 0.16379000
C -4.59954900 1.44854200 0.22239600	H 4.68020900 1.68569900 -0.91357300
H 4.59499800 1.62001600 -0.85603500	H -4.68008000 1.68607300 -0.91299600
H -4.59480700 1.62107300 -0.85582700	H 5.39802800 0.69065000 0.35634200
H 5.30177800 0.63501100 0.42716700	H -5.39798300 0.69066100 0.35657800
H -5.30173100 0.63635300 0.42751100	H 5.10216300 2.39906600 0.64321300
H 5.00559800 2.34599400 0.69772100	H -5.10209800 2.39898400 0.64398000
H -5.00506600 2.34727200 0.69792000	H 4.08787200 -3.42471500 -1.15624000
H 4.13308600 -3.48756000 -0.88689000	H 2.39148400 -3.00375300 -1.37007200
H 2.46133000 -3.09821800 -1.27902900	H 3.64954300 -2.08478900 -2.21041600
H 3.78313000 -2.17057300 -2.00050800	H -4.08778500 -3.42462800 -1.15636300
H -4.13422900 -3.48659000 -0.88660100	H -3.64990900 -2.08443900 -2.21040100
H -3.78420300 -2.16962300 -2.00022700	H -2.39151200 -3.00334800 -1.37048200
H -2.46246100 -3.09754200 -1.27898500	O 0.00090700 3.95286800 1.20768500
O 0.00206000 3.82818900 1.13474800	C 0.00012000 -0.80249600 2.04316700
C -0.00016800 -0.78607900 1.87804900	C 0.00077700 2.74333100 1.46561900
C 0.00117000 2.61810500 1.40934400	C -0.00000300 -2.17413500 -0.23703400
C -0.00035100 -2.05385700 -0.29547600	Re 0.00003000 -0.34861900 0.18543600
Mn -0.00015200 -0.37268400 0.15602900	K -0.00072400 3.24527100 -1.57111300
K 0.00051200 3.09771400 -1.61100400	O -0.00024000 1.83722000 0.56833200
O -0.00021700 1.69742300 0.53481200	H 0.00151700 2.40735300 2.51978100
H 0.00156800 2.30961800 2.47375300	
1Mn-HCOO⁻...K⁺	1Re-HCOO⁻...K⁺
	
O 0.00000400 -3.19979000 0.82187400	O -0.00000200 -3.31661900 -0.72495500

P	2.27547400	-0.23187200	0.09063700	P	-2.36942600	-0.15226700	-0.15099000
P	-2.27547800	-0.23188400	0.09063000	P	2.36942500	-0.15223700	-0.15101800
C	2.44387000	0.49346100	1.80016400	C	-2.46164400	0.65356600	-1.83639900
C	-2.44388200	0.49346600	1.80014900	C	2.46162400	0.65359400	-1.83642800
H	2.52417800	1.57695800	1.65839100	H	-2.54545600	1.73003700	-1.64798000
H	-2.52418500	1.57696000	1.65836300	H	2.54542100	1.73006700	-1.64802100
H	3.35024500	0.17325200	2.31729100	H	-3.35399000	0.35986700	-2.39307800
H	-3.35026000	0.17326300	2.31727400	H	3.35397200	0.35989700	-2.39310600
C	1.18177500	0.14383300	2.57553200	C	-1.18592200	0.34028900	-2.61014400
C	-1.18179200	0.14384200	2.57552700	C	1.18590000	0.34028900	-2.61015700
H	1.16265700	0.73193500	3.51852500	H	-1.17194100	0.95714600	-3.53408900
H	-1.16267800	0.73195300	3.51851400	H	1.17189800	0.95712600	-3.53411400
H	1.24106300	-0.90821800	2.90973700	H	-1.23083700	-0.70268200	-2.97179600
H	-1.24108200	-0.90820600	2.90974300	H	1.23082100	-0.70268900	-2.97178600
N	-0.00000600	0.40408400	1.77313900	N	-0.00000800	0.58619500	-1.80487700
C	-3.16260500	1.06579300	-0.94745900	C	3.27692600	1.11269200	0.90733000
C	3.16260100	1.06581100	-0.94744100	C	-3.27692400	1.11266900	0.90735600
H	-2.53423200	1.94722400	-0.77785200	H	2.65361900	2.00131600	0.75265900
H	2.53420000	1.94723100	-0.77787800	H	-2.65361500	2.00129100	0.75268300
C	-3.42873600	-1.72043200	0.04775200	C	3.51893700	-1.63679100	-0.23756900
C	3.42875000	-1.72040600	0.04774500	C	-3.51890700	-1.63684700	-0.23751500
C	-3.42404300	-2.53447600	1.34099500	C	3.36978600	-2.42526200	-1.53779300
C	3.42408900	-2.53445000	1.34098900	C	-3.36981200	-2.42527200	-1.53777200
O	-0.00000700	-1.37246800	-2.87379300	O	-0.00001000	-1.40344900	3.05401800
H	4.43193400	-1.30201400	-0.08357900	H	-4.53186000	-1.22193200	-0.20336200
H	-4.43192800	-1.30205700	-0.08356400	H	4.53187900	-1.22184200	-0.20349400
C	3.11660800	-2.61966300	-1.14897200	C	-3.31869400	-2.55326300	0.96926500
C	-3.11658200	-2.61969100	-1.14896000	C	3.31882600	-2.55316900	0.96925700
H	3.09805200	-2.07646600	-2.09373900	H	-3.43301400	-2.03226600	1.91976000
H	-3.09804000	-2.07649800	-2.09372900	H	3.43322100	-2.03213900	1.91972600
H	2.14841200	-3.10754900	-1.02984200	H	-2.32473400	-3.00236200	0.95622800
H	-2.14837400	-3.10755600	-1.02983100	H	2.32486700	-3.00227200	0.95631500
H	3.87657100	-3.40307100	-1.22836300	H	-4.05425500	-3.36292900	0.94100400
H	-3.87653000	-3.40311400	-1.22834400	H	4.05438800	-3.36283200	0.94096400
C	-3.13772800	0.76912300	-2.44437500	C	3.24561700	0.79052400	2.39887300
C	3.13778600	0.76910200	-2.44435100	C	-3.24561200	0.79050700	2.39890100
H	-3.78019600	-0.07829100	-2.69645200	H	3.90433500	-0.04634100	2.64243500
H	3.78028300	-0.07830500	-2.69637900	H	-3.90433500	-0.04635100	2.64247000
H	-2.12964100	0.57373700	-2.80761900	H	2.23927600	0.55880000	2.74651700
H	2.12971500	0.57368800	-2.80762500	H	-2.23927200	0.55877300	2.74654400
H	-3.51424500	1.63715900	-2.99250000	H	3.59620200	1.65664900	2.96684600
H	3.51430200	1.63713200	-2.99248400	H	-3.59619100	1.65663600	2.96687200
C	-4.57930000	1.38813800	-0.47478400	C	4.69464300	1.42946100	0.43582800
C	4.57927200	1.38819600	-0.47472100	C	-4.69464100	1.42944500	0.43585800
H	-4.63334000	1.61409100	0.59262700	H	4.74667500	1.66760500	-0.62930800
H	4.63326300	1.61419900	0.59268200	H	-4.74667300	1.66760000	-0.62927500
H	-5.27216200	0.56824100	-0.68023200	H	5.37847600	0.59917500	0.62875800
H	5.27215300	0.56829900	-0.68010000	H	-5.37847500	0.59915800	0.62877900
H	-4.95320400	2.26299800	-1.01514400	H	5.08016700	2.29348900	0.98532700
H	4.95318800	2.26303600	-1.01510600	H	-5.08016300	2.29346700	0.98536700
H	-0.00002400	1.36708900	-0.88469900	H	-0.00003600	1.45247700	0.95344700
H	-4.12681500	-3.36764900	1.24302500	H	4.07087100	-3.26538700	-1.53095100
H	-2.44178800	-2.96091800	1.54738900	H	2.36647200	-2.83939200	-1.64353200
H	-3.73489100	-1.95022300	2.20870600	H	3.59124600	-1.82596200	-2.42275100
H	4.12687600	-3.36761000	1.24300900	H	-4.07086100	-3.26542700	-1.53091200
H	3.73493500	-1.95019200	2.20869600	H	-3.59135600	-1.82595300	-2.42269600
H	2.44184600	-2.96091200	1.54739500	H	-2.36648700	-2.83935500	-1.64359200
O	-0.00016400	3.37331600	-0.58587800	O	-0.00008700	3.46837000	0.65926400
C	0.00000100	-0.97447200	-1.78905500	C	0.00000100	-1.01350500	1.96149100
C	-0.00001500	2.43294900	-1.41077000	C	-0.00000100	2.54831200	1.49527000

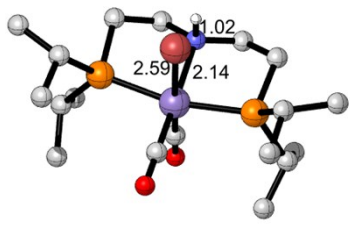
O	0.00013400	2.39022000	-2.62629600
C	-0.00000600	-2.09659800	0.45063700
Mn	-0.00000300	-0.44798900	-0.08727700
K	-0.00001100	3.18771200	1.91451400
Mn-TS(HCO₂⁻...K⁺)			
			
O	-0.00035800	-3.26583500	-0.18005700
P	2.25222600	-0.25127900	0.13015900
P	-2.25229500	-0.25098000	0.13007100
C	2.43464900	-0.24181300	1.98807700
C	-2.43473200	-0.24108900	1.98797400
H	2.50834700	0.80830000	2.29735400
H	-2.50822900	0.80908900	2.29711900
H	3.34824300	-0.72997600	2.33265400
H	-3.34844900	-0.72896300	2.33263500
C	1.17890800	-0.87346300	2.57090000
C	-1.17915300	-0.87289500	2.57100900
H	1.19480600	-0.75560100	3.67264300
H	-1.19509700	-0.75461800	3.67271000
H	1.21846900	-1.96649900	2.39702700
H	-1.21888200	-1.96598800	2.39757700
N	0.00002200	-0.26369800	1.99430400
C	-3.21007900	1.30584800	-0.34751200
C	3.21007600	1.30562600	-0.34705500
H	-2.55839100	2.09500000	0.04696900
H	2.55831600	2.09469300	0.04746600
C	-3.40167500	-1.62278900	-0.48062800
C	3.40154900	-1.62304400	-0.48074400
C	-3.44440000	-2.84650300	0.43361300
C	3.44373500	-2.84715400	0.43299900
O	0.00012300	-0.28748400	-3.06877600
H	4.40326400	-1.18023600	-0.49473300
H	-4.40330600	-1.17981300	-0.49515900
C	3.03917100	-2.04348500	-1.90567200
C	-3.03889100	-2.04383300	-1.90527800
H	2.98488100	-1.20255100	-2.59699800
H	-2.98353200	-1.20308100	-2.59674600
H	2.07355200	-2.54959500	-1.92896200
H	-2.07367500	-2.55073700	-1.92795400
H	3.79149100	-2.74189300	-2.28594400
H	-3.79158700	-2.74169500	-2.28580600
C	-3.30213600	1.49657400	-1.85956200
C	3.30239100	1.49660600	-1.85906500
H	-4.00355200	0.78541000	-2.30261700
H	4.00418000	0.78577400	-2.30205700
H	-2.33617900	1.37650000	-2.35015000
H	2.33659500	1.37624800	-2.34990200
H	-3.67444500	2.49958300	-2.08993900
H	3.67437500	2.49978800	-2.08921600
C	-4.58573300	1.44938800	0.30082400
C	4.58563700	1.44906100	0.30150800
H	-4.55395300	1.36258100	1.38877600
H	4.55366400	1.36231200	1.38945900
O	0.00010600	2.48245600	2.70231500
C	0.00000900	-2.19097300	-0.40437400
Re	0.00000500	-0.40451500	0.14056100
K	-0.00006800	3.36088000	-1.85102600
Re-TS(HCO₂⁻...K⁺)			
			
O	-0.00086700	-3.36698800	-0.18267500
P	2.35956400	-0.19658600	0.19356700
P	-2.36001900	-0.19553400	0.19332400
C	2.45583000	-0.05036300	2.05644800
C	-2.45664000	-0.05022400	2.05628600
H	2.53528300	1.02004200	2.28491200
H	-2.53628300	1.02004300	2.28535500
H	3.35115400	-0.52015800	2.46879000
H	-3.35201100	-0.52031500	2.46818700
C	1.18185900	-0.62625000	2.66291800
C	-1.18274900	-0.62635500	2.66270000
H	1.18970800	-0.43082700	3.75282700
H	-1.19065200	-0.43122200	3.75265900
H	1.20989900	-1.72756000	2.56215300
H	-1.21086900	-1.72763500	2.56161800
N	-0.00041500	-0.05650000	2.04227200
C	-3.32592800	1.33257500	-0.34663500
C	3.32631800	1.33070100	-0.34705000
H	-2.67712000	2.13595000	0.02434800
H	2.67786800	2.13461500	0.02332000
C	-3.50326700	-1.62097100	-0.26833500
C	3.50208100	-1.62291300	-0.26714300
C	-3.42620800	-2.79509100	0.70619900
C	3.42458200	-2.79630000	0.70823600
O	0.00004700	-0.41294600	-3.25860700
H	4.51646700	-1.21164600	-0.22518700
H	-4.51746500	-1.20927800	-0.22601800
C	3.22347600	-2.10135600	-1.69216700
C	-3.22486100	-2.09849700	-1.69369700
H	3.26060600	-1.29628800	-2.42597500
H	-3.26299400	-1.29310400	-2.42710000
H	2.23684300	-2.56090600	-1.75982400
H	-2.23784000	-2.55713300	-1.76196700
H	3.96623800	-2.85226900	-1.97928100
H	-3.96708800	-2.84991400	-1.98087000
C	-3.40472300	1.47155000	-1.86469400
C	3.40556500	1.46871400	-1.86517800
H	-4.11001900	0.75362200	-2.28991100
H	4.11035700	0.74997200	-2.28985800
H	-2.43430500	1.32280900	-2.33913200
H	2.43514300	1.32046700	-2.33978900
H	-3.76273700	2.47039700	-2.13204300
H	3.76444400	2.46712100	-2.13300700
C	-4.70358600	1.48934600	0.29334000
C	4.70390800	1.48713900	0.29315600
H	-4.67570100	1.42181200	1.38302700
H	4.67566800	1.42050200	1.38288800

H -5.28798200 0.69985000 -0.07251700	H -5.40433200 0.73385800 -0.07032200
H 5.28787200 0.69943000 -0.07167300	H 5.40434100 0.73097400 -0.06970500
H -5.01026100 2.42930400 0.05938800	H -5.12637600 2.46499200 0.03312400
H 5.01030700 2.42892100 0.06009900	H 5.12730100 2.46235000 0.03229900
H 0.00001500 1.37375300 -0.26769600	H 0.00033700 1.55433000 -0.36545600
H -4.12927200 -3.58779500 0.00971000	H -4.11060700 -3.58229700 0.37500200
H -2.46571300 -3.31989200 0.51962400	H -2.42477900 -3.22601300 0.73594000
H -3.80223700 -2.61271300 1.43756400	H -3.71449500 -2.52170300 1.72263700
H 4.12928300 -3.58802900 0.00946000	H 4.10825500 -3.58424900 0.37730100
H 3.80044500 -2.61372800 1.43743400	H 3.71350400 -2.52240200 1.72435700
H 2.46510500 -3.32087600 0.51778400	H 2.42284600 -3.22647100 0.73870600
O 0.00064300 3.77926600 -0.10348000	O 0.00844000 3.86463300 -0.23366100
C 0.00003000 -0.29815400 -1.90901600	C -0.00007800 -0.35541800 -2.09707400
C 0.00039500 3.10265900 -1.08021700	C 0.00386900 3.13530700 -1.17796900
O 0.00022000 2.85317400 -2.21826100	O 0.00003600 2.88022700 -2.31773100
C -0.00021100 -2.10142400 -0.13794000	C -0.00066300 -2.19836400 -0.14424700
Mn -0.00005500 -0.34801200 -0.14518300	Re -0.00023100 -0.29856200 -0.18415600
K 0.00008200 2.39758800 2.15104800	K -0.00092000 2.63043000 2.09101400
2Mn...K⁺...H₂O	2Re...K⁺...H₂O
	
O -0.00095800 -3.19103400 -0.40823600	O 0.00004400 -3.29711500 0.40916900
P -2.23608900 -0.11565100 -0.08943600	P 2.35006300 -0.06052200 0.14938900
P 2.23556400 -0.11663200 -0.08964800	P -2.35010300 -0.06047400 0.14940700
C -2.43326300 0.30250300 -1.89924200	C 2.45436900 0.45553600 1.94602200
C 2.43282300 0.30116700 -1.89951100	C -2.45437000 0.45559000 1.94603300
H -2.50998200 1.39446600 -1.97343100	H 2.53457900 1.54981400 1.95969300
H 2.50997900 1.39307900 -1.97392600	H -2.53450300 1.54987300 1.95966900
H -3.34809900 -0.10317100 -2.33581200	H 3.35130000 0.07398500 2.43872300
H 3.34744400 -0.10499300 -2.33607000	H -3.35131900 0.07409600 2.43875000
C -1.17935400 -0.18536700 -2.61165700	C 1.18203600 0.01128500 2.65925600
C 1.17857100 -0.18624900 -2.61166200	C -1.18204500 0.01131400 2.65926700
H -1.20029800 0.17144600 -3.66087400	H 1.19276000 0.42301200 3.68736700
H 1.19961600 0.17028600 -3.66097300	H -1.19276000 0.42305400 3.68737200
H -1.21931900 -1.29056600 -2.67972100	H 1.21279200 -1.08842300 2.78193500
H 1.21789500 -1.29148700 -2.67946200	H -1.21281300 -1.08839100 2.78195900
N -0.00021000 0.28401400 -1.91905000	N -0.00000400 0.44408300 1.93915300
C 3.12842600 1.34104600 0.71722800	C -3.26863800 1.36019300 -0.68854700
C -3.12790200 1.34256300 0.71766300	C 3.26869700 1.36006700 -0.68861200
H 2.48886100 2.17756500 0.41091400	H -2.62909000 2.20797600 -0.41321400
H -2.48796800 2.17869300 0.41105700	H 2.62924400 2.20792100 -0.41328300
C 3.42483800 -1.55293100 0.21650300	C -3.52871600 -1.52091500 -0.01927700
C -3.42615600 -1.55125000 0.21671300	C 3.52855800 -1.52105600 -0.01930100
C 3.44772500 -2.57535300 -0.91894600	C -3.42710000 -2.50311000 1.14649700
C -3.44940900 -2.57373500 -0.91868000	C 3.42685000 -2.50322800 1.14648300
O -0.00013900 -0.76717500 3.03788200	O 0.00001900 -0.89023500 -3.20898300
H -4.42358000 -1.10463100 0.28817900	H 4.53758400 -1.09478600 -0.01918300
H 4.42249200 -1.10683100 0.28812800	H -4.53769800 -1.09454400 -0.01911400
C -3.10601100 -2.24635200 1.54049700	C 3.29621800 -2.24810400 -1.34343000
C 3.10422800 -2.24794900 1.54022500	C -3.29652400 -2.24794400 -1.34344400
H -3.07469100 -1.55875600 2.38605700	H 3.38500300 -1.59157400 -2.20930500
H 3.07293400 -1.56035900 2.38579200	H -3.38536200 -1.59139000 -2.20929700
H -2.13830200 -2.74731400 1.49088600	H 2.29935100 -2.69035000 -1.36953800
H 2.13640000 -2.74865600 1.49044200	H -2.29968000 -2.69023500 -1.36964800

H	-3.86585800	-3.00505300	1.75380100	H	4.02871200	-3.05350500	-1.45680200
H	3.86382900	-3.00686000	1.75365900	H	-4.02906300	-3.05331000	-1.45677100
C	3.09473100	1.29219100	2.24198300	C	-3.24892100	1.26371300	-2.21107100
C	-3.09361500	1.29387600	2.24241200	C	3.24890400	1.26357400	-2.21113500
H	3.76973900	0.52618100	2.63101600	H	-3.93632900	0.49487400	-2.57127500
H	-3.76891300	0.52830500	2.63180200	H	3.93623500	0.49467400	-2.57135400
H	2.09309000	1.08259700	2.61869600	H	-2.25118000	1.02930700	-2.58408300
H	-2.09191600	1.08386400	2.61869000	H	2.25112700	1.02924900	-2.58410300
H	3.42408800	2.25043100	2.65663200	H	-3.56901700	2.21293000	-2.65256400
H	-3.42217600	2.25237600	2.65707000	H	3.56905800	2.21275900	-2.65265100
C	4.54394200	1.60640200	0.20908800	C	-4.67830300	1.62577200	-0.16590200
C	-4.54345200	1.60858600	0.20999700	C	4.67841700	1.62552600	-0.16604600
H	4.59780700	1.66350900	-0.88027900	H	-4.71608800	1.70955700	0.92264400
H	-4.59777700	1.66527300	-0.87937200	H	4.71627500	1.70934100	0.92249400
H	5.24211600	0.83243100	0.53717900	H	-5.37284300	0.83686400	-0.46471000
H	-5.24194400	0.83517900	0.53873900	H	5.37286700	0.83654300	-0.46486600
H	4.91360100	2.55648400	0.60899400	H	-5.06333200	2.56196500	-0.58327400
H	-4.91235500	2.55905700	0.60968000	H	5.06351500	2.56166800	-0.58346900
H	-0.00034700	1.26587100	0.58995800	H	-0.00002700	1.44894900	-0.67711500
H	4.15090800	-3.37625700	-0.66888200	H	-4.13117200	-3.32581800	0.98696800
H	2.46964300	-3.03451100	-1.06659200	H	-2.42909800	-2.93660200	1.21839900
H	3.77076600	-2.14544500	-1.86840300	H	-3.67347400	-2.04664200	2.10672900
H	-4.15301300	-3.37428500	-0.66866100	H	4.13075200	-3.32607100	0.98690500
H	-3.77213600	-2.14370000	-1.86818800	H	3.67338300	-2.04680100	2.10669200
H	-2.47152900	-3.03336700	-1.06620200	H	2.42876500	-2.93652900	1.21846300
H	0.00286400	2.63492800	1.23274900	H	-0.00009500	2.83124400	-1.34681800
O	0.00430000	3.62762200	1.17702200	O	-0.00004900	3.81681700	-1.25539900
C	-0.00067400	-2.03962700	-0.22769400	C	0.00002200	-2.14265800	0.22626900
C	-0.00026500	-0.60720300	1.88481100	C	0.00000100	-0.67058500	-2.06261400
H	0.01353500	3.95294100	2.07978700	H	-0.00038900	4.17582500	-2.14535100
K	0.00068500	2.93319500	-1.39269600	K	0.00036600	3.09387900	1.31349400
Mn	-0.00031200	-0.31850000	0.15304200	Re	-0.00001500	-0.27417900	-0.19760500
2Mn⁺...K⁺...H₂O-TS(H⁺ transfer, H₂ formation)				2Re⁺...K⁺...H₂O-TS(H⁺ transfer, H₂ formation)			
							
O	-0.02543100	-2.85365600	-1.46886500	O	0.12282200	-2.94610900	-1.53870400
P	-2.24852900	-0.06114600	-0.02260500	P	-2.35556600	-0.04104300	-0.09663100
P	2.24005200	-0.15412100	-0.01291200	P	2.37084600	0.01018200	-0.02391100
C	-2.36702700	1.09654600	-1.47435100	C	-2.44060100	1.07013600	-1.60125500
C	2.47961000	0.77008000	-1.62156300	C	2.44402800	1.18568500	-1.48349100
H	-2.29733000	2.09995300	-1.04040700	H	-2.56527200	2.08858400	-1.22970000
H	2.69897300	1.81816600	-1.36246300	H	2.36333700	2.18530200	-1.04261800
H	-3.31987700	1.03918500	-2.01706000	H	-3.31020500	0.84672400	-2.22440100
H	3.34545800	0.41618800	-2.19409500	H	3.38600700	1.15304300	-2.03998200
C	-1.16250600	0.83262600	-2.35975600	C	-1.14441300	0.91620600	-2.40120900
C	1.19097400	0.64768500	-2.42110900	C	1.21458200	0.90078500	-2.34785500
H	-1.16356000	1.56245100	-3.20103900	H	-1.14049500	1.67441400	-3.21660200
H	1.22881000	1.33274500	-3.29242600	H	1.21884900	1.55770500	-3.24107700
H	-1.27081300	-0.16042100	-2.84724700	H	-1.16025300	-0.06116300	-2.91473500
H	1.12594800	-0.37186100	-2.85157900	H	1.33570000	-0.12673100	-2.74042400
N	0.04992800	0.92647000	-1.57248200	N	0.02523500	1.07009200	-1.54466400
C	3.06023000	1.02498400	1.20801600	C	3.18443100	1.05019700	1.32204500
C	-3.11358800	0.95574600	1.31926100	C	-3.19321100	1.03661700	1.19145800

H	2.41735100	1.91356900	1.10419300
H	-2.41006100	1.79012100	1.42199600
C	3.43051900	-1.61204000	-0.09840600
C	-3.47813900	-1.45212900	-0.37810400
C	3.47957200	-2.26881600	-1.48250000
C	-3.50717400	-1.87615700	-1.84333900
O	-0.05693500	-1.97959100	2.59018100
H	-4.45919000	-1.04686800	-0.12358900
H	4.42584700	-1.21415700	0.11948600
C	-3.20476800	-2.66075100	0.51754500
C	3.07783500	-2.66243000	0.95374800
H	-3.12252000	-2.39860400	1.57497900
H	3.01557900	-2.24416100	1.96120700
H	-2.27814000	-3.15506800	0.22923200
H	2.11231600	-3.12103300	0.73976200
H	-4.01701900	-3.38826200	0.41373000
H	3.83669200	-3.44943100	0.96129300
C	2.93352700	0.56235800	2.65298000
C	-3.19349100	0.23238800	2.65985600
H	3.59585000	-0.28281400	2.86250500
H	-3.93005800	-0.57978900	2.63517700
H	1.91481200	0.26195100	2.89341500
H	-2.23437900	-0.18151900	2.95915600
H	3.21698000	1.37250800	3.33705000
H	-3.51823400	0.93278600	3.43760900
C	4.49444900	1.42035900	0.87610800
C	-4.47517900	1.51481300	0.90782600
H	4.62349500	1.74839900	-0.15988500
H	-4.43211200	2.10671000	-0.00535500
H	5.19013900	0.59337900	1.04208200
H	-5.22141300	0.72200100	0.76704200
H	4.81864000	2.23795400	1.52703100
H	-4.85716400	2.16739000	1.70178100
H	-0.00500800	0.80748200	1.29206600
H	4.20354700	-3.09295000	-1.46345800
H	2.51217100	-2.69488200	-1.75743900
H	3.79585100	-1.58697000	-2.26910600
H	-4.25907300	-2.66173200	-1.97986000
H	-3.75764600	-1.05666900	-2.52107100
H	-2.54324000	-2.29387500	-2.16048300
H	-0.12966400	1.70279100	1.23642500
O	-0.36823900	3.09975700	1.39714500
C	-0.01294700	-1.85104900	-0.87337900
C	-0.02920700	-1.36282600	1.60172500
Mn	-0.00233400	-0.40564200	0.12422800
H	-0.52711400	3.18517100	2.33907900
K	0.39473000	3.47655400	-0.94159700
2Mn-BH₄			
			
P	-2.28704300	0.10716700	-0.20303900
P	2.28697600	0.10728100	-0.20307600
C	-2.44799300	-0.40091000	-1.99266400
C	2.44783800	-0.40032500	-1.99282600
H	-2.47393600	0.52494500	-2.57203700
H	2.46991200	1.88407600	1.39764600
H	-2.59288300	1.95432900	1.10993700
C	3.59492200	-1.37012000	-0.38899800
C	-3.57195900	-1.41315200	-0.49386400
C	3.58609600	-1.81864500	-1.84725300
C	-3.27835500	-2.08910300	-1.82690500
O	-0.01466200	-2.23214100	2.61519500
H	-4.55346500	-0.91042400	-0.57130600
H	4.58389800	-0.94643500	-0.16916000
C	-3.62933200	-2.44668000	0.62996600
C	3.35047500	-2.56492700	0.53363200
H	-4.06553200	-2.03910600	1.55216700
H	3.39136800	-2.29382900	1.59130100
H	-2.62333900	-2.81864200	0.87429000
H	2.37115500	-3.00255400	0.34680500
H	-4.23417000	-3.29752200	0.33029400
H	4.11331700	-3.32973200	0.35157700
C	3.21408100	0.33636100	2.66813400
C	-3.02029200	0.53263200	2.62703500
H	3.98914000	-0.43216300	2.70392800
H	-3.67585700	-0.30366200	2.84945600
H	2.25571600	-0.12924100	2.90656200
H	-1.98660600	0.21995200	2.81390100
H	3.43468400	1.05793600	3.46077800
H	-3.26080300	1.33118700	3.33381000
C	4.55939800	1.60314000	0.95590700
C	-4.66401800	1.36436800	0.89110700
H	4.53717700	2.21407400	0.04325500
H	-4.86824800	1.44836800	-0.18127100
H	5.29655100	0.80924400	0.81063200
H	-5.32563300	0.59629700	1.29476200
H	4.93048800	2.23996000	1.76646200
H	-4.94915200	2.30581400	1.35157900
H	-0.05383600	0.79656900	1.60189200
H	4.36979800	-2.55797200	-2.00447800
H	2.63605500	-2.28649700	-2.11002200
H	3.76545100	-0.99774500	-2.55216500
H	-4.05106500	-2.82583800	-2.04220000
H	-3.25371900	-1.38026800	-2.65712700
H	-2.31688600	-2.61200000	-1.80521500
H	-0.06029400	1.80891500	1.20641100
O	-0.33163900	3.06178000	1.44202600
C	0.05953400	-1.93988300	-0.95710900
C	-0.01480200	-1.54625700	1.67629100
H	-0.46285800	3.05215700	2.39511400
K	-0.02833400	3.75466400	-0.88210700
Re	0.00638500	-0.38869200	0.14662400
2Re-3CO⁺			
			
P	0.72779700	0.28026600	1.89184200
P	0.72779700	0.28026600	-1.89184200
C	0.80015300	2.13832600	1.77325300
C	0.80015300	2.13832600	-1.77325300
H	1.62976400	2.38405200	1.10607500

H	2.47336600	0.52568300	-2.57197000	H	1.62976400	2.38405200	-1.10607500
H	-3.36837300	-0.94866900	-2.20032500	H	1.03325000	2.58915000	2.73985700
H	3.36837300	-0.94771600	-2.20076200	H	1.03325000	2.58915000	-2.73985700
C	-1.22624000	-1.21328300	-2.39045100	C	-0.50789400	2.70750400	1.25604500
C	1.22626400	-1.21295900	-2.39061300	C	-0.50789400	2.70750400	-1.25604500
H	-1.22067800	-1.38565400	-3.47550200	H	-0.41411800	3.78658300	1.09357600
H	1.22066700	-1.38521600	-3.47568100	H	-0.41411800	3.78658300	-1.09357600
H	-1.23180500	-2.19170900	-1.90344400	H	-1.28746100	2.56069500	2.00479400
H	1.23208300	-2.19143400	-1.90371000	H	-1.28746100	2.56069500	-2.00479400
N	-0.00005200	-0.51106100	-1.97556400	N	-0.99960600	2.06456100	0.00000000
C	3.21189500	1.74241900	-0.16989800	C	2.54923600	-0.18150900	-1.88803400
C	-3.21202600	1.74227400	-0.17050300	C	2.54923600	-0.18150900	1.88803400
H	2.56072500	2.36658700	-0.78817700	H	2.87078800	0.13863300	-0.89424000
H	-2.56120800	2.36595400	-0.78965600	H	2.87078800	0.13863300	0.89424000
C	3.41279300	-1.06119100	0.75682000	C	0.19273300	-0.12227400	-3.65229500
C	-3.41279100	-1.06108700	0.75718800	C	0.19273300	-0.12227400	3.65229500
C	3.41305600	-2.49671200	0.23352900	C	-0.82673400	0.84901900	-4.24368300
C	-3.41286500	-2.49680300	0.23443600	C	-0.82673400	0.84901900	4.24368300
H	-4.42010600	-0.65447600	0.61857800	H	1.11805900	-0.01399700	4.22588600
H	4.42006800	-0.65439300	0.61843800	H	1.11805900	-0.01399700	-4.22588600
C	-3.08598900	-1.04043500	2.25132700	C	-0.28093600	-1.57053800	3.78566100
C	3.08590100	-1.04120200	2.25095200	C	-0.28093600	-1.57053800	-3.78566100
H	-3.05603800	-0.03247900	2.66475400	H	0.42138700	-2.28974100	3.36501100
H	3.05561800	-0.03342200	2.66477400	H	0.42138700	-2.28974100	-3.36501100
H	-2.12107900	-1.50870100	2.44918200	H	-1.24667100	-1.72750800	3.30632300
H	2.12113500	-1.50985700	2.44857900	H	-1.24667100	-1.72750800	-3.30632300
H	-3.84588000	-1.60364900	2.80165700	H	-0.40195300	-1.81148600	4.84480000
H	3.84594600	-1.60439600	2.80109100	H	-0.40195300	-1.81148600	-4.84480000
C	3.27198700	2.36610000	1.22222500	C	3.39056200	0.58039100	-2.91167400
C	-3.27122500	2.36709300	1.22113800	C	3.39056200	0.58039100	2.91167400
H	3.96213100	1.83024500	1.87898300	H	3.29205000	1.66374000	-2.82668500
H	-3.96083800	1.83170600	1.87883600	H	3.29205000	1.66374000	2.82668500
H	2.29396600	2.40083200	1.70263900	H	3.15139500	0.29505000	-3.93794800
H	-2.29285500	2.40229900	1.70080200	H	3.15139500	0.29505000	3.93794800
H	3.63613700	3.39442000	1.14300100	H	4.44524700	0.33848500	-2.75612200
H	-3.63553200	3.39531300	1.14134300	H	4.44524700	0.33848500	2.75612200
C	4.59777400	1.69729600	-0.80970600	H	-1.02550500	0.56252200	-5.27954900
C	-4.59828600	1.69667000	-0.80945300	H	-1.02550500	0.56252200	5.27954900
H	4.58149800	1.30436000	-1.82802600	H	-1.78335300	0.81966200	-3.72111900
H	-4.58273600	1.30235700	-1.82725600	H	-1.78335300	0.81966200	3.72111900
H	5.30337500	1.09959800	-0.22604000	H	-0.46763900	1.87945600	-4.26505200
H	-5.30370100	1.09995700	-0.22456200	H	-0.46763900	1.87945600	4.26505200
H	5.00597900	2.71118100	-0.86108000	Re	-0.86069100	-0.21377400	0.00000000
H	-5.00624100	2.71059900	-0.86194300	C	-2.29334300	-0.39128700	1.29913000
H	0.00013300	1.75249800	-0.40475400	O	-3.21281000	-0.50892300	1.97601600
H	-0.00023200	0.41642800	-2.40867100	C	-2.29334300	-0.39128700	-1.29913000
H	4.11116100	-3.09561100	0.82625000	O	-3.21281000	-0.50892300	-1.97601600
H	2.43101900	-2.96237900	0.32710900	H	-2.00153000	2.22660800	0.00000000
H	3.73370200	-2.56741800	-0.80729300	C	2.77744100	-1.68774600	1.99788200
H	-4.11103500	-3.09552100	0.82726300	H	2.15303000	-2.26095700	1.31129400
H	-3.73335000	-2.56790600	-0.80641000	H	3.82128000	-1.91674600	1.77001200
H	-2.43082100	-2.96238000	0.32832700	H	2.58790400	-2.04628000	3.01112900
Mn	-0.00003600	0.08667200	0.06261900	C	2.77744100	-1.68774600	-1.99788200
C	0.00000100	0.74262800	1.70526700	H	2.58790400	-2.04628000	-3.01112900
C	0.00003400	-1.55315800	0.67503200	H	3.82128000	-1.91674600	-1.77001200
O	0.00005500	1.16810700	2.77978300	H	2.15303000	-2.26095700	-1.31129400
O	0.00009200	-2.63493800	1.10064700	C	-0.55931300	-2.11593900	0.00000000
H	-0.00064300	3.56831800	-1.06410800	O	-0.36650100	-3.24753700	0.00000000
H	1.00003200	2.18550300	-2.14374400				
H	-0.99962400	2.18466300	-2.14412000				

B	-0.00001300	2.43991600	-1.50228000	
2Mn-Br				
				
N	0.31783500	-2.00153800	0.00000000	
H	-0.68976700	-2.18504000	0.00000000	
P	0.11260200	-0.13854400	2.30446700	
P	0.11260200	-0.13854400	-2.30446700	
C	-1.43946600	0.24274000	-3.29466400	
C	-1.43946600	0.24274000	3.29466400	
C	1.50596400	0.49306000	-3.40744600	
C	1.50596400	0.49306000	3.40744600	
O	3.02455400	0.58820600	0.00000000	
C	0.17951400	-1.99995900	2.44042700	
C	0.17951400	-1.99995900	-2.44042700	
H	-0.86080000	-2.33902000	2.44497300	
H	-0.86080000	-2.33902000	-2.44497300	
H	0.64207000	-2.34527800	3.36646400	
H	0.64207000	-2.34527800	-3.36646400	
C	0.89425800	-2.57036700	1.22705800	
C	0.89425800	-2.57036700	-1.22705800	
H	0.81573900	-3.66640500	1.21768900	
H	0.81573900	-3.66640500	-1.21768900	
H	1.95751400	-2.31876000	1.24580600	
H	1.95751400	-2.31876000	-1.24580600	
H	-2.20097700	-0.25079300	-2.68351300	
H	-2.20097700	-0.25079300	2.68351300	
O	-0.35451700	3.01167800	0.00000000	
H	1.10811700	0.42396900	4.42495000	
H	1.10811700	0.42396900	-4.42495000	
C	1.81842100	1.96091600	3.11197700	
C	1.81842100	1.96091600	-3.11197700	
H	0.93116200	2.59392700	3.13308200	
H	0.93116200	2.59392700	-3.13308200	
H	2.28393500	2.07507100	2.13256500	
H	2.28393500	2.07507100	-2.13256500	
H	2.51955600	2.34566600	3.85893300	
H	2.51955600	2.34566600	-3.85893300	
C	-1.77703100	1.73047600	-3.32281300	
C	-1.77703100	1.73047600	3.32281300	
H	-1.08487200	2.29523000	-3.95256000	
H	-1.08487200	2.29523000	3.95256000	
H	-1.77525100	2.16634400	-2.32368300	
H	-1.77525100	2.16634400	2.32368300	
H	-2.77853400	1.86833200	-3.74057600	
H	-2.77853400	1.86833200	3.74057600	
C	-1.46371100	-0.35910400	-4.69748000	
C	-1.46371100	-0.35910400	4.69748000	
H	-1.25539700	-1.43098000	-4.70360500	
H	-1.25539700	-1.43098000	4.70360500	
H	-0.75297700	0.12806700	-5.37053900	
H	-0.75297700	0.12806700	5.37053900	
H	-2.45821800	-0.22051500	-5.13247900	
H	-2.45821800	-0.22051500	5.13247900	
C	2.78037300	-0.34774700	3.35030200	

H	2.61296200	-1.38619400	3.64236300
H	3.23283500	-0.33346100	2.35801500
H	3.51637000	0.06677200	4.04600100
C	2.78037300	-0.34774700	-3.35030200
H	3.23283500	-0.33346100	-2.35801500
H	2.61296200	-1.38619400	-3.64236300
H	3.51637000	0.06677200	-4.04600100
C	1.87604500	0.39762600	0.00000000
Mn	0.15548200	0.13049600	0.00000000
C	-0.15947400	1.87374700	0.00000000
Br	-2.38132100	-0.41376300	0.00000000

Table S15. Computed energetic data for all optimized structures

H₂ HF= -1.178636 ZPE= 0.010066 NImag= 0 Htot = -1.165265 Gtot = -1.180063	CH₃OH HF= -115.724973 ZPE= 0.051237 NImag= 0 Htot = -115.669468 Gtot = -115.696474
CH₂O HF= -114.500219 ZPE= 0.026657 NImag= 0 Htot = -114.469751 Gtot = -114.494561	H₂O HF= -76.430962 ZPE= 0.021369 NImag= 0 Htot = -76.405814 Gtot = -76.427232
HOCH₂OH HF= -190.954651 ZPE= 0.057504 NImag= 0 Htot = -190.892446 Gtot = -190.921351	HCOOH HF= -189.762022 ZPE= 0.033913 NImag= 0 Htot = -189.724004 Gtot = -189.75218
CO₂ HF= -188.580271 ZPE= 0.010286 NImag= 0 Htot = -188.566078 Gtot = -188.585337	OH⁻ HF= -75.784209 ZPE= 0.008406 NImag= 0 Htot = -75.764645 Gtot = -75.784209
CH₃O⁻ HF= -115.096466 ZPE= 0.034522 NImag= 0 Htot = -115.058095 Gtot = -115.083134	HOCH₂O⁻ HF= -190.351260 ZPE= -115.096466 NImag= 0 Htot = -190.305191 Gtot = -190.334819
HCOO⁻ HF= -189.198628 ZPE= 0.020097 NImag= 0 Htot = -189.174616 Gtot = -189.20167	K⁺ HF= -27.993433 ZPE= 0 NImag= 0 Htot = -27.991072 Gtot = -28.008609
1Mn(Cs) HF= 0.518281 ZPE= -1699.449469 NImag= 0 Htot = -1698.898247 Gtot = -1698.992970	1Re(Cs) HF= -1674.719010 ZPE= 0.518184 NImag= 0 Htot = -1674.167696 Gtot = -1674.264563
1Mn(C₁) HF= -1699.453006 ZPE= 0.518844 NImag= 0 Htot = -1698.901598 Gtot = -1698.994510	1Re(C₁) HF= -1674.723619 ZPE= 0.518168 NImag= 0 Htot = -1674.172510 Gtot = -1674.267165
2Mn(Cs)	2Re(Cs)

HF= -1700.652679 ZPE= 0.539668 NImag= 0 Htot = -1700.080142 Gtot = -1700.174062	HF= -1675.924273 ZPE= 0.538741 NImag= 0 Htot = -1675.448456 Gtot = -1675.448456
2Mn(C₁) HF= -1700.650496 ZPE= 0.540100 NImag= 0 Htot = -1700.077653 Gtot = -1700.171298	2Re(C₁) HF= -1675.921281 ZPE= 0.539520 NImag= 0 Htot = -1675.348643 Gtot = -1675.443802
1Mn-3CO HF= -1812.778476 ZPE= 0.527164 NImag= 0 Htot = -1812.216615 Gtot = -1812.314029	1Re-3CO HF= -1788.052511 ZPE= 0.526034 NImag= 0 Htot = -1787.49127 Gtot = -1787.590771
2Mn' HF= -1700.654227 ZPE= 0.539948 NImag= 0 Htot = -1700.081533 Gtot = -1700.175134	2Re' HF= -1675.925808 ZPE= 0.539121 NImag= 0 Htot = -1675.353532 Gtot = -1675.448561
2Mn-CO_{dis}-singlet HF= -1587.26375 ZPE= 0.528826 NImag= 0 Htot = -1586.703686 Gtot = -1586.793735	2Re-CO_{dis}-singlet HF= -1562.500509 ZPE= 0.529154 NImag= 0 Htot = -1561.940193 Gtot = -1562.030863
2Mn-CO_{dis}-triplet HF= -1587.272508 ZPE= 0.527835 NImag= 0 Htot = -1586.713001 Gtot = -1586.805486	2Re-CO_{dis}-triplet HF= -1562.472985 ZPE= 0.528109 NImag= 0 Htot = -1561.913082 Gtot = -1562.006229
2Mn-P_{dis}-singlet HF= -1700.599724 ZPE= 0.537802 NImag= 0 Htot = -1700.028135 Gtot = -1700.12678	2Re-P_{dis}-singlet HF= -1675.854295 ZPE= 0.537194 NImag= 0 Htot = -1675.282972 Gtot = -1675.383206
2Mn-P_{dis}-triplet HF= -1700.595402 ZPE= 0.535539 NImag= 0 Htot = -1700.025117 Gtot = -1700.127646	2Re-P_{dis}-triplet HF= -1675.817445 ZPE= 0.536266 NImag= 0 Htot = -1675.246586 Gtot = -1675.349045
1Mn+H₂(ads) HF= -1700.628105 ZPE= 0.534416 NImag= 0	1Re+H₂(ads) HF= -1675.897646 ZPE= 0.533991 NImag= 0

Htot = -1700.047533 Gtot = -1700.143182	Htot = -1675.319309 Gtot = -1675.41499
1Mn + H₂-TS(1M/2M) HF= -1700.613055 ZPE= 0.533793 NImag= -751.0487 Htot = -1700.046492 Gtot = -1700.139993	1Re+ H₂-TS(1M/2M) HF= -1675.878551 ZPE= 0.532873 NImag= -821.7513 Htot = -1675.312585 Gtot = -1675.407352
1Mn + H₂-TS(H₂O-H⁺) HF= -1777.062118 ZPE= 0.557329 NImag= -641.6928 Htot = -1776.469595 Gtot = -1776.567705	1Re + H₂-TS(H₂O-H⁺) HF= -1752.330942 ZPE= 0.555954 NImag= -859.2803 Htot = -1751.739455 Gtot = -1751.838944
1Mn + H₂-TS(CH₃OH-H⁺) HF= -1816.355819 ZPE= 0.584646 NImag= -679.9802 Htot = -1815.733945 Gtot = -1815.838862	1Re + H₂-TS(CH₃OH-H⁺) HF= -1791.624615 ZPE= 0.583592 NImag= -852.8398 Htot = -1791.003539 Gtot = -1791.108899
1Mn + H₂-TS(H₂O-H-H) HF= -1777.07145 ZPE= 0.560470 NImag= -611.5679 Htot = -1776.47571 Gtot = -1776.575059	1Re + H₂-TS(H₂O-H-H) HF= -1752.342904 ZPE= 0.558447 NImag= -1026.9988 Htot = -1751.749043 Gtot = -1751.848607
1Mn + H₂-TS(CH₃OH-H-H) HF= -1816.365651 ZPE= 0.587807 NImag= -824.9123 Htot = -1815.74091 Gtot = -1815.844116	1Re + H₂-TS(CH₃OH-H-H) HF= -1791.637069 ZPE= 0.586591 NImag= -963.4037 Htot = -1791.013452 Gtot = -1791.117123
Mn-TS1-H⁺ HF= -1815.167887 ZPE= 0.567588 NImag= -568.0086 Htot = -1814.564776 Gtot = -1814.663944	Re-TS1-H⁺ HF= -1790.436017 ZPE= 0.566525 NImag= -655.1028 Htot = -1789.83354 Gtot = -1789.935242
3Mn⁺-OCH₃⁻ HF= -1815.168153 ZPE= 0.569943 NImag= 0 Htot = -1814.562382 Gtot = -1814.662382	3Re⁺-OCH₃⁻ HF= -1790.436604 ZPE= 0.56911 NImag= 0 Htot = -1789.831292 Gtot = -1789.933731
Mn-TS1-H⁻ HF= -1815.159609 ZPE= 0.568379 NImag= -308.9818 Htot = -1814.555698 Gtot = -1814.65637	Re-TS1-H⁻ HF= -1790.43171 ZPE= 0.568067 NImag= -94.0183 Htot = -1789.827562 Gtot = -1789.92963
Mn-TS(CH₃OH)	Re-TS(CH₃OH)

HF= -1815.176411 ZPE= 0.569731 NImag= -69.8875 Htot = -1814.570915 Gtot = -1814.670483	HF= -1790.448978 ZPE= 0.569728 NImag= -72.4543 Htot = -1789.843328 Gtot = -1789.943867
2Mn-OCH₃ HF= -1815.197298 ZPE= 0.574322 NImag= 0 Htot = -1814.587064 Gtot = -1814.685938	2Re-OCH₃ HF= -1790.47004 ZPE= 0.574042 NImag= 0 Htot = -1789.859829 Gtot = -1789.959967
Mn-TS(H₂O) HF= -1775.888788 ZPE= 0.541074 NImag= -281.2206 Htot = -1775.313754 Gtot = -1775.409206	Re-TS(H₂O) HF= -1751.159322 ZPE= 0.540443 NImag= -711.3249 Htot = -1750.584638 Gtot = -1750.681149
2Mn-OH HF= -1775.907453 ZPE= 0.546161 NImag= 0 Htot = -1775.326707 Gtot = -1775.423548	2Re-OH HF= -1751.179324 ZPE= 0.545708 NImag= 0 Htot = -1750.598766 Gtot = -1750.696522
Mn-TS2-OH⁻ HF= -1890.412379 ZPE= 0.576605 NImag= -82.6811 Htot = -1889.798689 Gtot = -1889.900777	Re-TS2-OH⁻ HF= -1865.685247 ZPE= 0.576362 NImag= -62.3301 Htot = -1865.071694 Gtot = -1865.174796
3Mn⁺-O(H)CH₂O⁻ HF= -1890.413384 ZPE= 0.578031 NImag= 0 Htot = -1889.798315 Gtot = -1889.899819	3Re⁺-O(H)CH₂O⁻ HF= -1865.68561 ZPE= 0.577505 NImag= 0 Htot = -1865.070771 Gtot = -1865.173679
Mn-TS2-H⁺ HF= -1890.4064 ZPE= 0.575542 NImag= -194.1831 Htot = -1889.794794 Gtot = -1889.893853	Re-TS2-H⁺ HF= -1865.679154 ZPE= 0.575159 NImag= -209.9061 Htot = -1865.067704 Gtot = -1865.168234
2Mn-OCH₂OH HF= -1890.426087 ZPE= 0.579186 NImag= 0 Htot = -1889.809763 Gtot = -1889.911983	2Re-OCH₂OH HF= -1865.701763 ZPE= 0.579555 NImag= 0 Htot = -1865.084994 Gtot = -1865.188091
Mn-TS(HOCH₂OH) HF= -1890.405009 ZPE= 0.574239 NImag= -379.9445 Htot = -1889.793946	Re-TS(HOCH₂OH) HF= -1865.676735 ZPE= 0.573653 NImag= -853.5117 Htot = -1865.06588

Gtot = -1889.896722	Gtot = -1865.17025
Mn-TS3-H⁺ HF= -1890.403043 ZPE= 0.573149 NImag= -710.7507 Htot = -1889.793143 Gtot = -1889.894829	Re-TS3-H⁺ HF= -1865.666384 ZPE= 0.572181 NImag= -621.9052 Htot = -1865.057296 Gtot = -1865.160234
3Mn⁺-HCH(OH)O⁻ HF= -1890.402148 ZPE= 0.576154 NImag= 0 Htot = -1889.7893 Gtot = -1889.890491	3Re⁺-HCH(OH)O⁻ HF= -1865.672603 ZPE= 0.574583 NImag= 0 Htot = -1865.060691 Gtot = -1865.164743
Mn-TS3-H⁻ HF= -1890.40125 ZPE= 0.574868 NImag= -343.503 Htot = -1889.790023 Gtot = -1889.890987	Re-TS3-H⁻ HF= -1865.672769 ZPE= 0.57432 NImag= -106.6481 Htot = -1865.061773 Gtot = -1865.164898
Mn-TS4-H⁺ HF= -1889.221377 ZPE= 0.548958 NImag= -846.9354 Htot = -1888.636222 Gtot = -1888.737037	Re-TS4-H⁺ HF= -1864.488008 ZPE= 0.548023 NImag= -842.9237 Htot = -1863.903488 Gtot = -1864.005911
3Mn⁺-OOCH⁻ HF= -1889.235653 ZPE= 0.553974 NImag= 0 Htot = -1888.645064 Gtot = -1888.747353	3Re⁺-OOCH⁻ HF= -1864.502516 ZPE= 0.552814 NImag= 0 Htot = -1863.912723 Gtot = -1864.016806
Mn-TS4-H⁻ HF= -1889.227925 ZPE= 0.551696 NImag= -277.3506 Htot = -1888.639962 Gtot = -1888.741557	Re-TS4-H⁻ HF= -1864.499536 ZPE= 0.550964 NImag= -248.4703 Htot = -1863.911881 Gtot = -1864.015539
Mn-TS(HCOOH) HF= -1889.236287 ZPE= 0.550201 NImag= -1087.9661 Htot = -1888.649979 Gtot = -1888.75049	Re-TS(HCOOH) HF= -1864.512863 ZPE= 0.550607 NImag= -1276.3361 Htot = -1863.926106 Gtot = -1864.027642
2Mn-OOCH HF= -1889.264425 ZPE= 0.557677 NImag= 0 Htot = -1888.670734 Gtot = -1888.771243	2Re-OOCH HF= -1864.535657 ZPE= 0.556547 NImag= 0 Htot = -1863.942595 Gtot = -1864.045278
1Mn-TS(HOCH₂OH-H-H) HF= -1891.597243	1Re-TS(HOCH₂OH-H-H) HF= -1866.864234

ZPE= 0.593571 NImag= -816.6901 Htot = -1890.966016 Gtot = -1891.070576	ZPE= 0.592679 NImag= -1007.935 Htot = -1866.233805 Gtot = -1866.338895
1Mn-TS(HCOOH-H-H) HF= -1890.425967 ZPE= 0.571528 NImag= -573.181 Htot = -1889.817431 Gtot = -1889.920605	1Re-TS(HCOOH-H-H) HF= -1865.695816 ZPE= 0.570864 NImag= -515.6367 Htot = -1865.087665 Gtot = -1865.191908
1Mn-OCH₃⁻ HF= -1814.603205 ZPE= 0.555931 NImag= 0 Htot = -1814.011282 Gtot = -1814.111487	1Re-OCH₃⁻ HF= -1789.886676 ZPE= 0.555858 NImag= 0 Htot = -1789.294483 Gtot = -1789.396188
1Mn-HCH₂O⁻ HF= -1814.579527 ZPE= 0.553585 NImag= 0 Htot = -1813.989818 Gtot = -1814.090231	1Re-HCH₂O⁻ HF= -1789.85708 ZPE= 0.552597 NImag= 0 Htot = -1789.268006 Gtot = -1789.370128
1Mn-TS(HCH₂O) HF= -1814.573527 ZPE= 0.551317 NImag= -191.6029 Htot = -1813.986589 Gtot = -1814.086426	1Re-TS(HCH₂O) HF= -1789.855204 ZPE= 0.55097 NImag= -173.0548 Htot = -1789.268205 Gtot = -1789.36962
2Mn⁻ HF= -1700.064090 ZPE= 0.522158 NImag= 0 Htot = -1699.509112 Gtot = -1699.603267	2Re⁻ HF= -1675.345438 ZPE= 0.521477 NImag= 0 Htot = -1674.790685 Gtot = -1674.886406
1Mn-OCH₂OH⁻ HF= -1889.852144 ZPE= 0.563094 NImag= 0 Htot = -1889.2529 Gtot = -1889.352648	1Re-OCH₂OH⁻ HF= -1865.135131 ZPE= 0.563105 NImag= 0 Htot = -1864.535549 Gtot = -1864.63692
1Mn-HCH(OH)O⁻ HF= -1889.826031 ZPE= 0.559848 NImag= 0 Htot = -1889.229058 Gtot = -1889.331731	1Re-HCH(OH)O⁻ HF= -1865.10393 ZPE= 0.55823 NImag= 0 Htot = -1864.508273 Gtot = -1864.612318
Mn-TS(HCH(OH)O) HF= -1889.822954 ZPE= 0.55764 NImag= -533.4439 Htot = -1889.228957 Gtot = -1889.329503	Re-TS(HCH(OH)O) HF= -1865.103834 ZPE= 0.557089 NImag= -221.4282 Htot = -1864.50983 Gtot = -1864.612596

1Mn-OOCH⁻ HF= -1888.675114 ZPE= 0.539478 NImag= 0 Htot = -1888.098964 Gtot = -1888.202703	1Re-OOCH⁻ HF= -1863.940704 ZPE= 0.538211 NImag= 0 Htot = -1863.365406 Gtot = -1863.469796
1Mn-HCOO⁻ HF= -1888.666188 ZPE= 0.539184 NImag= 0 Htot = -1888.089806 Gtot = -1888.194815	1Re-HCOO⁻ HF= -1863.940704 ZPE= 0.538211 NImag= 0 Htot = -1863.365406 Gtot = -1863.469796
Mn-TS(HCO₂) HF= -1888.640779 ZPE= 0.534516 NImag= -401.8939 Htot = -1888.07014 Gtot = -1888.170835	Re-TS(HCO₂) HF= -1863.92489 ZPE= 0.534223 NImag= -308.4699 Htot = -1863.354074 Gtot = -1863.457501
2Mn⁻...H₂O HF= -1776.525063 ZPE= 0.547917 NImag= 0 Htot = -1775.941857 Gtot = -1776.040767	2Re⁻...H₂O HF= -1751.805464 ZPE= 0.547534 NImag= 0 Htot = -1751.222158 Gtot = -1751.323506
Mn-TS(H⁺ transfer, H₂ formation) HF= -1776.470123 ZPE= 0.543113 NImag= -923.0486 Htot = -1775.892289 Gtot = -1775.989477	Re-TS(H⁺ transfer, H₂ formation) HF= -1751.754579 ZPE= 0.541798 NImag= -1230.9719 Htot = -1751.177511 Gtot = -1751.276806
1Mn-OCH₃⁻...K⁺ HF= -1842.771521 ZPE= 0.559196 NImag= 0 Htot = -1842.17455 Gtot = -1842.277593	1Re-OCH₃⁻...K⁺ HF= -1818.052685 ZPE= 0.55905 NImag= 0 Htot = -1817.455579 Gtot = -1817.560245
1Mn-HCH₂O⁻...K⁺ HF= -1842.74821 ZPE= 0.556685 NImag= 0 Htot = -1842.153378 Gtot = -1842.258777	1Re-HCH₂O⁻...K⁺ HF= -1818.021442 ZPE= 0.555515 NImag= 0 Htot = -1817.42746 Gtot = -1817.534745
Mn-TS(HCH₂O⁻...K⁺) HF= -1842.73593 ZPE= 0.554045 NImag= -106.6981 Htot = -1842.145014 Gtot = -1842.246000	Re-TS(HCH₂O⁻...K⁺) HF= -1818.015343 ZPE= 0.553457 NImag= -126.9604 Htot = -1817.424599 Gtot = -1817.527760
2Mn⁻...K⁺ HF= -1728.219485 ZPE= 0.524233	2Re⁻...K⁺ HF= -1703.499134 ZPE= 0.523923

NImag= 0 Htot = -1727.66035 Gtot = -1727.760158	NImag= 0 Htot = -1702.940021 Gtot = -1703.040148
1Mn-OCH₂OH⁻...K⁺ HF= -1918.012225 ZPE= 0.564135 NImag= 0 Htot = -1917.409182 Gtot = -1917.515161	1Re-OCH₂OH⁻...K⁺ HF= -1893.292063 ZPE= 0.563879 NImag= 0 Htot = -1892.688966 Gtot = -1892.796554
1Mn-HCH(OH)O⁻...K⁺ HF= -1917.985244 ZPE= 0.561816 NImag= 0 Htot = -1917.38404 Gtot = -1917.492652	1Re-HCH(OH)O⁻...K⁺ HF= -1893.263431 ZPE= 0.561057 NImag= 0 Htot = -1892.662867 Gtot = -1892.772203
Mn-TS(HCH(OH)O⁻...K⁺) HF= -1917.980934 ZPE= 0.559565 NImag= -447.0465 Htot = -1917.382962 Gtot = -1917.488432	Re-TS(HCH(OH)O⁻...K⁺) HF= -1893.261033 ZPE= 0.559419 NImag= -170.3918 Htot = -1892.662938 Gtot = -1892.769537
1Mn-OOCH⁻...K⁺ HF= -1916.84528 ZPE= 0.541668 NImag= 0 Htot = -1916.265083 Gtot = -1916.371499	1Re-OOCH⁻...K⁺ HF= -1892.122009 ZPE= 0.540985 NImag= 0 Htot = -1891.542012 Gtot = -1891.651464
1Mn-HCOO⁻...K⁺ HF= -1916.817572 ZPE= 0.539182 NImag= 0 Htot = -1916.239332 Gtot = -1916.348229	1Re-HCOO⁻...K⁺ HF= -1892.088483 ZPE= 0.538299 NImag= 0 Htot = -1891.510979 Gtot = -1891.621063
Mn-TS(HCO₂⁻...K⁺) HF= -1916.799484 ZPE= 0.536362 NImag= -322.9417 Htot = -1916.22514 Gtot = -1916.329937	Re-TS(HCO₂⁻...K⁺) HF= -1892.079318 ZPE= 0.535577 NImag= -304.9531 Htot = -1891.505174 Gtot = -1891.6127
2Mn⁻...K⁺...H₂O HF= -1804.67299 ZPE= 0.548461 NImag= 0 Htot = -1804.08659 Gtot = -1804.191955	2Re⁻...K⁺...H₂O HF= -1779.953256 ZPE= 0.548106 NImag= 0 Htot = -1779.366765 Gtot = -1779.474167
2Mn⁻...K⁺...H₂O-TS(H⁺ transfer, H₂ formation) HF= -1804.648425 ZPE= 0.545059 NImag= -668.3 Htot = -1804.066463 Gtot = -1804.168785	2Re⁻...K⁺...H₂O-TS(H⁺ transfer, H₂ formation) HF= -1779.921449 ZPE= 0.543421 NImag= -1112.0452 Htot = -1779.340583 Gtot = -1779.445048
2Mn-BH₄	2Re-3CO⁺

HF= -1727.310549 ZPE= 0.572316 NImag= 0 Htot = -1726.702882 Gtot = -1726.800515	HF= -1788.48510474 ZPE= 0.543065 NImag= 0 Htot = -1787.907978 Gtot = -1788.003458
2Mn-Br HF= -4274.295901 ZPE= 0.534176 NImag= 0 Htot = -4273.727050 Gtot = -4273.825080	

Table S16. Coordinates of optimized structures in methanol

H₂-SMD(CH₃OH) H 0.00000000 0.00000000 0.37303400 H 0.00000000 0.00000000 -0.37303400	CH₃OH-SMD(CH₃OH) C 0.04771500 0.66542400 0.00000000 H 1.08923900 0.99109200 0.00000000 H -0.44405500 1.07197100 0.89085700 H -0.44405500 1.07197100 -0.89085700 O 0.04771500 -0.75892000 0.00000000 H -0.86914100 -1.05621900 0.00000000
CH₂O-SMD(CH₃OH) C 0.00000000 0.00000000 -0.53159600 H 0.00000000 0.93944800 -1.11152200 H 0.00000000 -0.93944800 -1.11152200 O 0.00000000 0.00000000 0.67657700	H₂O-SMD(CH₃OH) H 0.00000000 0.76099600 -0.47311800 O 0.00000000 0.00000000 0.11828000 H 0.00000000 -0.76099600 -0.47311800
HOCH₂OH-SMD(CH₃OH) C 0.00000000 0.00000000 0.52606300 H 0.89501600 0.05867300 1.15024300 H -0.89501600 -0.05867300 1.15024300 O 0.00000000 -1.17369900 -0.25299400 H 0.85120700 -1.24065200 -0.70448400 O 0.00000000 1.17369900 -0.25299400 H -0.85120700 1.24065200 -0.70448400	HCOOH-SMD(CH₃OH) C 0.00000000 0.41887400 0.00000000 H -0.34687900 1.45881800 0.00000000 O 1.16203800 0.08952400 0.00000000 O -1.03022900 -0.41884400 0.00000000 H -0.70759000 -1.33750500 0.00000000
CO₂-SMD(CH₃OH) C 0.00000000 0.00000000 -0.00002700 O 0.00000000 0.00000000 -1.15843300 O 0.00000000 0.00000000 1.15845400	OH-SMD(CH₃OH) H 0.00000000 0.00000000 -0.85559700 O 0.00000000 0.00000000 0.10695000
CH₃O⁻-SMD(CH₃OH) O 0.00000000 0.00000000 0.81302900 C 0.00000000 0.00000000 -0.57073000 H 0.00000000 1.01748900 -1.02661600 H 0.88117100 -0.50874400 -1.02661600 H -0.88117100 -0.50874400 -1.02661600	HOCH₂O-SMD(CH₃OH) C -0.15010500 0.48266800 0.04844400 H -0.09632300 1.24610800 -0.75805200 H -0.09195200 1.02677600 1.01945500 O 1.16885200 -0.17975400 -0.10244100 H 1.18548000 -0.87722600 0.56546600 O -1.18092400 -0.35670400 -0.03725000
HCOO⁻-SMD(CH₃OH) C 0.00000000 0.00000000 0.33833700 H 0.00000000 0.00000000 1.45411800 O 0.00000000 1.12419800 -0.21775900 O 0.00000000 -1.12419800 -0.21775900	K⁺-SMD(CH₃OH) K 0.00000000 0.00000000 0.00000000
1Mn(C1)-SMD(CH₃OH) C -2.46197300 -0.61929400 1.92722200 H -2.63308000 0.28104100 2.52160000 H -3.31985400 -1.28077400 2.06799700 C -1.15937600 -1.27310700 2.35094200 H -1.05248100 -1.18545300 3.44175300 H -1.19157100 -2.35229400 2.13898700 C 1.19826900 -1.05529200 2.44513800 H 1.38690100 -2.13336400 2.33078700 H 1.02026900 -0.89766300 3.51881500 C 2.42276900 -0.26258600 2.02464800 H 3.35348500 -0.77957400 2.26926300 H 2.43350500 0.70091500 2.53917900 C -3.29798200 1.49024800 0.03376600	1Re(C1)-SMD(CH₃OH) C -2.48294600 -0.64847600 1.98866800 H -2.63887900 0.25686500 2.57988200 H -3.33580900 -1.30870200 2.16333600 C -1.17570900 -1.30695300 2.39960800 H -1.06871500 -1.22108700 3.49019600 H -1.21534200 -2.38492100 2.18543100 C 1.19823100 -1.14719200 2.47346700 H 1.35504900 -2.22581100 2.32600800 H 1.03702100 -1.01356400 3.55267400 C 2.44913300 -0.38161100 2.07267900 H 3.35621100 -0.93566700 2.32500300 H 2.48586400 0.56798800 2.61140300 C -3.43093300 1.44257600 0.12251400

H -3.13837700	1.81199200	-1.00095500	H -3.32370100	1.75482000	-0.92180700
C -4.79453800	1.29760500	0.26374400	C -4.91054900	1.22336500	0.42583200
H -5.00058500	0.90368500	1.26349400	H -5.06098800	0.84206100	1.44016600
H -5.25218500	0.62832700	-0.46682600	H -5.38685000	0.53230600	-0.27182700
H -5.30399500	2.26374700	0.18373000	H -5.44319500	2.17735600	0.35421200
C -2.75079100	2.57869700	0.95644600	C -2.85543900	2.54750700	1.00596500
H -3.20075900	3.54184500	0.69678100	H -3.34995600	3.49600300	0.77521300
H -1.66672000	2.68516600	0.88445300	H -1.78259100	2.68367400	0.85675000
H -2.99748500	2.37654200	2.00240400	H -3.02474200	2.34294800	2.06676500
C -3.26333600	-1.33562900	-0.81378400	C -3.36769400	-1.38688800	-0.73779500
H -4.25951100	-1.33973700	-0.35948200	H -4.34843800	-1.42574100	-0.25279000
C -3.39538600	-0.93147900	-2.27913300	C -3.55068600	-0.97051400	-2.19397800
H -2.42190600	-0.87767500	-2.77179000	H -2.59005300	-0.87353700	-2.70585700
H -3.88798200	0.03591300	-2.40075800	H -4.08219400	-0.02132500	-2.29215900
H -3.99495800	-1.67504500	-2.81420200	H -4.13333500	-1.73042700	-2.72440200
C -2.67182300	-2.73457100	-0.66574500	C -2.72311600	-2.76536000	-0.62653700
H -3.28648800	-3.45415000	-1.21635900	H -3.33041000	-3.49957400	-1.16567100
H -2.64198200	-3.06010600	0.37661700	H -2.64458000	-3.10216400	0.40972000
H -1.65719800	-2.79053800	-1.06687500	H -1.72151000	-2.77673100	-1.06437800
C 3.28894100	1.64191300	-0.05193400	C 3.41659700	1.58715300	0.10762600
H 4.27378500	1.42175700	0.37324800	H 4.38027600	1.34527700	0.56815800
C 3.45044600	1.93963000	-1.54134900	C 3.64166400	1.94268600	-1.35994700
H 2.48567500	2.12778600	-2.01902400	H 2.69691900	2.15837600	-1.86649000
H 3.93900800	1.12571400	-2.08090700	H 4.14663200	1.14729200	-1.91198100
H 4.06425600	2.83623600	-1.67395900	H 4.26591700	2.83905100	-1.42956900
C 2.71120300	2.84555300	0.68774000	C 2.80278900	2.76181800	0.86401600
H 3.36552500	3.71076600	0.53977700	H 3.46001600	3.63286500	0.77647600
H 2.63203300	2.67878800	1.76414100	H 2.67427600	2.55798000	1.92917100
H 1.72045200	3.11373200	0.31451100	H 1.82897100	3.03825000	0.45301600
C 3.26263000	-1.24688700	-0.64160900	C 3.37030400	-1.28431700	-0.61419700
H 3.09088200	-1.05685200	-1.70655000	H 3.25487500	-1.02719300	-1.67269400
C 2.70854300	-2.63223900	-0.31198300	C 2.75055900	-2.66296800	-0.39264300
H 3.17100800	-3.37875300	-0.96528000	H 3.23770100	-3.39395600	-1.04551100
H 1.62739100	-2.69359700	-0.44910700	H 1.68118400	-2.67684100	-0.61533900
H 2.93690300	-2.91487800	0.71912800	H 2.88875200	-3.00160200	0.63762300
C 4.76353700	-1.19551600	-0.37048900	C 4.85556800	-1.29569200	-0.26650400
H 4.98546200	-1.31212200	0.69438400	H 5.01845900	-1.49889500	0.79593700
H 5.22532100	-0.26829900	-0.71373300	H 5.35581600	-0.35766700	-0.51360800
H 5.25694700	-2.01911200	-0.89731800	H 5.35575700	-2.09006200	-0.83022600
N 0.00280000	-0.67190800	1.68779500	N -0.00157700	-0.71487700	1.74647400
P -2.28119800	-0.08148600	0.16887300	P -2.38965600	-0.11314200	0.21868800
P 2.26944200	0.09403800	0.22088300	P 2.37985500	0.03787500	0.27176100
Mn -0.00463800	0.07162100	-0.05187200	Re -0.00088300	0.08438900	-0.12429700
C -0.12082900	1.56337300	-0.95309400	C -0.10503000	1.72741200	-1.04462200
C 0.12358900	-0.74443400	-1.57495300	C 0.11865400	-0.66559400	-1.83206900
O 0.25304100	-1.30269800	-2.59614800	O 0.22647400	-1.19076400	-2.88330500
O -0.23708500	2.55203000	-1.56828600	O -0.19928200	2.77759200	-1.56983200
2Mn(Cs)-SMD(CH₃OH)			2Re(Cs)-SMD(CH₃OH)		
P -2.24242800	0.08068600	-0.31232700	P -2.36802900	0.04052400	-0.35901300
P 2.24243200	0.08067900	-0.31232300	P 2.36802400	0.04051200	-0.35903900
C -2.42509400	-0.98109400	-1.83623400	C -2.44765700	-1.11817200	-1.82407200
C 2.42509400	-0.98108500	-1.83624200	C 2.44763000	-1.11818900	-1.82409500
H -2.42566500	-0.30840800	-2.69971600	H -2.44752800	-0.49042100	-2.72070100
H 2.42565700	-0.30839100	-2.69971800	H 2.44749700	-0.49044000	-2.72072600
H -3.36426300	-1.53588600	-1.85347000	H -3.36935700	-1.70195800	-1.83681800
H 3.36426500	-1.53587400	-1.85348800	H 3.36932800	-1.70197900	-1.83684600
C -1.22985800	-1.91153200	-1.92053500	C -1.23236900	-2.02768900	-1.84658900
C 1.22986200	-1.91152700	-1.92054300	C 1.23233500	-2.02769700	-1.84660100
H -1.21667300	-2.43426000	-2.88583800	H -1.21036000	-2.60376000	-2.77963200

H	1.21667400	-2.43425100	-2.88584800	H	1.21031200	-2.60376700	-2.77964300
H	-1.25810500	-2.66466000	-1.12980000	H	-1.24733800	-2.73418000	-1.01433400
H	1.25811400	-2.66465900	-1.12981200	H	1.24730600	-2.73419000	-1.01434700
N	0.00000000	-1.12211900	-1.74492300	N	-0.00001300	-1.21860200	-1.72763700
C	3.00299800	1.69616800	-0.91107400	C	3.18188100	1.57691300	-1.07098000
C	-3.00298900	1.69617200	-0.91109600	C	-3.18188500	1.57693100	-1.07094800
H	2.38464000	1.89403900	-1.79458000	H	2.52691000	1.77755700	-1.92679100
H	-2.38464100	1.89402100	-1.79461400	H	-2.52689800	1.77759300	-1.92674200
C	3.49555400	-0.61336400	0.90946700	C	3.58779500	-0.63554500	0.89988300
C	-3.49554700	-0.61334000	0.90947600	C	-3.58779800	-0.63553200	0.89991000
C	3.49500400	-2.13906600	0.95710400	C	3.52977000	-2.15584200	1.01603400
C	-3.49501500	-2.13904200	0.95710600	C	-3.52982600	-2.15583500	1.01600200
H	-4.47494200	-0.28804600	0.54600000	H	-4.57787200	-0.35713800	0.52656700
H	4.47495000	-0.28808500	0.54597900	H	4.57787200	-0.35719900	0.52650800
C	-3.27497600	-0.03716000	2.30646400	C	-3.37217200	0.01512200	2.26441500
C	3.27501000	-0.03717200	2.30645400	C	3.37222200	0.01516600	2.26436900
H	-3.27808100	1.05409300	2.31823500	H	-3.41087500	1.10500300	2.22384300
H	3.27813200	1.05408100	2.31821700	H	3.41096500	1.10504500	2.22375700
H	-2.32278600	-0.37375500	2.72429200	H	-2.40340800	-0.26979100	2.68238600
H	2.32282100	-0.37374900	2.72429800	H	2.40345700	-0.26969600	2.68237000
H	-4.07035500	-0.37775300	2.97776000	H	-4.14880200	-0.31938900	2.95995200
H	4.07039300	-0.37777200	2.97774200	H	4.14885400	-0.31934900	2.95990300
C	2.81279600	2.86188000	0.05366700	C	3.11692300	2.78295400	-0.14016300
C	-2.81276600	2.86190000	0.05362100	C	-3.11695600	2.78296000	-0.14011300
H	3.41884500	2.74707900	0.95556600	H	3.79291800	2.67243800	0.71107400
H	-3.41881800	2.74712600	0.95552200	H	-3.79296000	2.67242500	0.71111400
H	1.77004400	2.97777300	0.35470400	H	2.10785500	2.95171400	0.24206100
H	-1.77001200	2.97778100	0.35465800	H	-2.10789500	2.95172700	0.24212800
H	3.12457200	3.79358000	-0.43000600	H	3.42313600	3.68295400	-0.68322900
H	-3.12452500	3.79359600	-0.43007000	H	-3.42317200	3.68296400	-0.68317000
C	4.45767500	1.58562400	-1.35900000	C	4.59950400	1.35194500	-1.58903000
C	-4.45767300	1.58563300	-1.35900100	C	-4.59949500	1.35196200	-1.58903400
H	4.62500800	0.75139500	-2.04440100	H	4.67124200	0.49139900	-2.25844600
H	-4.62502300	0.75139600	-2.04438700	H	-4.67121600	0.49141600	-2.25845000
H	5.13581900	1.46814900	-0.50953800	H	5.31134900	1.20813500	-0.77197500
H	-5.13580600	1.46817700	-0.50952700	H	-5.31136000	1.20815400	-0.77199600
H	4.75169400	2.50239500	-1.88101200	H	4.92741700	2.23271200	-2.15092500
H	-4.75169100	2.50239900	-1.88102200	H	-4.92739400	2.23272900	-2.15093800
H	0.00001100	1.31108500	-0.88559700	H	-0.00000300	1.41832200	-1.10220400
H	-0.00000300	-0.40922000	-2.47111700	H	-0.00001500	-0.57178800	-2.51434800
H	4.24284400	-2.47835500	1.68176900	H	4.25499000	-2.48818400	1.76607700
H	2.52938900	-2.53570600	1.27644600	H	2.54519100	-2.49961600	1.33988800
H	3.74910600	-2.58919900	-0.00432300	H	3.77812900	-2.65797000	0.07942200
H	-4.24285300	-2.47832600	1.68177500	H	-4.25503600	-2.48817800	1.76605500
H	-3.74912800	-2.58916800	-0.00432200	H	-3.77823300	-2.65791800	0.07937900
H	-2.52940100	-2.53569400	1.27643800	H	-2.54525000	-2.49966000	1.33981300
Mn	0.00000200	0.02308000	0.07414500	Re	-0.00000400	0.12037300	0.10199100
C	0.00000400	1.11051300	1.42504800	C	0.00000300	1.36561400	1.51047100
C	0.00000000	-1.37369000	1.13750900	C	-0.00000600	-1.32948600	1.34813100
O	-0.00000600	1.84375100	2.34002900	O	0.00008300	2.14974400	2.39026900
O	-0.00009300	-2.24481100	1.92375000	O	0.00008000	-2.18130200	2.15839500
1Mn+H₂(ads)-SMD(CH₃OH)				1Re+H₂(ads)-SMD(CH₃OH)			
P	-0.05054400	-0.32863500	2.28339100	P	0.03066800	-0.35946200	2.39495600
P	-0.05054400	-0.32863500	-2.28339100	P	0.03066800	-0.35946200	-2.39495600
C	1.09447100	-1.77904300	2.43146700	C	1.23102100	-1.77303400	2.44818200
C	1.09447100	-1.77904300	-2.43146700	C	1.23102100	-1.77303400	-2.44818200
H	0.45896100	-2.66958300	2.45466000	H	0.62327000	-2.68283000	2.46900600
H	0.45896100	-2.66958300	-2.45466000	H	0.62327000	-2.68283000	-2.46900600
H	1.68041300	-1.76033200	3.35232200	H	1.84278800	-1.75822100	3.35238500

H	1.68041300	-1.76033200	-3.35232200	H	1.84278800	-1.75822100	-3.35238500
C	1.95839300	-1.80373500	1.18162900	C	2.07240900	-1.75785900	1.18207700
C	1.95839300	-1.80373500	-1.18162900	C	2.07240900	-1.75785900	-1.18207700
H	2.52207700	-2.75405800	1.16377200	H	2.65529100	-2.69492400	1.14671800
H	2.52207700	-2.75405800	-1.16377200	H	2.65529100	-2.69492400	-1.14671800
H	2.72847000	-1.00795900	1.25711100	H	2.82445500	-0.94571800	1.25252400
H	2.72847000	-1.00795900	-1.25711100	H	2.82445500	-0.94571800	-1.25252400
N	1.13334600	-1.68163900	0.00000000	N	1.24151500	-1.63825100	0.00000000
C	-1.60677400	-0.96669400	-3.12740800	C	-1.45915600	-1.08689600	-3.27963500
C	-1.60677400	-0.96669400	3.12740800	C	-1.45915600	-1.08689600	3.27963500
H	-1.83641700	-1.84917100	-2.51722500	H	-1.66793100	-1.96121000	-2.65082700
H	-1.83641700	-1.84917100	2.51722500	H	-1.66793100	-1.96121000	2.65082700
C	0.59678900	1.01049400	-3.43650300	C	0.68827100	0.97988500	-3.53207600
C	0.59678900	1.01049400	3.43650300	C	0.68827100	0.97988500	3.53207600
C	2.12084700	1.08605700	-3.49029900	C	2.20140300	1.15442300	-3.43448900
C	2.12084700	1.08605700	3.49029900	C	2.20140300	1.15442300	3.43448900
H	0.24345700	0.71223100	4.42832300	H	0.45243000	0.62703500	4.54083800
H	0.24345700	0.71223100	-4.42832300	H	0.45243000	0.62703500	-4.54083800
C	0.00085600	2.37672700	3.10324600	C	-0.02877400	2.30770600	3.29724900
C	0.00085600	2.37672700	-3.10324600	C	-0.02877400	2.30770600	-3.29724900
H	-1.08958700	2.36418600	3.06621900	H	-1.11298100	2.22318900	3.38589200
H	-1.08958700	2.36418600	-3.06621900	H	-1.11298100	2.22318900	-3.38589200
H	0.36517000	2.74729200	2.14196400	H	0.19541000	2.70757000	2.30587500
H	0.36517000	2.74729200	-2.14196400	H	0.19541000	2.70757000	-2.30587500
H	0.29690700	3.10069100	3.86957800	H	0.30773900	3.04121000	4.03712900
H	0.29690700	3.10069100	-3.86957800	H	0.30773900	3.04121000	-4.03712900
C	-2.79086900	-0.00983700	-3.03564800	C	-2.69271400	-0.19041600	-3.26345300
C	-2.79086900	-0.00983700	3.03564800	C	-2.69271400	-0.19041600	3.26345300
H	-2.64465600	0.87231000	-3.66375800	H	-2.57913800	0.66156200	-3.93776300
H	-2.64465600	0.87231000	3.66375800	H	-2.57913800	0.66156200	3.93776300
H	-2.97265800	0.32620500	-2.01281500	H	-2.91587000	0.19114700	-2.26488800
H	-2.97265800	0.32620500	2.01281500	H	-2.91587000	0.19114700	2.26488800
H	-3.69778600	-0.51237600	-3.38714200	H	-3.56279200	-0.76030700	-3.60491100
H	-3.69778600	-0.51237600	3.38714200	H	-3.56279200	-0.76030700	3.60491100
C	-1.38519200	-1.43311000	-4.56381400	C	-1.15350300	-1.57860700	-4.69184300
C	-1.38519200	-1.43311000	4.56381400	C	-1.15350300	-1.57860700	4.69184300
H	-0.53993900	-2.11884900	-4.65586500	H	-0.28309100	-2.23758900	-4.72808100
H	-0.53993900	-2.11884900	4.65586500	H	-0.28309100	-2.23758900	4.72808100
H	-1.21788900	-0.59228900	-5.24216000	H	-0.98164100	-0.74752100	-5.38092900
H	-1.21788900	-0.59228900	5.24216000	H	-0.98164100	-0.74752100	5.38092900
H	-2.27710100	-1.96051300	-4.91777900	H	-2.00970200	-2.14367600	-5.07428700
H	-2.27710100	-1.96051300	4.91777900	H	-2.00970200	-2.14367600	5.07428700
H	-1.39247100	-1.17279200	-0.40126700	H	-1.45813000	-1.33141400	-0.40578100
H	-1.39247100	-1.17279200	0.40126700	H	-1.45813000	-1.33141400	0.40578100
H	2.41363800	1.85936700	-4.20830200	H	2.51738400	1.92795800	-4.14214100
H	2.55305400	1.35702100	-2.52563100	H	2.51334000	1.47668700	-2.43927000
H	2.57502600	0.14976800	-3.81813800	H	2.74466000	0.24186400	-3.68503500
H	2.41363800	1.85936700	4.20830200	H	2.51738400	1.92795800	4.14214100
H	2.57502600	0.14976800	3.81813800	H	2.74466000	0.24186400	3.68503500
H	2.55305400	1.35702100	2.52563100	H	2.51334000	1.47668700	2.43927000
C	1.21809900	1.06323500	0.00000000	C	1.08672000	1.42296200	0.00000000
C	-1.27133900	1.30806500	0.00000000	C	-1.54984200	1.33216700	0.00000000
O	2.12362100	1.79188600	0.00000000	O	1.83154100	2.32289800	0.00000000
O	-1.96975800	2.24395200	0.00000000	O	-2.37096200	2.17346900	0.00000000
Mn	-0.14112600	-0.03346400	0.00000000	Re	-0.17380000	0.01890500	0.00000000
1Mn + H₂-TS(1M/2M)-SMD(CH₃OH)				1Re+ H₂-TS(1M/2M)-SMD(CH₃OH)			
P	-2.27499300	0.05237800	-0.30891800	P	-2.38682600	-0.02969400	-0.36446700
P	2.27501400	0.05235900	-0.30891100	P	2.38682800	-0.02971200	-0.36443900
C	-2.43290600	-1.00775400	-1.82785500	C	-2.44612000	-1.19400400	-1.81733200

C	2.43294800	-1.00786100	-1.82778900	C	2.44615600	-1.19414300	-1.81720600
H	-2.45422900	-0.32475700	-2.68244600	H	-2.45829200	-0.56706900	-2.71392100
H	2.45434000	-0.32491200	-2.68241600	H	2.45842000	-0.56727500	-2.71384100
H	-3.35770100	-1.58720200	-1.84163600	H	-3.36038100	-1.79102300	-1.81752200
H	3.35771800	-1.58735100	-1.84149700	H	3.36038700	-1.79120800	-1.81729800
C	-1.20077900	-1.89320100	-1.91175900	C	-1.20401500	-2.07393100	-1.82617400
C	1.20078400	-1.89325800	-1.91169900	C	1.20400500	-2.07400100	-1.82606700
H	-1.19555000	-2.40423900	-2.88985200	H	-1.17114000	-2.61892400	-2.78402700
H	1.19556200	-2.40432800	-2.88977600	H	1.17115100	-2.61904900	-2.78388900
H	-1.26990300	-2.69163600	-1.14881300	H	-1.29286400	-2.84413200	-1.03854900
H	1.26985200	-2.69167100	-1.14872500	H	1.29277000	-2.84415600	-1.03838600
N	0.00001700	-1.10670500	-1.74989300	N	0.00001000	-1.28590300	-1.65812700
C	3.05409100	1.65897200	-0.90465400	C	3.21782800	1.49914400	-1.07564000
C	-3.05411100	1.65901400	-0.90455800	C	-3.21788300	1.49919700	-1.07553000
H	2.42321500	1.88598700	-1.77240100	H	2.64410700	1.63198000	-2.00061700
H	-2.42319500	1.88614400	-1.77224600	H	-2.64429100	1.63202800	-2.00058800
C	3.47599300	-0.64087800	0.95803400	C	3.56735400	-0.73843400	0.90575600
C	-3.47596900	-0.64095600	0.95798000	C	-3.56734900	-0.73860900	0.90561500
C	3.49190500	-2.16688700	0.99453300	C	3.34315700	-2.23161700	1.12555200
C	-3.49187400	-2.16696800	0.99437500	C	-3.34293900	-2.23175900	1.12540200
H	-4.46269400	-0.30220800	0.62775100	H	-4.56337500	-0.60490700	0.47222100
H	4.46271700	-0.30214600	0.62778600	H	4.56339900	-0.60458200	0.47245600
C	-3.20616900	-0.07095500	2.34900000	C	-3.49350800	0.02719800	2.22320100
C	3.20618100	-0.07078000	2.34901200	C	3.49328100	0.02737500	2.22332800
H	-3.18509700	1.01992700	2.36068500	H	-3.70352100	1.09087200	2.10089000
H	3.18511900	1.02010400	2.36062100	H	3.70316200	1.09107600	2.10102600
H	-2.25349500	-0.42914800	2.74673800	H	-2.50694800	-0.07012600	2.68355400
H	2.25349800	-0.42893800	2.74676100	H	2.50669200	-0.07007900	2.68358700
H	-3.99395300	-0.39424200	3.03734000	H	-4.22992200	-0.37702800	2.92527000
H	3.99395300	-0.39402600	3.03738500	H	4.22969000	-0.37673900	2.92546800
C	2.93247600	2.82000500	0.07663700	C	3.03360000	2.75956700	-0.23756000
C	-2.93261700	2.81996400	0.07684600	C	-3.03353100	2.75963100	-0.23749600
H	3.56251600	2.67391100	0.95726400	H	3.58618100	2.71302100	0.70362900
H	-3.56271100	2.67376600	0.95741800	H	-3.58612800	2.71318500	0.70369000
H	1.90583500	2.97390800	0.41222100	H	1.98357100	2.94677900	-0.00671100
H	-1.90600700	2.97388200	0.41251400	H	-1.98348700	2.94675400	-0.00664900
H	3.26411700	3.74374700	-0.40881400	H	3.41149000	3.62364800	-0.79382400
H	-3.26426500	3.74373300	-0.40854800	H	-3.41133100	3.62372400	-0.79380100
C	4.49362400	1.50418100	-1.38921300	C	4.68220000	1.28568500	-1.44778200
C	-4.49360700	1.50419300	-1.38922100	C	-4.68230700	1.28575500	-1.44748500
H	4.61479100	0.67757100	-2.09279000	H	4.83588600	0.38706600	-2.04982400
H	-4.61467600	0.67767300	-2.09291800	H	-4.83609300	0.38710100	-2.04945000
H	5.18552700	1.34748800	-0.55743300	H	5.31777700	1.21456000	-0.56128200
H	-5.18554900	1.34733900	-0.55750400	H	-5.31777400	1.21470000	-0.56090100
H	4.80723000	2.41983400	-1.90139200	H	5.03835400	2.13889900	-2.03413600
H	-4.80724200	2.41989600	-1.90129200	H	-5.03851000	2.13893800	-2.03385500
H	0.00002600	1.23737300	-1.22399500	H	0.00008100	1.12823100	-1.60559900
H	0.00002900	0.41931900	-1.64546900	H	-0.00008600	0.25898000	-1.86213100
H	4.22591600	-2.50047000	1.73556400	H	4.06657500	-2.59911300	1.86061200
H	2.52412000	-2.57914400	1.28620400	H	2.34477800	-2.43892700	1.51488800
H	3.77568700	-2.60512800	0.03618100	H	3.48224800	-2.81212600	0.21184400
H	-4.22588200	-2.50060400	1.73538400	H	-4.06633500	-2.59938100	1.86042100
H	-3.77565700	-2.60514500	0.03599400	H	-3.48190000	-2.81227300	0.21167500
H	-2.52408700	-2.57924100	1.28601700	H	-2.34454300	-2.43891700	1.51477300
Mn	0.00001500	0.06543700	0.01655700	C	0.00002000	1.56984000	1.28861000
C	-0.00003000	1.23687600	1.31617200	C	0.00000100	-1.01863500	1.55648600
C	0.00001100	-1.25924800	1.16214700	O	0.00002900	2.44631800	2.07111400
O	-0.00004400	1.97946400	2.21762000	O	0.00001100	-1.71445700	2.50149100
O	-0.00000200	-2.13844800	1.92675100	Re	0.00000100	0.12391300	0.06408500
1Mn + H₂-TS(H₂O-H⁺)-SMD(CH₃OH)				1Re + H₂-TS(H₂O-H⁺)-SMD(CH₃OH)			

O	-0.00020100	-2.24191700	-1.84293400	O	-0.00039000	-2.33829700	-1.95830300
P	-2.28620200	0.16145700	0.01160300	P	-2.39982500	0.21940500	-0.01894600
P	2.28626200	0.16139900	0.01150600	P	2.39980200	0.21886900	-0.01925500
C	-2.44544900	1.43118300	-1.32976400	C	-2.46336700	1.64256300	-1.21063800
C	2.44554300	1.43097100	-1.33001200	C	2.46385800	1.64089100	-1.21233600
H	-2.50621300	2.39966300	-0.82619200	H	-2.51382200	2.54828000	-0.60035100
H	2.50660400	2.39950100	-0.82657300	H	2.51579400	2.54715800	-0.60299900
H	-3.35426800	1.30757800	-1.92050400	H	-3.35763800	1.61341100	-1.83525700
H	3.35424700	1.30707400	-1.92086700	H	3.35763200	1.61015500	-1.83757700
C	-1.19242200	1.38029900	-2.18804700	C	-1.19711700	1.66499000	-2.05013900
C	1.19240200	1.38022700	-2.18814200	C	1.19704900	1.66378800	-2.05099300
H	-1.18580500	2.25513800	-2.85922200	H	-1.17689600	2.59821100	-2.63379500
H	1.18577800	2.25509800	-2.85927500	H	1.17706900	2.59675300	-2.63506900
H	-1.21676900	0.49466700	-2.84281600	H	-1.20838300	0.84147300	-2.77712600
H	1.21662800	0.49462600	-2.84295600	H	1.20728700	0.83995000	-2.77763300
N	0.00002200	1.38496500	-1.34404700	N	0.00023000	1.58483400	-1.20363700
C	3.11624200	1.02919400	1.45998700	C	3.27847500	0.93271700	1.47816000
C	-3.11622100	1.02910000	1.46014800	C	-3.27873200	0.93183700	1.47902100
H	2.51001700	1.94004500	1.53697500	H	2.65138500	1.80689000	1.69152700
H	-2.51011200	1.94002300	1.53716000	H	-2.65156600	1.80567300	1.69354500
C	3.43511000	-1.26369800	-0.41777800	C	3.53060400	-1.12292700	-0.68135000
C	-3.43507300	-1.26359300	-0.41778700	C	-3.53069600	-1.12155200	-0.68263300
C	3.49846000	-1.56644800	-1.91297100	C	3.46149800	-1.26944200	-2.19889500
C	-3.49874800	-1.56608100	-1.91301800	C	-3.46131200	-1.26657600	-2.20031100
O	0.00007700	-2.09514400	2.26801100	O	-0.00022900	-2.39061800	2.27596100
H	-4.42567500	-0.92107300	-0.10383700	H	-4.53861200	-0.78547100	-0.42043300
H	4.42577500	-0.92111400	-0.10409700	H	4.53853700	-0.78684100	-0.41921800
C	-3.08764700	-2.52172800	0.37533400	C	-3.26578700	-2.45816500	0.00684100
C	3.08784900	-2.52169400	0.37563100	C	3.26521700	-2.45885200	0.00926900
H	-3.03978200	-2.34209300	1.45033300	H	-3.31937600	-2.38945000	1.09449900
H	3.04057500	-2.34196200	1.45064000	H	3.31808100	-2.38913300	1.09690000
H	-2.12853800	-2.93921300	0.06059600	H	-2.28037600	-2.84957200	-0.25556500
H	2.12849800	-2.93902600	0.06142600	H	2.27995300	-2.85045400	-0.25341500
H	-3.85319800	-3.28496600	0.20175800	H	-4.01271600	-3.19035200	-0.31633000
H	3.85316900	-3.28509000	0.20172500	H	4.01232700	-3.19137100	-0.31272100
C	2.99915600	0.27517000	2.78055200	C	3.25275200	0.02176000	2.70096100
C	-2.99895800	0.27510800	2.78070700	C	-3.25352100	0.01958000	2.70087100
H	3.60495300	-0.63433600	2.78394000	H	3.91881100	-0.83542900	2.57759700
H	-3.60419300	-0.63477000	2.78400000	H	-3.92032000	-0.83692100	2.57670400
H	1.96797200	-0.00117000	3.01000400	H	2.25027400	-0.35238900	2.91942400
H	-1.96764100	-0.00057700	3.01034200	H	-2.25131100	-0.35561600	2.91875900
H	3.36124700	0.90955300	3.59599800	H	3.59888900	0.57873600	3.57737800
H	-3.36158000	0.90927100	3.59609100	H	-3.59902900	0.57592100	3.57793700
C	4.55893100	1.44679100	1.18783200	C	4.69376100	1.42135200	1.18229300
C	-4.55897800	1.44649000	1.18803000	C	-4.69384400	1.42107400	1.18329500
H	4.66794800	1.99430700	0.24889700	H	4.73598200	2.08777500	0.31785200
H	-4.66820900	1.99345800	0.24879900	H	-4.73563400	2.08872700	0.31978600
H	5.23427000	0.58769100	1.16223000	H	5.38083700	0.58939000	1.00684000
H	-5.23427000	0.58733200	1.16304900	H	-5.38096700	0.58945400	1.00640300
H	4.90409000	2.10422000	1.99246100	H	5.07342800	1.97812600	2.04499000
H	-4.90401800	2.10436300	1.99234500	H	-5.07376600	1.97667600	2.04663700
H	0.40461900	1.16824300	1.21308100	H	0.41019800	1.12594700	1.49846500
H	0.00010500	2.63523600	-0.69191900	H	0.00112000	2.69285200	-0.48776900
H	4.20454600	-2.38663100	-2.07975000	H	4.15911600	-2.05270200	-2.51276500
H	2.53276400	-1.88289600	-2.31080000	H	2.46698000	-1.56482600	-2.53817700
H	3.84804600	-0.71485500	-2.49879700	H	3.74459700	-0.35390700	-2.72073400
H	-4.20498500	-2.38613400	-2.07979300	H	-4.15950400	-2.04893100	-2.51515700
H	-3.84831800	-0.71433900	-2.49863900	H	-3.74352100	-0.35025600	-2.72124100
H	-2.53317400	-1.88261000	-2.31108200	H	-2.46695800	-1.56241500	-2.53967800

H -0.40480000 1.16821900 1.21268600	H -0.41019000 1.12600600 1.49841300
O 0.00024800 3.64405500 -0.18133900	O 0.00169900 3.70546000 0.15298700
C -0.00012800 -1.38405600 -1.06133900	C -0.00024400 -1.48534000 -1.16502000
C 0.00000200 -1.28132400 1.43474300	C -0.00018900 -1.52756600 1.48320000
Mn -0.00004700 -0.10251400 0.13454500	Re -0.00006000 -0.15032400 0.17791200
H -0.00158200 4.29138400 -0.89390800	H 0.00646800 4.42167700 -0.49031400
1Mn + H₂-TS(CH₃OH-H⁺)-SMD(CH₃OH)	1Re + H₂-TS(CH₃OH-H⁺)-SMD(CH₃OH)
O 0.01389800 -2.12897800 -2.11903700	O 0.01633900 -2.31900800 -2.12819500
P -2.28568000 -0.00908300 0.04677700	P -2.39771600 0.07316300 0.00216800
P 2.29293100 0.01391300 0.04565900	P 2.40339500 0.09792400 0.00267600
C -2.45027200 1.45058000 -1.08613100	C -2.46887200 1.57900400 -1.08417400
C 2.44258100 1.47480700 -1.08778800	C 2.45760800 1.60641200 -1.08115100
H -2.51120900 2.33333500 -0.44405700	H -2.52159200 2.43851800 -0.41042600
H 2.49547800 2.35872600 -0.44658100	H 2.49955800 2.46575400 -0.40637000
H -3.35960500 1.41316200 -1.68793600	H -3.36448200 1.59140500 -1.70774900
H 3.35147000 1.44586500 -1.69078000	H 3.35338600 1.63042200 -1.70413700
C -1.19804400 1.51841200 -1.94276000	C -1.20416200 1.65987300 -1.92282800
C 1.18896500 1.53017000 -1.94323600	C 1.19282300 1.67432400 -1.92078400
H -1.19573700 2.46571200 -2.50516900	H -1.19127300 2.62226300 -2.45577100
H 1.17730900 2.47704400 -2.50606600	H 1.17026000 2.63693700 -2.45287400
H -1.21673800 0.71420400 -2.69397100	H -1.20921300 0.87577900 -2.69264200
H 1.21514700 0.72595000 -2.69420900	H 1.20725700 0.89109700 -2.69135300
N -0.00385900 1.42220900 -1.10513700	N -0.00554200 1.53950300 -1.08268200
C 3.12953900 0.64479000 1.60737500	C 3.27258700 0.69831000 1.55423800
C -3.12850100 0.61279000 1.60893100	C -3.27167300 0.66662200 1.55382900
H 2.53255800 1.54033800 1.82014800	H 2.64653200 1.55735300 1.82499000
H -2.54075000 1.51451400 1.82158700	H -2.65525800 1.53359600 1.82151600
C 3.44285100 -1.31787400 -0.61812700	C 3.54492000 -1.17830100 -0.76174000
C -3.42244300 -1.35163000 -0.61800700	C -3.52677700 -1.21534500 -0.76015200
C 3.47846000 -1.38929900 -2.14286400	C 3.46682700 -1.21403500 -2.28539000
C -3.45604900 -1.42376600 -2.14277500	C -3.44554300 -1.25530100 -2.28354500
O 0.01742800 -2.56772000 1.94394400	O 0.01788100 -2.70781800 2.07149200
H -4.41951200 -1.05656100 -0.27722100	H -4.53582600 -0.89443000 -0.48368400
H 4.43676400 -1.01365900 -0.27620700	H 4.55073600 -0.85001500 -0.48230300
C -3.09118200 -2.71647100 -0.01813200	C -3.27250600 -2.59807400 -0.16449100
C 3.12326000 -2.68568800 -0.01869500	C 3.30066000 -2.56480500 -0.17069600
H -3.07005600 -2.70368600 1.07273500	H -3.31601600 -2.60256300 0.92570900
H 3.09984000 -2.67288600 1.07211800	H 3.34221900 -2.57227600 0.91959100
H -2.12340400 -3.08287100 -0.36910500	H -2.29459800 -2.98273900 -0.46281900
H 2.15958800 -3.06102000 -0.37147000	H 2.32623600 -2.95583300 -0.47193400
H -3.85018100 -3.44336800 -0.32520700	H -4.03074700 -3.29798700 -0.52996500
H 3.88960100 -3.40552200 -0.32415100	H 4.06493300 -3.25768500 -0.53698700
C 3.00217800 -0.29860400 2.79869500	C 3.23058100 -0.29718900 2.70871800
C -2.99078600 -0.32902300 2.80035200	C -3.21596500 -0.32577600 2.71039300
H 3.60200000 -1.20210200 2.66538700	H 3.89625700 -1.14589600 2.53440600
H -3.58076600 -1.23904900 2.66746400	H -3.87400900 -1.18117600 2.54006100
H 1.96794800 -0.59824300 2.97897100	H 2.22414800 -0.68208700 2.88614000
H -1.95334700 -0.61737300 2.98060200	H -2.20524600 -0.70062000 2.88487600
H 3.36453900 0.20238000 3.70210000	H 3.56560000 0.19561800 3.62686300
H -3.35842100 0.16825000 3.70367500	H -3.55246300 0.16569200 3.62870500
C 4.57725200 1.08095300 1.39931900	C 4.69138300 1.20232200 1.30600600
C -4.58067600 1.03413000 1.40149300	C -4.69681600 1.15306100 1.30699100
H 4.69477100 1.74881800 0.54302900	H 4.74182300 1.92624400 0.48953400
H -4.70524900 1.70155200 0.54587200	H -4.75780100 1.87238900 0.48721000
H 5.24287400 0.22526600 1.25889600	H 5.37874000 0.38306400 1.07987100
H -5.23757600 0.17185700 1.26032300	H -5.37505000 0.32471700 1.08651500
H 4.92584500 1.61935200 2.28658700	H 5.06407700 1.69775400 2.20825600
H -4.93461600 1.56818400 2.28927200	H -5.07300700 1.64838700 2.20785000
H 0.40505800 0.81177200 1.39143800	H 0.40834700 0.87767300 1.57971300

H -0.01252200	2.50900500	-0.25943000	H -0.01600900	2.56758200	-0.26805400
H 4.19747300	-2.15776100	-2.44528500	H 4.17382000	-1.96108000	-2.66074600
H 2.51097300	-1.66518100	-2.56521900	H 2.47424800	-1.49945800	-2.63834500
H 3.79671900	-0.45047400	-2.59870200	H 3.73214900	-0.25837500	-2.74056000
H -4.17017600	-2.19662700	-2.44555600	H -4.14661400	-2.00845400	-2.65780100
H -3.77936100	-0.48711500	-2.59954000	H -3.71665500	-0.30299700	-2.74226900
H -2.48650200	-1.69416700	-2.56391700	H -2.45036400	-1.53495400	-2.63375600
H -0.40540400	0.80958200	1.38994300	H -0.41132200	0.87071900	1.58165700
O -0.01551700	3.40241700	0.46859000	O -0.02180700	3.48970200	0.50837600
C -0.10551900	4.61485400	-0.23553100	C -0.11387500	4.72330900	-0.15212000
H 0.71435600	4.75170100	-0.95885200	H 0.70681100	4.89050200	-0.86994100
H -1.05040600	4.71750300	-0.79343900	H -1.05704300	4.84422100	-0.71158900
H -0.05684400	5.46205900	0.46158300	H -0.07118700	5.55296400	0.56871400
C 0.01019200	-1.38028900	-1.23251100	C 0.01168500	-1.52754400	-1.27357800
C 0.01240400	-1.63919100	1.24155700	C 0.01283400	-1.78005500	1.35588100
Mn 0.00498400	-0.27840200	0.13219200	Re 0.00478200	-0.29945000	0.16813600
1Mn + H₂-interm(H₂O-H₂)-SMD(CH₃OH)			1Re + H₂-interm(H₂O-H₂)-SMD(CH₃OH)		
O -0.00266800	-2.36838100	-1.69941600	O 0.00098400	-2.39040400	-1.89298800
P -2.29538400	0.15922400	0.00513900	P -2.40339500	0.21110200	-0.02579000
P 2.29460800	0.15554400	0.00405300	P 2.40337800	0.21249700	-0.02530800
C -2.44599500	1.38535300	-1.37845800	C -2.46490000	1.59778100	-1.26144400
C 2.44810700	1.37608400	-1.38428300	C 2.46331900	1.60106000	-1.25889900
H -2.48299800	2.37246100	-0.90975000	H -2.49940200	2.52357700	-0.68065200
H 2.49133900	2.36469800	-0.91943600	H 2.49493400	2.52586800	-0.67631100
H -3.36229300	1.25867400	-1.95636900	H -3.36546400	1.55739400	-1.87571800
H 3.36241100	1.24262200	-1.96382100	H 3.36466800	1.56403600	-1.87225800
C -1.21427500	1.29219300	-2.25919000	C -1.21577700	1.58995300	-2.12390200
C 1.21399300	1.28576100	-2.26202900	C 1.21512700	1.59227400	-2.12264100
H -1.20499600	2.12826000	-2.97081400	H -1.19581800	2.49400400	-2.74571400
H 1.20628600	2.12043900	-2.97530100	H 1.19467000	2.49686300	-2.74366100
H -1.21468200	0.36645700	-2.84178300	H -1.20812300	0.72778300	-2.79587300
H 1.20941600	0.35882000	-2.84269100	H 1.20920900	0.73070800	-2.79541000
N 0.00090600	1.33042500	-1.42636400	N -0.00069600	1.54609400	-1.28242900
C 3.12257200	1.08037900	1.41671700	C 3.28246900	0.97035900	1.44847700
C -3.12386500	1.07895400	1.42074300	C -3.28183500	0.97089900	1.44732700
H 2.52043400	1.99645800	1.45206300	H 2.65000600	1.84460100	1.64382700
H -2.51963800	1.99334300	1.46254800	H -2.64898200	1.84523400	1.64100700
C 3.43860800	-1.28373600	-0.38188200	C 3.52914600	-1.14908900	-0.65225900
C -3.44044700	-1.27763900	-0.38669600	C -3.52858700	-1.15186700	-0.65057900
C 3.48185100	-1.64918600	-1.86378400	C 3.46705100	-1.32946700	-2.16629700
C -3.48503500	-1.63604300	-1.87025900	C -3.46615100	-1.33479000	-2.16432300
O -0.00167600	-1.98204600	2.36225800	O 0.00071900	-2.30915600	2.35768300
H -4.43376400	-0.91984600	-0.09982700	H -4.53677100	-0.81501200	-0.39059500
H 4.43234100	-0.92513300	-0.09748200	H 4.53711600	-0.81220100	-0.39148800
C -3.10654300	-2.50411400	0.45989400	C -3.25196900	-2.46837100	0.07249500
C 3.10460100	-2.50612900	0.47049600	C 3.25318400	-2.46691800	0.06858800
H -3.07641300	-2.28298500	1.52768300	H -3.30672700	-2.37259700	1.15809600
H 3.07487500	-2.28001400	1.53726100	H 3.30616600	-2.37257900	1.15439000
H -2.14280200	-2.93318600	0.17718200	H -2.26354800	-2.85872100	-0.17990800
H 2.14055300	-2.93600900	0.18997600	H 2.26573000	-2.85835500	-0.18583200
H -3.86970500	-3.27316700	0.30319500	H -3.99322700	-3.21395400	-0.23221300
H 3.86735900	-3.27625100	0.31713000	H 3.99592200	-3.21107600	-0.23603800
C 2.99842600	0.38372000	2.76772600	C 3.26699500	0.08532200	2.69045700
C -3.00447200	0.37481200	2.76830900	C -3.26620200	0.08766000	2.69058200
H 3.59604200	-0.53007300	2.80947000	H 3.93606700	-0.77148200	2.58180000
H -3.60446700	-0.53768300	2.80407400	H -3.93646400	-0.76844500	2.58380300
H 1.96488500	0.12822500	3.00963300	H 2.26725400	-0.28796000	2.92262500
H -1.97214600	0.11542300	3.01120800	H -2.26674000	-0.28663200	2.92227800
H 3.36696000	1.04985200	3.55421200	H 3.61537400	0.66289300	3.55239300

H -3.37308900	1.03773300	3.55746400	H -3.61296600	0.66690700	3.55204100
C 4.56807600	1.47798700	1.13002500	C 4.69325800	1.46089100	1.13546200
C -4.56777300	1.48162000	1.13299000	C -4.69257800	1.46139400	1.13409400
H 4.68366600	1.98374600	0.16876800	H 4.72673600	2.11637700	0.26250400
H -4.67962100	1.99468300	0.17518600	H -4.72623000	2.11521900	0.25986800
H 5.23917300	0.61547900	1.14551800	H 5.38346100	0.63026200	0.96644100
H -5.24076800	0.62047100	1.14028400	H -5.38307300	0.63062400	0.96697400
H 4.91257300	2.16857700	1.90650400	H 5.07531500	2.03091600	1.98828500
H -4.91294500	2.16722800	1.91357300	H -5.07409000	2.03317600	1.98598300
H 0.40772500	1.20427300	1.15176800	H 0.41225400	1.16641300	1.45531400
H 0.00475700	2.28230500	-0.94363000	H -0.00203900	2.45481800	-0.70533400
H 4.20269600	-2.46079600	-2.00664500	H 4.15915300	-2.12613600	-2.45741000
H 2.51706600	-2.00407000	-2.23009300	H 2.47191700	-1.62374800	-2.50481500
H 3.80335200	-0.81702100	-2.49191500	H 3.76223200	-0.42910000	-2.70772900
H -4.20539000	-2.44753000	-2.01627600	H -4.15732600	-2.13276800	-2.45406400
H -3.80792200	-0.80108700	-2.49398300	H -3.76238600	-0.43576400	-2.70743200
H -2.52039900	-1.98838700	-2.23943400	H -2.47069300	-1.62854500	-2.50227500
H -0.40654500	1.20453500	1.15235900	H -0.41245400	1.16587200	1.45575800
O 0.01856900	3.79074100	-0.24758800	O -0.00517400	3.84705000	0.13276200
C -0.00158600	-1.45525900	-0.98709300	C 0.00070800	-1.52042600	-1.12194700
C -0.00116900	-1.21923200	1.48697100	C 0.00059700	-1.47998400	1.53310200
Mn -0.00054400	-0.09857600	0.13363800	Re 0.00018300	-0.14651800	0.18777200
H 0.02132400	4.43270900	-0.96531500	H -0.00959600	4.55369700	-0.52150000
1Mn + H₂-interm(CH₃OH-H₂)-SMD(CH₃OH)			1Re + H₂-interm(CH₃OH-H₂)-SMD(CH₃OH)		
O 0.01641800	-2.28618300	-2.00085800	O 0.01606900	-2.38446100	-2.06862800
P -2.29018500	-0.02415500	0.03627000	P -2.40021700	0.06305300	-0.00386600
P 2.29825500	0.00285300	0.03565500	P 2.40622500	0.08880200	-0.00333800
C -2.45208400	1.39290000	-1.15385200	C -2.47040600	1.52774700	-1.14815200
C 2.44313800	1.42286400	-1.15316900	C 2.45944500	1.55675100	-1.14441900
H -2.49975500	2.30200300	-0.54848600	H -2.51560700	2.41312600	-0.50822500
H 2.47850400	2.33258000	-0.54768400	H 2.49140700	2.44183500	-0.50310000
H -3.36630400	1.33911700	-1.74608000	H -3.36938600	1.51970100	-1.76635600
H 3.35816100	1.38111700	-1.74519500	H 3.35934600	1.56191800	-1.76134700
C -1.21853500	1.42971300	-2.03499000	C -1.21959000	1.58306700	-2.00574900
C 1.20953200	1.44447100	-2.03470400	C 1.20939700	1.59792000	-2.00388200
H -1.21074800	2.35283900	-2.62867100	H -1.20336600	2.52400500	-2.56972500
H 1.19101400	2.36685000	-2.62916700	H 1.18332900	2.53865100	-2.56770700
H -1.21575300	0.58967000	-2.73482700	H -1.20628300	0.76539800	-2.73149800
H 1.21723400	0.60412100	-2.73415900	H 1.20673200	0.78051500	-2.73005300
N -0.00405700	1.35692500	-1.20219000	N -0.00507000	1.49049900	-1.16732400
C 3.11791900	0.70871400	1.57207100	C 3.26977100	0.75705200	1.52168300
C -3.11704400	0.67355400	1.57263100	C -3.26946000	0.72569000	1.52051800
H 2.52811500	1.62133800	1.72244600	H 2.63691400	1.62091400	1.75894000
H -2.53644600	1.59214200	1.72293300	H -2.64656600	1.59795900	1.75358100
C 3.45565500	-1.34352500	-0.57664300	C 3.54865000	-1.21497900	-0.71648900
C -3.43216800	-1.38489700	-0.57340900	C -3.52971100	-1.25374200	-0.71375900
C 3.47768700	-1.48069200	-2.09699400	C 3.47784600	-1.30452500	-2.23818000
C -3.45566800	-1.52455900	-2.09348300	C -3.45751000	-1.34757000	-2.23516800
O 0.01982400	-2.48167900	2.05121100	O 0.01574000	-2.65602500	2.14153600
H -4.42787400	-1.06451100	-0.25243900	H -4.53733400	-0.92460200	-0.44189600
H 4.44794600	-1.01145200	-0.25706600	H 4.55308300	-0.87767900	-0.44294200
C -3.11691400	-2.72296900	0.09228700	C -3.26666600	-2.61242400	-0.06849400
C 3.15758300	-2.68602100	0.08805400	C 3.29688800	-2.57781200	-0.07559200
H -3.10747200	-2.66057000	1.18170900	H -3.30868900	-2.57693200	1.02120800
H 3.14969800	-2.62497600	1.17755600	H 3.33887500	-2.54550100	1.01422100
H -2.14932700	-3.11319800	-0.23227200	H -2.28700500	-3.00241800	-0.35393400
H 2.19402000	-3.08717400	-0.23500900	H 2.32016700	-2.97418900	-0.36209500
H -3.87913200	-3.45670600	-0.18899500	H -4.02194500	-3.32892000	-0.40668800
H 3.92784400	-3.41034700	-0.19568900	H 4.05766300	-3.28722300	-0.41637600

C	2.95643400	-0.16321300	2.81220900	C	3.23708600	-0.19638400	2.71141100
C	-2.94666700	-0.19639700	2.81298800	C	-3.22327700	-0.22302100	2.71353300
H	3.53662300	-1.08605200	2.73967900	H	3.90831300	-1.04589400	2.56487500
H	-3.51801900	-1.12480000	2.74107600	H	-3.88482100	-1.08078400	2.57130400
H	1.91346000	-0.42805900	2.99560400	H	2.23409200	-0.58180700	2.90661600
H	-1.90112700	-0.45109700	2.99621100	H	-2.21543900	-0.59599500	2.90788500
H	3.31875000	0.38160200	3.68977300	H	3.57190200	0.33177100	3.60965200
H	-3.31393100	0.34528200	3.69043500	H	-3.56232600	0.30436600	3.61064000
C	4.57358700	1.11561900	1.36220800	C	4.68492100	1.26080500	1.25248700
C	-4.57671800	1.06575200	1.36259600	C	-4.69104600	1.21127500	1.25187200
H	4.71207600	1.73070000	0.47021100	H	4.73101200	1.95325900	0.40893300
H	-4.72084600	1.68109000	0.47168700	H	-4.74715000	1.89818600	0.40440400
H	5.23157700	0.24632000	1.28359200	H	5.37746900	0.43759700	1.05861300
H	-5.22574000	0.18992400	1.28177800	H	-5.37423000	0.37880800	1.06435100
H	4.91319700	1.70208700	2.22185900	H	5.05357100	1.79333700	2.13492900
H	-4.92292100	1.64710400	2.22309200	H	-5.06394200	1.74451100	2.13210100
H	0.40641400	0.85010800	1.33010800	H	0.40875100	0.89915300	1.56033800
H	-0.01141700	2.22066300	-0.57813400	H	-0.01262400	2.35312000	-0.52228400
H	4.19541100	-2.26066800	-2.37110300	H	4.18734100	-2.06366400	-2.58290100
H	2.50750400	-1.77603400	-2.49951300	H	2.48739400	-1.60357300	-2.58575200
H	3.79147600	-0.56235300	-2.59577900	H	3.74482900	-0.36533600	-2.72523000
H	-4.16632300	-2.31193300	-2.36484800	H	-4.16006000	-2.11422200	-2.57747700
H	-3.77927100	-0.61031100	-2.59355200	H	-3.73284800	-0.41251700	-2.72551600
H	-2.48346200	-1.81150200	-2.49717800	H	-2.46434500	-1.63883800	-2.58157800
H	-0.40760800	0.84709100	1.32881700	H	-0.41223200	0.89420900	1.56015700
O	-0.03069200	3.56599600	0.41041800	O	-0.02730500	3.62465400	0.47150400
C	-0.11025100	4.77137200	-0.27322400	C	-0.11059600	4.85711400	-0.16340200
H	0.70406300	4.91930400	-1.01330100	H	0.71011700	5.04177900	-0.88722300
H	-1.05340500	4.89982500	-0.84484700	H	-1.04892700	5.00058100	-0.73836600
H	-0.05609800	5.65519000	0.39535300	H	-0.07097200	5.71047900	0.54355600
C	0.01212000	-1.47550500	-1.17372900	C	0.01174000	-1.57244000	-1.23601200
C	0.01401400	-1.59691100	1.29956200	C	0.01187900	-1.75336900	1.39830300
Mn	0.00572500	-0.28847800	0.12631600	Re	0.00502600	-0.30662200	0.17470600
1Mn + H₂-TS(H₂O-H-H)-SMD(CH₃OH)				1Re + H₂-TS(H₂O-H-H)-SMD(CH₃OH)			
O	-0.00169000	2.94095300	0.28609700	O	0.00154900	2.98696800	-0.82133800
P	-2.28432300	-0.15425200	0.10440800	P	2.39031900	-0.20762300	-0.12891400
P	2.28465000	-0.14377800	0.10643700	P	-2.39056700	-0.20146200	-0.12904300
C	-2.43564300	-0.55409700	1.91448700	C	2.45536500	-0.98668700	-1.81928400
C	2.44083300	-0.51625800	1.92233200	C	-2.45990900	-0.96521000	-1.82639000
H	-2.44408700	-1.64452900	1.99446200	H	2.47116100	-2.06814300	-1.66055000
H	2.46398900	-1.60548300	2.01669100	H	-2.48037000	-2.04838400	-1.67676600
H	-3.36424700	-0.18501300	2.35122000	H	3.36770000	-0.72112100	-2.35545600
H	3.36393200	-0.12947800	2.35510800	H	-3.37091700	-0.69153100	-2.36061100
C	-1.22391500	-0.00166500	2.64129200	C	1.22389900	-0.60966900	-2.62506800
C	1.21987900	0.02637400	2.64106800	C	-1.22512900	-0.59004400	-2.62736900
H	-1.19952500	-0.37855700	3.67190600	H	1.19655600	-1.19718600	-3.55106600
H	1.19890400	-0.34074400	3.67531600	H	-1.20072500	-1.16972200	-3.55838700
H	-1.25858100	1.08970900	2.69126400	H	1.24329800	0.44693500	-2.90289600
H	1.23704200	1.11856800	2.68059800	H	-1.23478100	0.46902800	-2.89603600
N	0.00270200	-0.40038200	1.93086400	N	-0.00361700	-0.86183400	-1.84335500
C	3.09046900	-1.66004700	-0.65698000	C	-3.21262700	-1.52432500	0.91660400
C	-3.09362500	-1.65723900	-0.68116100	C	3.21321500	-1.51970300	0.92950900
H	2.44250100	-2.45728100	-0.27528400	H	-2.53964500	-2.37277900	0.74679400
H	-2.45038500	-2.46242100	-0.30938100	H	2.54390600	-2.37173300	0.76524600
C	3.46116600	1.27700300	-0.24924800	C	-3.56195700	1.26266800	-0.13902800
C	-3.46287100	1.27263300	-0.22005500	C	3.56217700	1.25580300	-0.15607300
C	3.49849400	2.32365500	0.86155700	C	-3.49716100	2.06163200	-1.43745300
C	-3.49071600	2.30186700	0.90724300	C	3.49163000	2.04420700	-1.46047400
O	-0.00399000	0.58211900	-3.01030000	O	0.00559100	1.24541500	3.02837300

H	-4.45358800	0.81155600	-0.27820000	H	4.56089500	0.81562800	-0.07376200
H	4.45144700	0.81525900	-0.30986500	H	-4.56050900	0.82237900	-0.05513400
C	-3.16454700	1.94794200	-1.55768400	C	3.32869000	2.17199300	1.04290900
C	3.14951900	1.93104000	-1.59434000	C	-3.32109200	2.16901600	1.06601800
H	-3.14034800	1.24351900	-2.39070500	H	3.36038500	1.64061200	1.99509700
H	3.12191800	1.21367900	-2.41606900	H	-3.35186100	1.63035100	2.01449200
H	-2.20663700	2.47270300	-1.53260500	H	2.36168100	2.67530900	0.97056500
H	2.18942200	2.45193400	-1.56981200	H	-2.35262000	2.66917600	0.99449800
H	-3.94154300	2.68834900	-1.77393900	H	4.10437600	2.94407500	1.06838600
H	3.92183800	2.67111500	-1.82774600	H	-4.09373500	2.94379900	1.09987100
C	3.02320200	-1.68672500	-2.18005000	C	-3.20789100	-1.20887300	2.40883300
C	-3.02465500	-1.66422400	-2.20441200	C	3.20492500	-1.19279300	2.41929600
H	3.68578400	-0.94157700	-2.62718400	H	-3.92356100	-0.42060100	2.65543300
H	-3.68138300	-0.90922000	-2.64355600	H	3.91677700	-0.40020000	2.66210100
H	2.01217200	-1.51243800	-2.55269400	H	-2.22289100	-0.89905900	2.76325400
H	-2.01192400	-1.49262100	-2.57357900	H	2.21788900	-0.88462700	2.76972800
H	3.34534900	-2.66781400	-2.54347000	H	-3.50015100	-2.10124000	2.97107700
H	-3.35277900	-2.63859300	-2.58046100	H	3.49915000	-2.07997600	2.98830500
C	4.51074200	-1.91879200	-0.16263900	C	-4.60930300	-1.91418700	0.44009900
C	-4.51549700	-1.91750200	-0.19182800	C	4.61203200	-1.90941600	0.45891100
H	4.58330200	-1.91532600	0.92696800	H	-4.63550500	-2.17877100	-0.61914300
H	-4.58911000	-1.92693600	0.89769600	H	4.64175100	-2.17794300	-0.59943300
H	5.21746700	-1.18185000	-0.55314800	H	-5.33355400	-1.11315800	0.61015000
H	-5.22043500	-1.17478400	-0.57466900	H	5.33541000	-1.10720900	0.62834400
H	4.84456000	-2.90198500	-0.51041000	H	-4.95378500	-2.78691700	1.00424700
H	-4.85072700	-2.89606100	-0.55107400	H	4.95517200	-2.78012400	1.02692900
H	0.01419400	-1.54641600	-0.71358400	H	-0.00644600	-1.51775100	1.12697500
H	0.01732600	-1.44321800	1.87371400	H	-0.01571300	-1.87957600	-1.56919000
H	4.21418800	3.10636600	0.58944400	H	-4.21746400	2.88448200	-1.38693100
H	2.52944200	2.80558300	1.00352900	H	-2.50998600	2.50171300	-1.59307800
H	3.82088500	1.91061200	1.81876700	H	-3.74972300	1.46215600	-2.31394000
H	-4.21005900	3.08780400	0.65457000	H	4.21125200	2.86822500	-1.41934900
H	-3.80342300	1.87318100	1.86075100	H	3.74153300	1.43800100	-2.33293500
H	-2.52108100	2.78300100	1.04803700	H	2.50344100	2.48192800	-1.61594800
H	-0.01233400	-1.90553900	0.05221900	H	0.01236700	-1.94778500	0.40581600
O	-0.07347000	-3.07734600	1.21373200	O	0.08602200	-3.34333300	-0.68040600
C	-0.00175800	1.78704700	0.14457100	C	0.00134600	1.87447300	-0.46654600
C	-0.00191500	0.35629400	-1.86891000	C	0.00359800	0.80158900	1.94574200
Mn	0.00019500	0.05881700	-0.14100700	Re	0.00022400	0.10352600	0.18515300
H	0.76606400	-3.53200800	1.08393100	H	-0.73467700	-3.80887100	-0.47479600
1Mn + H₂-TS(CH₃OH-H-H)-SMD(CH₃OH)				1Re + H₂-TS(CH₃OH-H-H)-SMD(CH₃OH)			
O	-0.01557400	-3.05293800	-0.44580800	O	-0.00655900	-3.02460700	-0.98964400
P	-2.29306600	0.01992100	-0.09370800	P	-2.40858200	0.10161700	-0.12447900
P	2.28618000	-0.00688100	-0.09318600	P	2.39686300	0.05750200	-0.10052500
C	-2.44637400	0.49043700	-1.88700900	C	-2.47280800	0.95386800	-1.77911800
C	2.43691500	0.48733400	-1.87973100	C	2.45549000	0.99492100	-1.70965300
H	-2.47473700	1.58268400	-1.92205400	H	-2.52908500	2.02574700	-1.57459100
H	2.44861000	1.58096300	-1.89907900	H	2.46605000	2.05570500	-1.44384600
H	-3.36661000	0.12158300	-2.34134100	H	-3.36495500	0.67965700	-2.34388100
H	3.36332600	0.13969800	-2.33838200	H	3.36880000	0.79030600	-2.27070700
C	-1.22494600	-0.01104200	-2.63435800	C	-1.21593800	0.65052300	-2.57780700
C	1.22131300	-0.01720300	-2.63329900	C	1.22740600	0.69377700	-2.55055200
H	-1.20496700	0.40850100	-3.64809300	H	-1.18660900	1.28917600	-3.46949900
H	1.20443500	0.40214700	-3.64717100	H	1.21142400	1.35610400	-3.42523600
H	-1.24084100	-1.09957700	-2.72783000	H	-1.20698800	-0.38897400	-2.91484200
H	1.23691300	-1.10574500	-2.72580500	H	1.24489300	-0.33578300	-2.91637800
N	-0.00083700	0.37145400	-1.90710700	N	-0.00568700	0.88671700	-1.76255100
C	3.11235600	1.44674700	0.76356900	C	3.27631000	1.23467500	1.06401900
C	-3.10652400	1.48776400	0.75198600	C	-3.24470100	1.35354700	0.99310700

H	2.48219800	2.27565600	0.42345800	H	2.62078600	2.11171700	1.01341400
H	-2.47448100	2.30909200	0.39665000	H	-2.61196600	2.23256800	0.82255100
C	3.45111300	-1.45918300	0.15488600	C	3.52698500	-1.42681700	-0.28524800
C	-3.46779400	-1.42187100	0.17520500	C	-3.56416500	-1.37123100	-0.22826000
C	3.46587400	-2.43521900	-1.01918800	C	3.44601300	-2.07255400	-1.66576000
C	-3.49558400	-2.41014300	-0.98827800	C	-3.46923800	-2.10786500	-1.56121000
O	-0.01656600	-0.87622600	2.97836900	O	-0.09625100	-1.51550400	2.96301600
H	-4.45864200	-0.96339200	0.24817600	H	-4.56766000	-0.94261300	-0.14633100
H	4.44574100	-1.00889800	0.22794900	H	4.53661300	-1.02374200	-0.15870500
C	-3.17103100	-2.14586500	1.48750200	C	-3.34513300	-2.33254600	0.93769200
C	3.15420400	-2.19426200	1.46106400	C	3.27447300	-2.45966600	0.81181000
H	-3.14957200	-1.47380300	2.34683100	H	-3.41056900	-1.84144600	1.90990900
H	3.14110400	-1.53099800	2.32739600	H	3.31417300	-2.03143500	1.81451900
H	-2.21212900	-2.66742800	1.44387600	H	-2.36846100	-2.81706500	0.87007200
H	2.19132600	-2.70820000	1.41593200	H	2.30069200	-2.93901200	0.68898100
H	-3.94690800	-2.89538100	1.67430000	H	-4.10816300	-3.11697100	0.91072500
H	3.92515100	-2.95142000	1.63701000	H	4.03839600	-3.24162100	0.75524800
C	3.03286000	1.38825300	2.28503500	C	3.30308300	0.74967700	2.50976500
C	-3.01842900	1.44751300	2.27370500	C	-3.17063000	0.99851000	2.47465300
H	3.67817900	0.60719300	2.69413300	H	4.00217300	-0.07936100	2.64350100
H	-3.66045500	0.67122400	2.69700400	H	-3.82984800	0.16375300	2.72439900
H	2.01581700	1.21216800	2.64007700	H	2.31930300	0.42705700	2.85718200
H	-1.99914400	1.27810200	2.62572400	H	-2.15721000	0.73970000	2.78824200
H	3.36989900	2.34128400	2.70527300	H	3.63595600	1.56401000	3.16083400
H	-3.35433300	2.40557900	2.68344200	H	-3.49434300	1.85782100	3.07040300
C	4.54091200	1.71036100	0.29583100	C	4.66722500	1.64989500	0.59281300
C	-4.53670900	1.75146200	0.28912900	C	-4.67117200	1.70102700	0.57686100
H	4.62418600	1.76422500	-0.79180700	H	4.66796300	2.02917200	-0.43119600
H	-4.62647300	1.78736000	-0.79878100	H	-4.74961900	1.96217900	-0.48091300
H	5.23409400	0.94438600	0.65337500	H	5.38151400	0.82471600	0.65219900
H	-5.23229000	0.99589900	0.66398600	H	-5.36376300	0.87985300	0.77917900
H	4.88405200	2.66904800	0.69840700	H	5.04340500	2.44982600	1.23863800
H	-4.87172100	2.71905400	0.67704700	H	-5.01631700	2.56490000	1.15389500
H	0.07746500	1.39584800	0.77585600	H	0.28472300	1.39186900	1.17479600
H	0.00707700	1.40213100	-1.81452800	H	-0.04063800	1.89561900	-1.43535100
H	4.18579100	-3.23301500	-0.80883100	H	4.13986200	-2.91862800	-1.70328500
H	2.49439000	-2.90809100	-1.17389800	H	2.44829400	-2.46087400	-1.87872400
H	3.77158100	-1.96358000	-1.95443700	H	3.72745500	-1.38708600	-2.46663000
H	-4.22093100	-3.19989000	-0.76642300	H	-4.18573200	-2.93567900	-1.56210700
H	-3.80168000	-1.94625900	-1.92723600	H	-3.71065700	-1.46988700	-2.41278400
H	-2.52872500	-2.89259900	-1.14213800	H	-2.47806200	-2.53590500	-1.72076500
H	-0.08090000	1.75321900	0.02091800	H	-0.24291200	1.69078300	0.62663700
O	-0.21175000	3.00694600	-1.02606800	O	-0.38909700	3.35492500	-0.69676400
C	-0.01321100	-1.90950800	-0.23942800	C	-0.01216900	-1.94049900	-0.56080700
C	-0.01266700	-0.58985800	1.85121100	C	-0.05818300	-1.00941500	1.90920100
Mn	-0.00483800	-0.19901900	0.14111000	C	0.48006000	4.19359300	-0.01918500
C	0.25976000	4.07174600	-0.27127900	H	0.78399400	3.80663700	0.97750100
H	0.45062300	3.80031800	0.78882700	H	1.42843200	4.38808600	-0.56099400
H	1.21221500	4.49259600	-0.64851100	H	0.04759600	5.19505900	0.18024400
H	-0.44964400	4.92098400	-0.23517200	Re	-0.01114100	-0.20985100	0.19213100
Mn-TS1-H⁺-SMD(CH₃OH)				Re-TS1-H⁺-SMD(CH₃OH)			
O	0.01055900	2.99064400	-0.53254000	O	-0.00092400	-2.99993200	-1.05093100
P	2.30438400	-0.04574700	-0.09645000	P	-2.41060800	0.10772300	-0.11081200
P	-2.29827400	-0.04446300	-0.08015600	P	2.40637700	0.10662600	-0.10697000
C	2.46512200	-0.68695300	-1.83183300	C	-2.48093300	1.06235800	-1.70707300
C	-2.45021500	-0.74802200	-1.79138800	C	2.46878800	1.09538100	-1.68252200
H	2.55909700	-1.77310400	-1.75550300	H	-2.56405200	2.11719200	-1.43238600
H	-2.50052600	-1.83399200	-1.67422200	H	2.53149700	2.14533600	-1.38331900
H	3.35735300	-0.31444900	-2.33722100	H	-3.35934400	0.80780900	-2.30263200

H	-3.36140300	-0.42826000	-2.29922200	H	3.35561700	0.87083300	-2.27798400
C	1.19973800	-0.33291600	-2.59478700	C	-1.20176900	0.83909200	-2.49660800
C	-1.20695200	-0.37691700	-2.58065100	C	1.19963200	0.86728900	-2.48641300
H	1.15910100	-0.92058200	-3.52331900	H	-1.16491100	1.56156000	-3.32478400
H	-1.16575500	-0.98120300	-3.49854700	H	1.16102200	1.60060000	-3.30488700
H	1.21016200	0.72326900	-2.88903900	H	-1.19916000	-0.16020400	-2.94888600
H	-1.24828500	0.67276300	-2.89470800	H	1.21443000	-0.12563300	-2.95251800
N	0.00525800	-0.60547300	-1.77686500	N	-0.00604500	1.00153400	-1.64622400
C	-3.13682800	-1.37904700	0.94754300	C	3.20986800	1.28817800	1.11228900
C	3.10753400	-1.43089800	0.89166400	C	-3.19432700	1.32088400	1.09081200
H	-2.54986400	-2.25948800	0.66740900	H	2.61716300	2.19464600	0.94487000
H	2.55922400	-2.29995200	0.51327000	H	-2.60595000	2.22367100	0.88877100
C	-3.43886100	1.44378500	0.00263200	C	3.57870500	-1.33811100	-0.31037900
C	3.46410600	1.42197500	0.04289000	C	-3.59160700	-1.33386200	-0.27979300
C	-3.39838600	2.30244000	-1.25949900	C	3.44674700	-2.00394200	-1.67740200
C	3.41376200	2.34817000	-1.17044600	C	-3.45772100	-2.03494000	-1.62893100
O	0.02361000	0.89279800	2.92893800	O	-0.00674200	-1.59590200	2.89740000
H	4.46475200	0.98166400	0.08352400	H	-4.59029900	-0.89118500	-0.22174000
H	-4.44384300	1.01942700	0.08574900	H	4.58008300	-0.90376700	-0.23724600
C	3.22125500	2.20226700	1.33301400	C	-3.42275300	-2.32863700	0.86482400
C	-3.16277600	2.28628100	1.24648700	C	3.40047300	-2.36039100	0.80844000
H	3.26655800	1.57109700	2.22201100	H	-3.52517200	-1.86427700	1.84705100
H	-3.20805500	1.70436800	2.16831600	H	3.50855900	-1.92250300	1.80208400
H	2.24752700	2.69734400	1.32089700	H	-2.44622900	-2.81736900	0.82157200
H	-2.18013500	2.76013700	1.19749300	H	2.41925400	-2.83797600	0.75472300
H	3.98526000	2.97912500	1.43996800	H	-4.18875400	-3.10667300	0.78590600
H	-3.91040000	3.08262600	1.32186300	H	4.15863700	-3.14374100	0.70874300
C	-3.00137700	-1.19466100	2.45514700	C	3.03817300	0.88431200	2.57318200
C	2.86896400	-1.35493300	2.39596500	C	-2.99655300	0.95470600	2.55834500
H	-3.57826100	-0.34026600	2.81658200	H	3.64732000	0.01481400	2.83068700
H	3.38245700	-0.50515900	2.85181000	H	-3.59527800	0.08756800	2.84649100
H	-1.96337200	-1.06264500	2.76504700	H	1.99876200	0.65481300	2.81744700
H	1.80820500	-1.28459000	2.64208800	H	-1.95190600	0.73749300	2.79136800
H	-3.38692900	-2.08417300	2.96398500	H	3.35842700	1.70813500	3.21911700
H	3.25783100	-2.26199300	2.87019400	H	-3.31204500	1.79213900	3.18889200
C	-4.58907300	-1.63657100	0.55227300	C	4.66622600	1.60604800	0.78626900
C	4.58701500	-1.63335400	0.57517900	C	-4.65665800	1.62813300	0.78160900
H	-4.71495600	-1.77876700	-0.52354600	H	4.80980800	1.88471400	-0.26044200
H	4.78637700	-1.67824900	-0.49828900	H	-4.81777500	1.88144300	-0.26906300
H	-5.24824700	-0.82399400	0.86843700	H	5.32184000	0.75985300	1.00724400
H	5.20495200	-0.84059000	1.00468400	H	-5.30630500	0.78582200	1.03302300
H	-4.94135200	-2.54807200	1.04620900	H	5.00322000	2.44764500	1.39999700
H	4.92545200	-2.57893600	1.01120500	H	-4.98569800	2.48363700	1.38019100
H	-0.16011600	-2.38658800	0.56219600	H	-0.03165000	2.24988100	-1.31339800
H	0.03244700	-1.84024500	-1.56631200	H	4.15979600	-2.83235800	-1.74098500
C	-0.06827400	-3.32529500	-0.03558400	H	2.44900100	-2.41886200	-1.83217100
H	-4.10788100	3.12911500	-1.14994900	H	3.66807200	-1.32126500	-2.49931300
H	-2.41255300	2.73893900	-1.42882600	H	-4.17074300	-2.86466700	-1.67220700
H	-3.68521800	1.74526400	-2.15309300	H	-3.67777400	-1.37413000	-2.46880200
H	4.13573400	3.15879300	-1.02716300	H	-2.45984200	-2.45366000	-1.77150000
H	3.68007000	1.83879700	-2.09804600	O	-0.07051800	3.44738000	-1.10577100
H	2.43182500	2.80589700	-1.29980700	C	-0.00169900	-1.91766600	-0.58228900
O	0.06042800	-3.08855400	-1.39928600	Re	-0.00245900	-0.22950900	0.14568600
H	-0.96449400	-3.91885800	0.21096300	C	-0.00429300	-1.06032100	1.85310900
C	0.00988800	1.85372000	-0.27132900	C	0.08525100	3.66701500	0.26389200
Mn	0.00759700	0.17151900	0.09575000	H	1.03349200	4.17372300	0.50687000
C	0.01653200	0.56489100	1.81110800	H	-0.72093700	4.29073200	0.68108200
H	0.79506400	-3.86389600	0.38910300	H	0.08023400	2.72585000	0.84824000
3Mn⁺-OCH₃⁻-SMD(CH₃OH)				3Re⁺-OCH₃⁻-SMD(CH₃OH)			

O	-0.01126200	2.97492800	0.05708500	O	0.00799400	3.01645700	-0.83141900
P	2.30471500	-0.05235400	-0.12605400	P	2.41250600	-0.11422000	-0.11308500
P	-2.31032100	-0.06041000	-0.13151500	P	-2.41171200	-0.11479200	-0.12047700
C	2.45918000	-0.34016100	-1.95521700	C	2.46831300	-0.99314900	-1.75348200
C	-2.45668500	-0.37367700	-1.95747000	C	-2.46306500	-0.99878300	-1.75845000
H	2.52761900	-1.42235900	-2.09444000	H	2.48914900	-2.06289100	-1.52758800
H	-2.51183600	-1.45812900	-2.08490700	H	-2.48705500	-2.06863500	-1.53386700
H	3.36085500	0.10484000	-2.37821300	H	3.37323100	-0.75836500	-2.31638900
H	-3.36302400	0.05526900	-2.38727400	H	-3.36566200	-0.76052000	-2.32379200
C	1.21302300	0.18563400	-2.64172400	C	1.22491200	-0.67463600	-2.56760800
C	-1.21613800	0.16041700	-2.64784900	C	-1.21735100	-0.68012300	-2.56988900
H	1.18487900	-0.16156600	-3.68243200	H	1.19348200	-1.32381300	-3.45194000
H	-1.18161600	-0.19728000	-3.68480200	H	-1.18211400	-1.33160900	-3.45238100
H	1.20751400	1.27824600	-2.66082200	H	1.23812100	0.35993000	-2.91932000
H	-1.22563000	1.25277100	-2.67848100	H	-1.23227900	0.35342900	-2.92438500
N	0.00120200	-0.27020000	-1.92931100	N	0.00366000	-0.88478400	-1.75978600
C	-3.20618900	-1.55528200	0.57507900	C	-3.26743600	-1.33681500	1.01721900
C	3.21842400	-1.54373000	0.56336200	C	3.26490200	-1.34098000	1.02057700
H	-2.71943100	-2.37026200	0.03088000	H	-2.67663100	-2.24039500	0.83226500
H	2.70971800	-2.36255400	0.04564100	H	2.61071600	-2.21447400	0.91848100
C	-3.42734100	1.40206200	0.24437800	C	-3.55565100	1.35893700	-0.28767300
C	3.40842200	1.41460600	0.27626200	C	3.55092600	1.36786000	-0.25051200
C	-3.34766800	2.51298700	-0.79945300	C	-3.38382600	2.08956200	-1.61692100
C	3.34420900	2.53086600	-0.76301800	C	3.42905300	2.08131500	-1.59438300
O	-0.00518600	0.23862500	3.03476800	O	-0.00538200	1.39511800	2.99555000
H	4.42260900	1.00571400	0.25841600	H	4.56047900	0.95184300	-0.17504700
H	-4.43977500	0.99009500	0.21030400	H	-4.56283400	0.93131800	-0.26469300
C	3.13105200	1.95049600	1.67956400	C	3.33645700	2.34677700	0.90196400
C	-3.17620300	1.94370400	1.65043500	C	-3.40422800	2.32339000	0.88601800
H	3.18693800	1.17335200	2.44355800	H	3.42287100	1.87421000	1.88143600
H	-3.24868800	1.16907100	2.41586400	H	-3.56420400	1.84113600	1.85149700
H	2.14456800	2.41443900	1.74599000	H	2.35356300	2.81879500	0.84072700
H	-2.19010200	2.40610100	1.73425700	H	-2.41217200	2.78108100	0.89727200
H	3.87312300	2.71497400	1.93167800	H	4.08962400	3.13939700	0.84908200
H	-3.92163200	2.71032200	1.88541200	H	-4.14079400	3.12773700	0.79252000
C	-2.95813400	-1.77970100	2.06237000	C	-3.13417200	-0.99375400	2.49764500
C	3.02670700	-1.74795900	2.06235900	C	3.25688700	-0.91947800	2.48651800
H	-3.41095200	-0.99856700	2.67730200	H	-3.74181300	-0.12923500	2.77400800
H	3.54017200	-0.98129500	2.64741200	H	3.95335400	-0.09903800	2.67472900
H	-1.89319300	-1.82337800	2.29644500	H	-2.09958200	-0.78627100	2.77908800
H	1.97349400	-1.74465600	2.34819100	H	2.26464100	-0.60941700	2.82087900
H	-3.40405000	-2.73238900	2.36600400	H	-3.48052000	-1.84015700	3.09918600
H	3.44756300	-2.71533800	2.35491100	H	3.57112900	-1.76240200	3.10993800
C	-4.69535300	-1.60437000	0.24174600	C	-4.71590200	-1.62886300	0.63677100
C	4.69522000	-1.60322800	0.17964200	C	4.66628800	-1.73650200	0.56359200
H	-4.89501600	-1.42595100	-0.81774600	H	-4.82991000	-1.88220600	-0.41993400
H	4.86024200	-1.44543500	-0.88883500	H	4.69035200	-2.07240100	-0.47530600
H	-5.26844700	-0.87888500	0.82448500	H	-5.37112300	-0.78251400	0.85809800
H	5.28921000	-0.86879000	0.72931600	H	5.37595900	-0.91236700	0.67317100
H	-5.08609600	-2.59727900	0.48687000	H	-5.07931600	-2.48157900	1.21927600
H	5.09205100	-2.59242100	0.43010300	H	5.03026900	-2.56217500	1.18356500
H	-0.11476900	-1.77641400	0.20492800	H	-0.18499600	-2.38807100	0.71858300
H	0.01561300	-1.33048400	-1.93319400	H	0.00422800	-1.94153400	-1.48978500
C	-0.00788800	-2.87430500	-0.22014000	C	-0.05931400	-3.42231700	0.29049900
H	-4.04785200	3.30878500	-0.52464000	H	-4.10501400	2.91191000	-1.66509000
H	-2.35417700	2.95925900	-0.85585900	H	-2.38757500	2.52327300	-1.71953400
H	-3.62676100	2.16802900	-1.79663500	H	-3.57046200	1.44493500	-2.47731200
H	4.03704300	3.32715700	-0.47156100	H	4.13871700	2.91460800	-1.62027300
H	3.64147500	2.19251100	-1.75716900	H	3.66245100	1.43053900	-2.43848100
H	2.35048400	2.97472000	-0.83427400	H	2.43139900	2.49842200	-1.74439000

O 0.05167700 -2.95593500 -1.55686100	O -0.01524700 -3.45108200 -1.08595600
H -0.89286700 -3.34387200 0.24594300	H -0.90581100 -3.99259400 0.72133600
C -0.00568900 1.81018600 0.06549900	C 0.00649500 1.90483200 -0.44347700
Mn -0.00489500 0.07841200 0.12160000	Re 0.00170700 0.17238100 0.18045300
C -0.00472100 0.14795600 1.87459500	C -0.00178600 0.90852500 1.92964400
H 0.88159200 -3.23572200 0.32365100	H 0.85267900 -3.81852700 0.77856700
Mn-TS1-H-SMD(CH₃OH)	Re-TS1-H-SMD(CH₃OH)
O -0.03791100 3.05539500 -0.24882500	O -0.00045500 -3.15254300 -0.42905000
P 2.26636600 -0.02310900 -0.09065300	P -2.38695800 0.10089800 -0.15205600
P -2.27919100 -0.06909800 -0.09325500	P 2.38669500 0.10035800 -0.15187300
C 2.44405800 -0.48027500 -1.88826600	C -2.46103100 0.67110000 -1.92646300
C -2.43036100 -0.58970600 -1.87510000	C 2.46113700 0.67031500 -1.92635900
H 2.49620500 -1.57209900 -1.93414600	H -2.48760400 1.76476400 -1.90238100
H -2.42086500 -1.68414300 -1.88676900	H 2.48827200 1.76396200 -1.90255400
H 3.35943500 -0.09107100 -2.33587900	H -3.36899400 0.33508200 -2.42971600
H -3.36515700 -0.26487700 -2.33456800	H 3.36896200 0.33374200 -2.42948700
C 1.21702300 0.00086100 -2.63791500	C -1.22756300 0.21023800 -2.68229400
C -1.22944600 -0.06548200 -2.63820500	C 1.22753300 0.20977500 -2.68220500
H 1.20834600 -0.40692800 -3.65696000	H -1.20698800 0.66648300 -3.67930500
H -1.20635300 -0.48749100 -3.65118400	H 1.20713200 0.66593300 -3.67926000
H 1.20269200 1.09018100 -2.71502100	H -1.22367300 -0.87396400 -2.80877500
H -1.26482500 1.02217200 -2.73113600	H 1.22332800 -0.87443700 -2.80856700
N 0.00403600 -0.41819600 -1.91128700	N 0.00002000 0.57887000 -1.94048100
C -3.17943800 -1.48498900 0.76229300	C 3.30198400 1.49428600 0.71430800
C 3.18169500 -1.45339400 0.72311100	C -3.30201900 1.49513000 0.71396600
H -2.62263500 -2.34415900 0.37623600	H 2.73059200 2.36262400 0.37084200
H 2.64927700 -2.30771000 0.29350700	H -2.73027700 2.36328300 0.37063000
C -3.45021600 1.39325700 0.09413900	C 3.52723000 -1.38633800 -0.02753300
C 3.40863700 1.45329200 0.15562800	C -3.52794200 -1.38546100 -0.02791200
C -3.40201800 2.36736600 -1.08058500	C 3.42101600 -2.32680900 -1.22503700
C 3.35119300 2.46424600 -0.98698500	C -3.42125500 -2.32633000 -1.22506900
O -0.00919500 0.58528400 3.02149500	O -0.00003900 -0.79797600 3.18660200
H 4.41840500 1.03338000 0.17495300	H -4.53989800 -0.97028400 -0.01562400
H -4.45246800 0.95601600 0.11909400	H 4.53927600 -0.97141500 -0.01450100
C 3.14636700 2.13771600 1.49634800	C -3.29576500 -2.14243200 1.27814400
C -3.21205700 2.12616500 1.41358200	C 3.29415000 -2.14368500 1.27817100
H 3.19201500 1.44532700 2.33896700	H -3.37239000 -1.49976100 2.15676500
H -3.24504200 1.46056300 2.27794600	H 3.36893200 -1.50106800 2.15699200
H 2.16588900 2.61934200 1.51220700	H -2.30951700 -2.61260800 1.29319000
H -2.24429900 2.63262800 1.41854800	H 2.30837000 -2.61487300 1.29185600
H 3.89890200 2.91477000 1.66690200	H -4.04427200 -2.93492600 1.38103900
H -3.98434000 2.88954000 1.55558000	H 4.04335500 -2.93540000 1.38198300
C -3.03654100 -1.48590200 2.27994000	C 3.19803700 1.43669500 2.23414400
C 3.01337700 -1.51327200 2.23708100	C -3.19853800 1.43752500 2.23383200
H -3.59378200 -0.66754200 2.74226600	H 3.79608500 0.62239500 2.65023700
H 3.55379800 -0.70670500 2.73866700	H -3.79756500 0.62387600 2.64976600
H -1.99392700 -1.40946400 2.59313200	H 2.16623900 1.30839200 2.56895500
H 1.96500800 -1.45770500 2.53509700	H -2.16699000 1.30813700 2.56899800
H -3.43703800 -2.42065000 2.68633200	H 3.57565600 2.36990700 2.66461900
H 3.41707600 -2.45810200 2.61595200	H -3.57528900 2.37115400 2.66416100
C -4.63772000 -1.65131200 0.34334300	C 4.74712100 1.67426100 0.25800500
C 4.65013900 -1.57600500 0.32450200	C -4.74697200 1.67567500 0.25728900
H -4.76856300 -1.62676600 -0.74099300	H 4.84411900 1.69808100 -0.82990400
H 4.79899200 -1.51340900 -0.75607600	H -4.84366400 1.69972500 -0.83063800
H -5.27845000 -0.88162900 0.78112900	H 5.39669900 0.88300200 0.64065100
H 5.26660700 -0.80793300 0.79838900	H -5.39696500 0.88459900 0.63960400
H -5.01053400 -2.61861100 0.69650300	H 5.13514600 2.62340400 0.64211400
H 5.03684500 -2.54662400 0.65275800	H -5.13476700 2.62488700 0.64146200
H -0.01398500 -1.45247100 0.47113600	H -0.00040300 1.62395000 0.57422400

H	0.03276100	-1.43770600	-1.85789900	H	0.00028300	1.60024600	-1.85830000
C	0.07024700	-3.43572600	-0.14148100	C	0.00175900	3.42463700	0.03575100
H	-4.10891500	3.18390600	-0.89822300	H	4.10305100	-3.17070200	-1.07775700
H	-2.41466500	2.81480700	-1.20572700	H	2.41547300	-2.73638700	-1.33626600
H	-3.68769600	1.89895300	-2.02420900	H	3.70143500	-1.84426900	-2.16305400
H	4.04286900	3.28622400	-0.77322100	H	-4.10366900	-3.16994400	-1.07796100
H	3.65140500	2.03268300	-1.94354800	H	-3.70092100	-1.84396000	-2.16340000
H	2.35725800	2.89876700	-1.10423400	H	-2.41577500	-2.73627200	-1.33550700
O	0.25030500	-3.49083300	-1.35145100	O	0.00442500	3.52777000	-1.19202300
H	-0.93677300	-3.50563700	0.29318900	H	0.92894800	3.50537000	0.62042600
C	-0.02444700	1.88885900	-0.14578700	C	-0.00031800	-1.99589600	-0.22426100
Mn	-0.00999000	0.16236500	0.14436000	Re	-0.00016100	-0.14358600	0.19809500
C	-0.01049700	0.41043800	1.86407700	C	-0.00015300	-0.54917300	2.03665900
H	0.90482400	-3.49408100	0.57184300	H	-0.92779100	3.50623000	0.61654000
Mn-TS(CH₃OH)-SMD(CH₃OH)				Re-TS(CH₃OH)-SMD(CH₃OH)			
P	2.32585300	0.05326200	0.15267700	P	-2.42289400	-0.05387700	0.21594300
P	-2.29093500	0.04152900	0.13792900	P	2.40522500	-0.02579600	0.20084200
C	2.46551900	0.13207600	2.00645500	C	-2.46638700	-0.38638400	2.04620900
C	-2.42031000	0.26125700	1.97835800	C	2.44959900	-0.43561200	2.01365600
H	2.53792600	1.19213900	2.26465200	H	-2.50981400	-1.47298100	2.15904800
H	-2.41550200	1.34150300	2.15312400	H	2.47255700	-1.52746300	2.07741500
H	3.36724800	-0.35790100	2.37715400	H	-3.36468000	0.02783200	2.50816000
H	-3.35155600	-0.13358700	2.38845900	H	3.35798800	-0.06122900	2.49044200
C	1.20668800	-0.46105900	2.62245000	C	-1.20438000	0.14661200	2.71045100
C	-1.19830800	-0.36637100	2.63181900	C	1.20240300	0.08966200	2.70931200
H	1.18162400	-0.20890500	3.69487900	H	-1.14810800	-0.26149600	3.73123100
H	-1.16807300	-0.07139800	3.69326800	H	1.14890900	-0.35643100	3.71431100
H	1.24318600	-1.56038700	2.56889300	H	-1.26155500	1.23854400	2.81875100
H	-1.29235400	-1.46306100	2.62495700	H	1.28142400	1.17499300	2.85997200
N	0.01928900	0.05368300	1.95355000	N	-0.00849700	-0.23678800	1.96009800
C	-3.24606100	1.52041000	-0.52371100	C	3.42976200	-1.40905400	-0.54915500
C	3.21188200	1.62881000	-0.36460800	C	-3.41832800	-1.48963200	-0.47282300
H	-2.59403900	2.35517100	-0.25875100	H	2.82058700	-2.28244600	-0.29570900
H	2.58689800	2.38478200	0.11839300	H	-2.80845300	-2.33949000	-0.15007200
C	-3.38864400	-1.41900500	-0.31823900	C	3.44834900	1.52527800	0.03622100
C	3.46095500	-1.33298600	-0.41981600	C	-3.48541700	1.47224700	-0.02016000
C	-3.37250900	-2.54579100	0.71174700	C	3.10690800	2.57295200	1.09393700
C	3.46433100	-2.54585800	0.50794600	C	-3.15971900	2.56722300	0.99343500
O	0.02133200	0.15193700	-3.03174100	O	-0.02548900	-0.49891300	-3.23756900
H	4.46413800	-0.89608900	-0.39806400	H	-4.50679100	1.12792300	0.17266000
H	-4.40033400	-1.00122800	-0.33851400	H	4.47085900	1.18055400	0.22296600
C	3.14985900	-1.74905200	-1.85728700	C	-3.41712200	2.01613100	-1.44547000
C	-3.06867400	-1.95827700	-1.71223900	C	3.39116300	2.13433900	-1.36328700
H	3.14657600	-0.90572700	-2.54974400	H	-3.68959500	1.27193000	-2.19413500
H	-3.06838600	-1.18137000	-2.47734500	H	3.65996300	1.42536400	-2.14647300
H	2.17941900	-2.24506100	-1.92983900	H	-2.41917400	2.38660900	-1.68777000
H	-2.09721600	-2.45470600	-1.73907300	H	2.39907800	2.52751100	-1.59156400
H	3.90861300	-2.45785500	-2.20521300	H	-4.11393500	2.85484100	-1.54572000
H	-3.82318000	-2.69965400	-1.99592600	H	4.09657600	2.96998000	-1.42000200
C	-3.39597900	1.51891700	-2.04264000	C	3.53329000	-1.34291300	-2.07035600
C	3.18066600	1.88811400	-1.86759100	C	-3.48713600	-1.51813900	-1.99694100
H	-4.11289400	0.76588300	-2.37882500	H	4.24684500	-0.58130700	-2.39207400
H	3.81528700	1.18640000	-2.41466400	H	-4.18672100	-0.77412700	-2.38462200
H	-2.44819700	1.34540500	-2.55575600	H	2.57312600	-1.13409500	-2.54481000
H	2.17089500	1.82838500	-2.27816100	H	-2.51407400	-1.34618700	-2.45946200
H	-3.77520300	2.49280400	-2.36896400	H	3.89186200	-2.30352000	-2.45340700
H	3.56222400	2.89419300	-2.07117700	H	-3.84384100	-2.49907700	-2.32678500
C	-4.59671900	1.74336000	0.15373200	C	4.80658400	-1.58629700	0.08547200
C	4.63232700	1.75654500	0.18067600	C	-4.80821600	-1.63586600	0.14090100

H -4.51064900	1.85661400	1.23621400	H 4.75935000	-1.70006100	1.17050400
H 4.68931800	1.58789700	1.25844800	H -4.78617900	-1.67056400	1.23225300
H -5.29767000	0.92861600	-0.04820600	H 5.46893000	-0.74683300	-0.14148300
H 5.32309000	1.06407800	-0.30804400	H -5.47357100	-0.82299900	-0.16170900
H -5.04982300	2.66108100	-0.23604600	H 5.27852500	-2.48817500	-0.31829800
H 5.00376000	2.76890200	-0.01075200	H -5.26088700	-2.57022400	-0.20724300
H 0.09930900	1.36306400	1.50194900	H -0.10890300	-1.56835900	1.52344600
H -4.05443700	-3.33820300	0.38555300	H 3.75096300	3.44672300	0.95087900
H 4.15243700	-3.29925100	0.11013100	H -3.81144500	3.42808400	0.81196400
H -2.38154900	-2.99164400	0.81578300	H 2.07192300	2.91324000	1.01412000
H 2.47998400	-3.01128400	0.58240700	H -2.12776000	2.91303500	0.90332300
H -3.70548300	-2.21643600	1.69753100	H 3.27284700	2.21067100	2.10992600
H 3.80256000	-2.29792100	1.51561100	H -3.32558600	2.24625500	2.02319600
O 0.22571200	2.05898100	0.62433600	O -0.32421600	-2.32024700	0.71615200
C 0.01847400	0.12258900	-1.86383100	C -0.02034900	-0.29394300	-2.08096900
C -0.41711500	3.31019900	0.70935800	C 0.48369400	-3.48018200	0.69370900
H 0.20464900	4.02087800	1.27064900	H 0.00144500	-4.29593600	1.24869600
H -0.57551700	3.72551800	-0.29101900	H 0.63008300	-3.82080600	-0.33613100
H -1.38891400	3.25272200	1.21567600	H 1.47028200	-3.31120300	1.14098200
C 0.02388700	-1.75473700	-0.23387700	C -0.00701900	1.83575900	-0.54130100
O 0.04028600	-2.92203600	-0.27926800	O -0.01340400	2.99676600	-0.74830000
Mn 0.01491200	-0.03311700	-0.11809700	Re -0.01199700	0.01772800	-0.21118000
2Mn-OCH₃-SMD(CH₃OH)			2Re-OCH₃-SMD(CH₃OH)		
N -0.66955200	1.92262600	0.00000000	N -0.57033300	2.02230700	0.00000000
H 3.23841200	-0.22536000	0.88030000	H 3.30734400	-0.35556000	0.88218000
H 0.26468900	2.33908100	0.00000000	H 0.36016900	2.44741700	0.00000000
C 3.04994600	0.41410500	0.00000000	C 3.15345100	0.28845500	0.00000000
P 0.00490900	0.21251300	2.31556100	P 0.00568000	0.26926200	2.40526500
P 0.00490900	0.21251300	-2.31556100	P 0.00568000	0.26926200	-2.40526500
C 1.62527000	0.23564000	-3.26593300	C 1.62915300	0.26938100	-3.34497400
C 1.62527000	0.23564000	3.26593300	C 1.62915300	0.26938100	3.34497400
C -1.15236100	-0.75547900	-3.44259600	C -1.20042300	-0.62611300	-3.53054900
C -1.15236100	-0.75547900	3.44259600	C -1.20042300	-0.62611300	3.53054900
O -2.63040500	-1.25275000	0.00000000	O -2.81683600	-1.25383900	0.00000000
C -0.52292000	1.99255400	2.43267600	C -0.45432400	2.07524100	2.45288600
C -0.52292000	1.99255400	-2.43267600	C -0.45432400	2.07524100	-2.45288600
H 0.39686300	2.58517400	2.41818500	H 0.48959900	2.62913200	2.44778700
H 0.39686300	2.58517400	-2.41818500	H 0.48959900	2.62913200	-2.44778700
H -1.04349800	2.22168200	3.36355400	H -0.98245300	2.34518100	3.36856100
H -1.04349800	2.22168200	-3.36355400	H -0.98245300	2.34518100	-3.36856100
C -1.36641100	2.34745800	1.22404300	C -1.26557700	2.45950300	1.22886600
C -1.36641100	2.34745800	-1.22404300	C -1.26557700	2.45950300	-1.22886600
H -1.55605100	3.42832100	1.19892900	H -1.41312100	3.54590900	1.20509900
H -1.55605100	3.42832100	-1.19892900	H -1.41312100	3.54590900	-1.20509900
H -2.33511600	1.84341600	1.25370600	H -2.25111300	1.98990600	1.23859100
H -2.33511600	1.84341600	-1.25370600	H -2.25111300	1.98990600	-1.23859100
H 2.27085000	0.80838000	-2.59397100	H 2.28193400	0.82027500	-2.66040100
H 2.27085000	0.80838000	2.59397100	H 2.28193400	0.82027500	2.66040100
O 1.15696100	-2.76734100	0.00000000	O 1.00237100	-3.04794100	0.00000000
H -0.75076700	-0.60348900	4.44972200	H -0.82520200	-0.44664800	4.54308200
H -0.75076700	-0.60348900	-4.44972200	H -0.82520200	-0.44664800	-4.54308200
C -1.10671200	-2.25184700	3.13171200	C -1.18964600	-2.13207100	3.27133000
C -1.10671200	-2.25184700	-3.13171200	C -1.18964600	-2.13207100	-3.27133000
H -0.09078800	-2.64876200	3.11358200	H -0.18462700	-2.55609800	3.27346400
H -0.09078800	-2.64876200	-3.11358200	H -0.18462700	-2.55609800	-3.27346400
H -1.56931800	-2.47505800	2.16815300	H -1.65246600	-2.37208200	2.31174900
H -1.56931800	-2.47505800	-2.16815300	H -1.65246600	-2.37208200	-2.31174900
H -1.66186500	-2.80204500	3.89877900	H -1.76521700	-2.63936400	4.05256100
H -1.66186500	-2.80204500	-3.89877900	H -1.76521700	-2.63936400	-4.05256100

C	2.22948900	-1.15436100	-3.44579200
C	2.22948900	-1.15436100	3.44579200
H	1.67565100	-1.73827900	-4.18573000
H	1.67565100	-1.73827900	4.18573000
H	2.25765300	-1.72433500	-2.51524400
H	2.25765300	-1.72433500	2.51524400
H	3.25768800	-1.06262500	-3.81070600
H	3.25768800	-1.06262500	3.81070600
C	1.55930500	0.96827800	-4.60439300
C	1.55930500	0.96827800	4.60439300
H	1.20760800	1.99698100	-4.50617300
H	1.20760800	1.99698100	4.50617300
H	0.91261500	0.45493600	-5.32140300
H	0.91261500	0.45493600	5.32140300
H	2.56130700	1.00751600	-5.04488000
H	2.56130700	1.00751600	5.04488000
C	-2.59239400	-0.24808500	3.43541600
H	-2.67215200	0.78969000	3.76410400
H	-3.05274700	-0.33175500	2.44896800
H	-3.18955600	-0.85370600	4.12542600
C	-2.59239400	-0.24808500	-3.43541600
H	-3.05274700	-0.33175500	-2.44896800
H	-2.67215200	0.78969000	-3.76410400
H	-3.18955600	-0.85370600	-4.12542600
O	1.79267800	1.00553200	0.00000000
H	3.23841200	-0.22536000	-0.88030000
C	-1.56339500	-0.77180900	0.00000000
Mn	0.03139800	-0.07832600	0.00000000
C	0.72974300	-1.68061700	0.00000000
H	3.84556800	1.18043700	0.00000000
Mn-TS(H₂O)-SMD(CH₃OH)			
P	-2.30092100	0.06218900	-0.22374700
P	2.30679400	0.05350900	-0.25212600
C	-2.44517900	-0.62526100	-1.94580200
C	2.44846600	-0.65502400	-1.96565400
H	-2.49114600	0.23886600	-2.61522200
H	2.51234300	0.19650500	-2.64942100
H	-3.35857100	-1.20413700	-2.09416400
H	3.35279100	-1.25153900	-2.09974900
C	-1.20006100	-1.44249500	-2.25058500
C	1.19034900	-1.45727900	-2.25865800
H	-1.17788000	-1.66727000	-3.32977800
H	1.15637200	-1.68487400	-3.33687900
H	-1.26035700	-2.41772700	-1.73973000
H	1.24344800	-2.43174600	-1.74570700
N	0.00110500	-0.71982500	-1.85778700
C	3.18766500	1.70771000	-0.46627600
C	-3.17241900	1.71910100	-0.41332800
H	2.71305000	2.09898000	-1.37358100
H	-2.55584900	2.19745400	-1.18026500
C	3.45087500	-0.96240500	0.83753500
C	-3.43751700	-0.95212500	0.87831600
C	3.38052200	-2.46221600	0.55979000
C	-3.45628100	-2.43907500	0.53192000
O	0.04046700	1.45970400	2.62266600
H	-4.43956000	-0.55465800	0.69130300
H	4.45847800	-0.62680600	0.57665800
C	-3.10753200	-0.74320000	2.35609600
C	3.21079700	-0.66815400	2.31686300
C	2.20409200	-1.13172300	-3.53402200
C	2.20409200	-1.13172300	3.53402200
H	1.64717900	-1.69424000	-4.28796800
H	1.64717900	-1.69424000	4.28796800
H	2.20620400	-1.71145800	-2.60877400
H	2.20620400	-1.71145800	2.60877400
H	3.23878000	-1.05833800	-3.88386400
H	3.23878000	-1.05833800	3.88386400
C	1.58479700	1.01996900	-4.67401700
C	1.58479700	1.01996900	4.67401700
H	1.24456600	2.05155600	-4.56560000
H	1.24456600	2.05155600	4.56560000
H	0.93854100	0.52321800	-5.40278800
H	0.93854100	0.52321800	5.40278800
H	2.59115200	1.05240100	-5.10451800
H	2.59115200	1.05240100	5.10451800
C	-2.62168000	-0.07551800	3.44848400
H	-2.68361500	0.97049400	3.75423800
H	-3.03497800	-0.16557200	2.44179300
H	-3.26844200	-0.64967000	4.12010200
C	-2.62168000	-0.07551800	-3.44848400
H	-3.03497800	-0.16557200	-2.44179300
H	-2.68361500	0.97049400	-3.75423800
H	-3.26844200	-0.64967000	-4.12010200
O	1.92003100	0.93927000	0.00000000
H	3.30734400	-0.35556000	-0.88218000
C	-1.71921300	-0.81917000	0.00000000
Re	0.02877700	-0.14554200	0.00000000
C	0.64526800	-1.92762400	0.00000000
H	3.97705000	1.02220600	0.00000000
Re-TS(H₂O)-SMD(CH₃OH)			
P	2.39960600	0.03706300	0.27965000
P	-2.40310500	0.04599700	0.30427200
C	2.45363300	-0.59925800	2.02826500
C	-2.45517900	-0.60053000	2.05000000
H	2.47194300	0.28637100	2.67030000
H	-2.48580000	0.27768200	2.70203400
H	3.36483700	-1.16625100	2.22796200
H	-3.36086100	-1.17999300	2.23991000
C	1.20636600	-1.41846500	2.33278200
C	-1.20270600	-1.41527900	2.34636200
H	1.16871600	-1.60412800	3.41771500
H	-1.15447000	-1.59828100	3.43133300
H	1.27724700	-2.40772900	1.85525800
H	-1.27824700	-2.40578100	1.87233200
N	-0.00015900	-0.71678300	1.90413300
C	-3.31088500	1.68497100	0.47366000
C	3.27824700	1.68929400	0.43246300
H	-2.78119900	2.14714600	1.31465600
H	2.59911200	2.23017400	1.09927000
C	-3.53321900	-1.06966100	-0.69269500
C	3.52899200	-1.05830900	-0.73830200
C	-3.32036900	-2.54698900	-0.37236300
C	3.39549700	-2.53332800	-0.37000900
O	-0.00605700	1.65970200	-2.77307100
H	4.54410500	-0.73281300	-0.48947900
H	-4.54728400	-0.80120400	-0.38120900
C	3.30134600	-0.85260500	-2.23502700
C	-3.39700600	-0.81020700	-2.19099400

H	-3.07300800	0.31101100	2.63591100	H	3.36607400	0.19419100	-2.53398200
H	3.28061900	0.39592800	2.54937800	H	-3.58912400	0.23033100	-2.45731400
H	-2.14593300	-1.19032400	2.61661400	H	2.32195300	-1.22655500	-2.54018300
H	2.22705600	-1.01783700	2.63883000	H	-2.39852000	-1.06964300	-2.55054600
H	-3.87346600	-1.22372700	2.97373400	H	4.05990600	-1.40542000	-2.79878700
H	3.96155100	-1.18749100	2.92143200	H	-4.11831300	-1.42803200	-2.73574800
C	2.92373100	2.70274400	0.65855400	C	-3.14452200	2.60437600	-0.73117200
C	-3.12016500	2.59222800	0.83619500	C	3.35363000	2.45958300	-0.88204700
H	3.37712100	2.38627100	1.60068900	H	-3.67617400	2.23072500	-1.60897900
H	-3.74786200	2.19554300	1.63821300	H	4.08096900	2.01961500	-1.56855000
H	1.85587900	2.85139000	0.82790300	H	-2.09427700	2.73342300	-0.99893400
H	-2.10397300	2.70307100	1.21891800	H	2.38752100	2.50521000	-1.38854100
H	3.35802700	3.67361500	0.39805000	H	-3.55628700	3.59154500	-0.49763900
H	-3.49526700	3.59296700	0.59761500	H	3.67589100	3.48697800	-0.68449700
C	4.67970000	1.58513100	-0.76578800	C	-4.77624100	1.54032600	0.87460800
C	-4.59779400	1.61427600	-0.95034700	C	4.64822100	1.60696200	1.10017900
H	4.89225500	0.85470200	-1.55050300	H	-4.91403000	0.87146200	1.72775000
H	-4.66338700	1.00875000	-1.85706300	H	4.61545000	1.10915400	2.07159000
H	5.24947200	1.30580800	0.12404800	H	-5.38516200	1.16729800	0.04726700
H	-5.28569300	1.19519800	-0.21126600	H	5.37545900	1.08401000	0.47324400
H	5.06347400	2.55286400	-1.10493900	H	-5.17635000	2.51955400	1.15649500
H	-4.96592700	2.61517000	-1.19965800	H	5.03258500	2.61897900	1.26528300
H	-0.00715300	0.65179300	-1.94853200	H	0.02218200	0.72534500	2.08146300
H	4.10297800	-2.97664300	1.20228500	H	-4.01401500	-3.14582200	-0.97161700
H	-4.14927600	-2.95477400	1.20511900	H	4.07183100	-3.12374300	-0.99668500
H	2.39627300	-2.87791000	0.77940200	H	-2.30907300	-2.87746000	-0.61553200
H	-2.47640800	-2.90419900	0.65557000	H	2.38228000	-2.90187900	-0.54382200
H	3.63436000	-2.70743700	-0.47298700	H	-3.51443500	-2.77829400	0.67640700
H	-3.79688900	-2.62531500	-0.48804400	H	3.65955400	-2.73002900	0.67039000
O	-0.10129300	1.70676000	-1.43245900	O	0.12389600	1.71986000	1.60852900
C	0.02304100	0.94713800	1.57256800	C	-0.00413000	1.08014800	-1.75002700
H	0.70845100	2.21381000	-1.55466200	H	-0.68818300	2.21849000	1.75364900
C	0.00560800	-1.43725900	0.88871500	C	-0.01284500	-1.45697000	-1.14823200
O	-0.00279400	-2.46808900	1.43924000	O	-0.01091600	-2.44631800	-1.78973900
Mn	0.00615600	0.07352000	0.05147300	Re	-0.00387400	0.09088900	-0.13347300
2Mn-OH-SMD(CH₃OH)				2Re-OH-SMD(CH₃OH)			
N	0.00376200	-0.88998000	-1.82234100	N	0.00356600	-0.88322900	-1.89193200
H	-0.00462000	-0.03812000	-2.38611200	H	-0.00363600	-0.04220300	-2.47413800
P	-2.30509300	0.06218400	-0.24223100	P	-2.39889200	0.03045400	-0.29906300
P	2.31068600	0.06932700	-0.24445600	P	2.40387300	0.03517200	-0.30149700
C	3.20362800	1.69110000	-0.57271100	C	3.28461200	1.65833800	-0.62871600
C	-3.19669900	1.68363700	-0.57620600	C	-3.28856300	1.64712900	-0.64052800
C	3.46030900	-0.87953600	0.90334100	C	3.54854700	-0.96405300	0.79902900
C	-3.45803700	-0.88117800	0.90689900	C	-3.54347900	-0.96263500	0.80712800
O	0.00325500	-2.35928500	1.60397000	O	-0.00163300	-2.45361600	1.77938200
C	-2.43334600	-0.76639900	-1.90608900	C	-2.45078300	-0.77944600	-1.97826100
C	2.44031200	-0.75338000	-1.91119100	C	2.45678900	-0.76468600	-1.98507600
H	-2.43859900	0.03692800	-2.64907600	H	-2.45517300	0.03395900	-2.71040200
H	2.44055000	0.05269800	-2.65147800	H	2.45363000	0.05262600	-2.71294700
H	-3.35855800	-1.33100600	-2.02867100	H	-3.36382200	-1.35743000	-2.12799800
H	3.36797100	-1.31317300	-2.03803900	H	3.37296200	-1.33617800	-2.14112200
C	-1.22000900	-1.64866900	-2.12888800	C	-1.22457000	-1.64742100	-2.19633900
C	1.23061400	-1.64046700	-2.13514500	C	1.23486600	-1.63901500	-2.20298000
H	-1.19750600	-2.00428600	-3.16709700	H	-1.19568300	-1.99763600	-3.23509800
H	1.20749000	-1.99250100	-3.17453100	H	1.20486600	-1.98650800	-3.24260400
H	-1.24458700	-2.52766200	-1.48063200	H	-1.23979200	-2.52559700	-1.54825300
H	1.26126600	-2.52163900	-1.49018600	H	1.25695600	-2.51888300	-1.55735900
H	2.57265800	2.13023500	-1.35157300	H	2.63617900	2.10141100	-1.39139200
H	-2.56206700	2.12074800	-1.35319100	H	-2.65363500	2.08057800	-1.42062500

O	0.00418100	1.60931200	2.54366100	O	0.00555100	1.71644700	2.73007300
H	-4.46125600	-0.51225900	0.67235600	H	-4.55468400	-0.65081800	0.52815600
H	4.46399100	-0.50929500	0.67314800	H	4.55979100	-0.65000800	0.52237200
C	-3.15641600	-0.55809400	2.36997600	C	-3.31577700	-0.62209800	2.27851900
C	3.15528900	-0.56367600	2.36735200	C	3.32006300	-0.63393200	2.27284900
H	-3.16570000	0.51353500	2.57591600	H	-3.40202700	0.44632600	2.48249500
H	3.16250600	0.50699100	2.57825800	H	3.40609200	0.43285400	2.48495800
H	-2.18105300	-0.94744000	2.66974800	H	-2.32759900	-0.94737200	2.61198000
H	2.18001900	-0.95584900	2.66350400	H	2.33174300	-0.96175700	2.60338300
H	-3.91088200	-1.02390200	3.01256200	H	-4.06160600	-1.13746300	2.89237600
H	3.90926100	-1.03137800	3.00915100	H	4.06556800	-1.15383200	2.88329800
C	3.19787500	2.63879800	0.62275700	C	3.28472600	2.58930700	0.57952400
C	-3.19845000	2.63125600	0.61936300	C	-3.28119000	2.59468000	0.55496400
H	3.84733300	2.28184600	1.42609300	H	3.97083600	2.24432800	1.35693300
H	-3.86298300	2.27941600	1.41257900	H	-3.96435900	2.25901800	1.33901200
H	2.19623800	2.78418600	1.03231600	H	2.29003200	2.68747600	1.01983900
H	-2.20230200	2.76580500	1.04577300	H	-2.28565900	2.69696800	0.99330600
H	3.57441000	3.61964300	0.31432600	H	3.61511800	3.58723400	0.27386900
H	-3.56078500	3.61606300	0.30676900	H	-3.61211500	3.58911100	0.23892800
C	4.61269900	1.52842400	-1.13650700	C	4.68437600	1.50547500	-1.21597900
C	-4.60273000	1.52094600	-1.14751300	C	-4.69288000	1.48242600	-1.21400900
H	4.64389300	0.87514600	-2.01111100	H	4.70295100	0.86097700	-2.09765800
H	-4.62912900	0.86829600	-2.02267200	H	-4.71684100	0.82282700	-2.08425500
H	5.31021600	1.13389600	-0.39281300	H	5.39212400	1.10426500	-0.48584200
H	-5.30368100	1.12578700	-0.40743400	H	-5.39385100	1.09277900	-0.47139800
H	4.99432400	2.50698200	-1.44713300	H	5.05940100	2.48784200	-1.52192400
H	-4.98290800	2.49966000	-1.45937600	H	-5.07175900	2.45886000	-1.53366300
C	-3.45130900	-2.39064600	0.67606600	C	-3.43196400	-2.46730400	0.57506500
H	-3.75651300	-2.66093100	-0.33647600	H	-3.69276500	-2.75377500	-0.44534900
H	-2.47105400	-2.83133000	0.86806200	H	-2.42867300	-2.83919700	0.79175000
H	-4.16046400	-2.86163400	1.36503300	H	-4.12525100	-2.98550000	1.24561900
C	3.45494400	-2.38786200	0.66512200	C	3.43726300	-2.46728400	0.55790700
H	2.47467500	-2.83023200	0.85295200	H	2.43382900	-2.84006700	0.77263800
H	3.76240400	-2.65290600	-0.34812000	H	3.69771400	-2.74776300	-0.46425200
H	4.16304600	-2.86168600	1.35322700	H	4.13043700	-2.98964700	1.22534400
O	-0.01401700	1.71576300	-1.24424200	O	0.02936900	1.80440600	-1.26145400
C	0.00441900	-1.37589900	0.96872600	C	0.00060300	-1.46626000	1.13234300
Mn	-0.00087700	0.10006600	0.05120200	Re	-0.00017000	0.11364300	0.12365900
C	0.00125900	1.02436100	1.53267400	C	0.00219900	1.10474400	1.72595000
H	-0.37937600	2.48229800	-0.79467700	H	-0.53352100	2.51154600	-0.93484200
Mn-TS2-OH-SMD(CH₃OH)				Re-TS2-OH-SMD(CH₃OH)			
P	-2.29351200	-0.07450400	-0.07134100	P	2.40420100	0.06272000	0.14192600
P	2.32288100	0.00979200	-0.07515300	P	-2.40222700	0.01528400	0.13491800
C	-2.45245900	0.63732100	-1.78435000	C	2.44073900	0.89939900	1.80692700
C	2.43239500	0.80689000	-1.75415100	C	-2.47991400	0.76727100	1.83895800
H	-2.51529500	1.72288400	-1.66455500	H	2.42739800	1.97657700	1.61474800
H	2.41059200	1.88789200	-1.58523700	H	-2.53420700	1.85051500	1.69734800
H	-3.36040500	0.31152700	-2.29335800	H	3.35664300	0.67889700	2.35791800
H	3.36448500	0.57619900	-2.27222000	H	-3.37724600	0.46468900	2.38066800
C	-1.21521700	0.28784100	-2.58929600	C	1.21943400	0.51453100	2.62319000
C	1.22864900	0.39973400	-2.58311500	C	-1.23134500	0.42224600	2.63104200
H	-1.21444500	0.83771700	-3.53901800	H	1.19114300	1.09927400	3.55044600
H	1.19810600	0.97777300	-3.51551400	H	-1.22288700	0.97980200	3.57529400
H	-1.18504500	-0.77870900	-2.82413100	H	1.24470800	-0.54214900	2.89552100
H	1.27633500	-0.65776200	-2.85238100	H	-1.19620500	-0.64234200	2.87084600
N	-0.00730100	0.61326600	-1.80964200	N	-0.01856100	0.74891400	1.84785700
C	3.21293100	1.27145700	0.99564100	C	-3.30816600	1.30425300	-0.88305000
C	-3.21411200	1.21258800	0.94356400	C	3.31159000	1.30507700	-0.93136100
H	2.56424200	2.14495400	0.88400300	H	-2.68197100	2.18594800	-0.71319600

H	-2.62152500	2.11097600	0.74323600	H	2.66381100	2.18268400	-0.83541300
C	3.48180900	-1.47204700	-0.11722400	C	-3.52022100	-1.49206300	0.16243800
C	-3.40242000	-1.59436400	-0.01645700	C	3.54573600	-1.42094000	0.27113000
C	3.47140700	-2.21994300	-1.44794800	C	-3.41496400	-2.29161100	1.45826300
C	-3.39831900	-2.40616700	-1.30969100	C	3.41872600	-2.16028800	1.60030900
O	0.04108800	-1.23972200	2.88041500	O	0.01865200	-1.34735200	-3.03776400
H	-4.41310100	-1.19997800	0.12607100	H	4.55598900	-1.00447900	0.21064900
H	4.48199500	-1.04978800	0.02102700	H	-4.53603100	-1.09085300	0.09265700
C	-3.05943900	-2.48193300	1.17975200	C	3.34359100	-2.37930000	-0.90103600
C	3.19856400	-2.42758100	1.04160700	C	-3.26247300	-2.38547600	-1.04891600
H	-3.05199200	-1.93427900	2.12366900	H	3.44419100	-1.88914600	-1.87059200
H	3.19745300	-1.92662000	2.01095200	H	-3.34401900	-1.84781800	-1.99494300
H	-2.08172900	-2.95394600	1.05910400	H	2.35814800	-2.84818000	-0.86196500
H	2.23436500	-2.92617900	0.92100400	H	-2.26727200	-2.83280900	-1.00261500
H	-3.80291700	-3.28106200	1.26844400	H	4.09329200	-3.17573400	-0.85373200
H	3.96988100	-3.20427000	1.07299600	H	-3.99437500	-3.19959400	-1.06661600
C	3.23938300	0.89745000	2.47433700	C	-3.29755800	1.00262200	-2.37831200
C	-3.17172900	0.93966700	2.44398500	C	3.35084000	0.90841500	-2.40411800
H	3.91641100	0.06173700	2.66840400	H	-3.97257500	0.18054300	-2.62899100
H	-3.79693900	0.08549400	2.71603300	H	4.06525400	0.10137500	-2.58391800
H	2.25023600	0.63092000	2.85155800	H	-2.29901600	0.74680200	-2.73929800
H	-2.15860600	0.74423000	2.80228100	H	2.37460700	0.58508200	-2.77220000
H	3.59986900	1.74909100	3.06052900	H	-3.63836900	1.88328600	-2.93219400
H	-3.55548300	1.80920400	2.98739400	H	3.66958400	1.76473900	-3.00681400
C	4.60729000	1.64561900	0.49917400	C	-4.71813200	1.61419700	-0.38875700
C	-4.64220200	1.47660600	0.47408000	C	4.69923700	1.68487900	-0.42193200
H	4.61235500	1.95988300	-0.54679500	H	-4.74836400	1.85391700	0.67644700
H	-5.30638600	0.63698000	0.69515300	H	5.40793200	0.85757400	-0.51172600
H	5.31797700	0.82226500	0.61001700	H	-5.40533500	0.78384600	-0.57095500
H	-5.04155100	2.34998100	1.00046100	H	5.09180700	2.51197400	-1.02263300
H	4.99008500	2.48270900	1.09273400	H	-5.10998100	2.48176500	-0.92999300
H	-4.70240400	1.68529500	-0.59621200	H	4.69016400	2.01425000	0.61939600
H	4.19142000	-3.04375600	-1.40153200	H	-4.11287800	-3.13423500	1.41591800
H	-4.08357900	-3.25348900	-1.20165800	H	4.13170200	-2.99120400	1.61558000
H	2.49391900	-2.65445800	-1.66534500	H	-2.41464700	-2.70404000	1.60163300
H	-2.41103100	-2.81322000	-1.53525000	H	2.42214600	-2.58418400	1.73703700
H	3.75980300	-1.58511400	-2.28769400	H	-3.67405600	-1.70081200	2.33878600
H	-3.73489300	-1.82568000	-2.17074700	H	3.64480400	-1.52434700	2.45793000
C	0.02951200	-0.81413400	1.79428100	C	0.01704200	-0.90572900	-1.94948700
C	0.04114800	-1.86057600	-0.42668100	C	0.02162100	-1.97729100	0.43359100
O	0.05609200	-2.97491700	-0.78194400	O	0.03361600	-3.09990500	0.79409500
H	-0.56486800	1.89304000	1.48435600	H	0.54800900	1.99250200	-1.61922400
O	0.00685900	1.78850500	0.71918200	O	-0.04351800	1.89441100	-0.86615000
C	-0.00659800	3.82823300	-0.08073800	C	0.09443400	3.78296400	0.03862300
H	1.08875800	3.77960500	-0.01289800	H	-0.45213600	4.18946900	-0.82388600
H	-0.52592800	4.10635900	0.84836600	H	1.18693800	3.74441000	-0.07501400
O	-0.57718700	3.87227700	-1.16827000	O	-0.43015700	3.73246900	1.15488500
H	-0.05627500	1.60305100	-1.56690700	H	-0.05968900	1.75146600	1.64358200
Mn	0.01513200	-0.22131000	0.14931500	Re	0.00751000	-0.21543800	-0.19639600
3Mn⁺-O(H)CH₂O⁻-SMD(CH₃OH)				3Re⁺-O(H)CH₂O⁻-SMD(CH₃OH)			
P	2.31502100	0.02661500	-0.08940000	P	2.41354000	-0.00156700	0.16424100
P	-2.32468800	-0.02899900	-0.09805600	P	-2.41856100	0.04979500	0.16966600
C	2.47637900	-0.43550900	-1.88353400	C	2.49049000	0.49673100	1.95775400
C	-2.43759900	-0.66029000	-1.84320000	C	-2.45410300	0.73435300	1.90033800
H	2.59514600	-1.52095700	-1.91280200	H	2.60705300	1.58318100	1.96720000
H	-2.44673100	-1.75215100	-1.77918200	H	-2.45263800	1.82382000	1.79955700
H	3.35697000	0.00333700	-2.35373600	H	3.35758800	0.07299400	2.46621900
H	-3.35839400	-0.35619800	-2.34365200	H	-3.36434600	0.45627500	2.43473500
C	1.20991400	-0.03739200	-2.61906700	C	1.20951200	0.11318700	2.67921300

C	-1.21731300	-0.20331400	-2.62141700	C	-1.22489300	0.28983100	2.67616300
H	1.21551600	-0.46480600	-3.63004400	H	1.21021000	0.55066400	3.68529200
H	-1.19587600	-0.69090500	-3.60441300	H	-1.20109800	0.79555300	3.64921800
H	1.14271600	1.04846100	-2.72353900	H	1.13281200	-0.97110800	2.79096200
H	-1.25043300	0.87561500	-2.79324200	H	-1.25637800	-0.78555600	2.86529700
N	0.02074600	-0.50469600	-1.87999700	N	0.02018200	0.58147000	1.93555800
C	-3.28349400	-1.33028200	0.86228200	C	-3.41060300	1.32154500	-0.79012000
C	3.28214400	-1.35169500	0.74886400	C	3.38687300	1.38211400	-0.65116900
H	-2.65709000	-2.21658600	0.73492400	H	-2.82184400	2.22888300	-0.62561700
H	2.70777100	-2.23941800	0.46242300	H	2.80364500	2.26223100	-0.35716300
C	-3.42405100	1.49563000	0.00587000	C	-3.48324700	-1.49736400	0.17093300
C	3.38518100	1.55384000	0.17586500	C	3.48392600	-1.53002500	-0.03893100
C	-3.43383800	2.34605000	-1.26212100	C	-3.34991500	-2.32479100	1.44639700
C	3.41986000	2.50722300	-1.01638000	C	3.42674500	-2.48203500	1.15313900
O	-0.03657400	0.88215000	2.96981800	O	-0.02866400	-0.96481700	-3.15249300
H	4.39561400	1.15644900	0.30924200	H	4.50373800	-1.13978300	-0.10705200
H	-4.43243400	1.09305600	0.14211700	H	-4.50979100	-1.12119400	0.12286900
C	2.99509400	2.29783900	1.45248100	C	3.16060900	-2.26323300	-1.33940800
C	-3.08408600	2.35044800	1.22729600	C	-3.22218100	-2.35047700	-1.06874500
H	2.96194400	1.64606300	2.32695400	H	3.20122700	-1.61077900	-2.21320300
H	-3.05198200	1.77447200	2.15317400	H	-3.33045800	-1.78814000	-1.99722900
H	2.01933400	2.77820000	1.35357400	H	2.16632900	-2.71301300	-1.30393400
H	-2.12098900	2.85125300	1.11109400	H	-2.21872600	-2.77986600	-1.05342500
H	3.73070100	3.08326200	1.65444200	H	3.88630000	-3.06836000	-1.49300500
H	-3.84578900	3.12756400	1.34955400	H	-3.93799200	-3.17842200	-1.09869300
C	-3.37030600	-1.03259700	2.35600800	C	-3.43577800	1.05290300	-2.29188200
C	3.27715500	-1.23972900	2.27067100	C	3.38671300	1.29002200	-2.17415300
H	-4.03565000	-0.19078700	2.56276600	H	-4.07246900	0.20051100	-2.54078300
H	3.90040400	-0.41000700	2.61357600	H	4.01998500	0.47244200	-2.52736200
H	-2.39444300	-0.81498100	2.79457200	H	-2.43761100	0.86457300	-2.69403400
H	2.27226900	-1.09505500	2.67536800	H	2.38303600	1.13926900	-2.58042600
H	-3.78001700	-1.90417100	2.87659900	H	-3.84505600	1.92561600	-2.81071600
H	3.68443400	-2.15606100	2.70947700	H	3.78410600	2.21690000	-2.59963300
C	-4.66147000	-1.63579900	0.28121500	C	-4.81407900	1.55749800	-0.24023600
C	4.70106800	-1.53173600	0.21520400	C	4.80099400	1.55917300	-0.10509600
H	-4.62162600	-1.89876000	-0.77778400	H	-4.81535400	1.76398300	0.83222200
H	5.35523400	-0.70464300	0.50273800	H	4.82250300	1.64183900	0.98374300
H	-5.35276200	-0.79693800	0.39805700	H	-5.47177900	0.70404100	-0.42391700
H	5.13257200	-2.44552000	0.63707200	H	5.45801500	0.73658800	-0.39896900
H	-5.09721700	-2.48795500	0.81345500	H	-5.26054900	2.42253000	-0.74147700
H	4.73082700	-1.62922000	-0.87199700	H	5.23398700	2.47918400	-0.51128000
H	-4.11928900	3.18805900	-1.11988000	H	-4.02481000	-3.18475800	1.38429600
H	4.08094200	3.34748400	-0.77945000	H	4.08150300	-3.33707900	0.95571700
H	-2.44990000	2.76180900	-1.48596300	H	-2.33920000	-2.71338500	1.58081800
H	2.43660100	2.92208200	-1.24351600	H	2.42174500	-2.87268100	1.32040500
H	-3.77971000	1.79141200	-2.13613300	H	-3.62454500	-1.76114100	2.33987800
H	3.81089400	2.03578700	-1.91935100	H	3.77404200	-2.01723700	2.07728200
C	-0.02431700	0.55439800	1.85344500	C	-0.02223100	-0.61855400	-2.03276000
C	-0.01620000	1.79157500	-0.27844000	C	-0.00497600	-1.91110900	0.23150700
O	-0.02387300	2.92429600	-0.55376200	O	-0.00009000	-3.05819800	0.48966300
H	0.67771000	-2.16898900	1.30263000	H	0.77474800	2.38299100	-1.29309600
O	-0.05942600	-1.98860000	0.71035500	O	-0.05513800	2.20885700	-0.83397400
C	-0.21809100	-3.21782000	-0.17476500	C	-0.26678200	3.34723900	0.15076100
H	-1.29214500	-3.16244700	-0.42383800	H	-1.35319800	3.26353200	0.32749000
H	-0.07409200	-4.04804100	0.54438700	H	-0.08402500	4.24332200	-0.47344500
O	0.59421100	-3.23056400	-1.21663400	O	0.48491200	3.26064800	1.23453600
H	0.12059600	-1.53359200	-1.78642100	H	0.11527600	1.61633600	1.81991700
Mn	-0.00890900	0.10996700	0.15394800	Re	-0.00710000	-0.10896600	-0.21093700
Mn-TS2-H⁺-SMD(CH₃OH)				Re-TS2-H⁺-SMD(CH₃OH)			

P	2.31429700	-0.03742000	-0.09497500	P	2.42267200	-0.00365800	0.17611800
P	-2.31136200	0.02211100	-0.10124100	P	-2.42187900	0.04563200	0.16460000
C	2.42983500	-0.70124200	-1.82391400	C	2.49627400	0.59374000	1.93661400
C	-2.47721900	-0.42713000	-1.89567500	C	-2.46086000	0.86890400	1.83150200
H	2.44017800	-1.79125200	-1.73503600	H	2.66904000	1.67108300	1.88462300
H	-2.63373500	-1.50744800	-1.93121500	H	-2.50260600	1.94494200	1.63995300
H	3.35111400	-0.40567000	-2.32961300	H	3.33432000	0.15780300	2.48293500
H	-3.34003000	0.04355400	-2.36952800	H	-3.35645300	0.60463300	2.39768400
C	1.19179700	-0.26187900	-2.58969200	C	1.18045100	0.31507200	2.64740800
C	-1.17691300	-0.06649100	-2.59873300	C	-1.20681700	0.53229300	2.62253500
H	1.16859200	-0.78830000	-3.55894300	H	1.18179600	0.84421400	3.61168200
H	-1.17972900	-0.52110500	-3.60376800	H	-1.18580500	1.15255300	3.53076800
H	1.27078600	0.81099400	-2.83344100	H	1.09110800	-0.75488300	2.87225900
H	-1.13206700	1.02326500	-2.76199000	H	-1.24675100	-0.51146400	2.95728300
N	-0.02490000	-0.53608200	-1.83327900	N	0.02221900	0.74571100	1.84684600
C	-3.28822300	-1.35567300	0.73278600	C	-3.40986000	1.24463200	-0.89247200
C	3.28267700	-1.30146700	0.90949800	C	3.40729900	1.33451700	-0.70564300
H	-2.72854300	-2.24532700	0.42358100	H	-2.78394300	2.14173900	-0.84964900
H	2.64026500	-2.18461900	0.86672100	H	2.83287900	2.23018600	-0.44234200
C	-3.38180200	1.54843400	0.17540500	C	-3.48866800	-1.49335000	0.27611700
C	3.41166800	1.49299600	-0.01506900	C	3.48145300	-1.54672200	0.04322100
C	-3.38393900	2.54102200	-0.98511600	C	-3.34012600	-2.23723400	1.60073300
C	3.43656300	2.31139200	-1.30391100	C	3.38537600	-2.46747600	1.25683200
O	0.02742000	0.89666100	2.96742200	O	-0.03361600	-1.22409000	-3.08030800
H	4.41921100	1.09511200	0.14219900	H	4.50716800	-1.16922500	-0.00871100
H	-4.39739500	1.15208600	0.26767700	H	-4.51377100	-1.11306500	0.21862500
C	3.06198400	2.38089600	1.17967600	C	3.18244300	-2.30918100	-1.24621600
C	-3.02298100	2.25500400	1.48176200	C	-3.24742400	-2.42694500	-0.90843200
H	3.00765900	1.82806300	2.11825100	H	3.27811200	-1.68512200	-2.13610000
H	-3.06296200	1.59036800	2.34613300	H	-3.35193600	-1.92528600	-1.87105500
H	2.10693800	2.88949600	1.03560500	H	2.17249200	-2.72454300	-1.23663900
H	-2.02081000	2.68720700	1.43760400	H	-2.25075300	-2.87043500	-0.86695300
H	3.83038300	3.15251300	1.29629600	H	3.88588400	-3.14176900	-1.34881900
H	-3.72855700	3.07301200	1.66134500	H	-3.97498100	-3.24470100	-0.88037600
C	-3.26908400	-1.27710300	2.25696700	C	-3.50456300	0.82552100	-2.35630400
C	3.43256400	-0.90996200	2.37700300	C	3.39292600	1.19197700	-2.22410600
H	-3.92494000	-0.48378000	2.62393200	H	-4.19513900	-0.01004000	-2.49384200
H	4.13701500	-0.08401900	2.50462100	H	4.03655500	0.37503600	-2.55948300
H	-2.26765200	-1.09551000	2.65560000	H	-2.53315400	0.54159600	-2.76749800
H	2.48182500	-0.62281500	2.83119800	H	2.38660600	1.00907400	-2.60996300
H	-3.63003300	-2.21947900	2.68141400	H	-3.88713200	1.66212200	-2.94957500
H	3.82585700	-1.76104500	2.94228100	H	3.76629200	2.11178000	-2.68535600
C	-4.71558400	-1.51368200	0.21336600	C	-4.78343200	1.59004900	-0.32489300
C	4.63340100	-1.66969100	0.30068700	C	4.82594400	1.51611100	-0.17382100
H	-4.76364400	-1.55961700	-0.87669100	H	-4.74116400	1.91155400	0.71787800
H	4.54161000	-2.06742100	-0.71197100	H	4.85494000	1.63018200	0.91207400
H	-5.36423000	-0.70086900	0.54992800	H	-5.47459000	0.74568400	-0.39231700
H	5.31850900	-0.81818500	0.27044600	H	5.47322500	0.67905500	-0.44708300
H	-5.14151800	-2.44614900	0.59888900	H	-5.22104900	2.41074600	-0.90287000
H	5.10855300	-2.44295100	0.91378800	H	5.26612900	2.41954600	-0.60876100
H	-4.13682000	3.31198300	-0.78970500	H	-4.02048100	-3.09532400	1.60453700
H	4.13370400	3.14718000	-1.18185300	H	4.04181200	-3.32961100	1.09988400
H	-2.42309500	3.04508200	-1.09669600	H	-2.32920700	-2.62315600	1.74196900
H	2.45844000	2.73435400	-1.53962200	H	2.37458900	-2.84953200	1.40521900
H	-3.64010400	2.07682200	-1.93856000	H	-3.59714300	-1.61551100	2.45995400
H	3.77468000	1.72997900	-2.16347500	H	3.70845600	-1.98008500	2.17810600
O	0.06202000	-2.06654100	0.77486800	C	-0.02088900	-0.77085300	-1.99792300
C	0.01714500	0.54469900	1.85427700	C	-0.01056800	-1.88835100	0.31851300
C	0.22671800	-3.15389600	-0.16013900	O	-0.01267500	-3.02332800	0.63457000
H	-0.04773700	-4.08901800	0.33811000	H	0.84919300	2.59215800	-1.40364700

H	1.29920400	-3.16651100	-0.38035300	O	-0.01596600	2.39890800	-1.02294100
C	0.01632600	1.76800300	-0.30088800	C	-0.27423700	3.35835000	0.04740200
O	0.02871700	2.89227600	-0.61628000	H	-1.35972800	3.26522000	0.19565400
Mn	0.00555700	0.10231200	0.15314800	H	-0.06566700	4.35951600	-0.35948900
O	-0.53447700	-2.97382700	-1.29154600	O	0.44865500	3.11550800	1.16848400
H	-0.28037600	-1.92894300	-1.61850900	H	0.18365100	1.92948400	1.56100900
H	-0.69824800	-2.25055400	1.33740100	Re	-0.00253000	-0.12157400	-0.21060100
2Mn-OCH₂OH-SMD(CH₃OH)				2Re-OCH₂OH-SMD(CH₃OH)			
P	2.32100600	-0.08220300	0.18564900	P	2.40776100	-0.06938500	0.24878400
P	-2.31180500	-0.10005800	0.18300800	P	-2.40592000	-0.07541900	0.24908100
C	2.44010700	-0.31924400	2.02745000	C	2.45484200	-0.23747900	2.10462400
C	-2.42921900	-0.33363100	2.02523400	C	-2.45229800	-0.24576600	2.10465400
H	2.42645400	0.68236600	2.46731700	H	2.44581500	0.78106800	2.50457600
H	-2.42018200	0.66897500	2.46289000	H	-2.44605700	0.77220200	2.50591700
H	3.37120700	-0.79923500	2.33182500	H	3.37175800	-0.71640000	2.45154300
H	-3.35786900	-0.81753500	2.33088400	H	-3.36792000	-0.72777600	2.45069900
C	1.23205600	-1.09539600	2.51435700	C	1.23224200	-0.98518800	2.60583800
C	-1.21717100	-1.10263200	2.51349800	C	-1.22763500	-0.99083100	2.60462200
H	1.21076500	-1.11384900	3.61145900	H	1.20655700	-0.96799100	3.70186700
H	-1.19675500	-1.12051400	3.61063200	H	-1.20199400	-0.97553200	3.70068900
H	1.25841000	-2.13050900	2.16676300	H	1.24722200	-2.02870000	2.28745000
H	-1.23691500	-2.13799700	2.16625100	H	-1.23893300	-2.03376000	2.28419900
N	0.00577300	-0.47091100	1.99052400	N	0.00120200	-0.36810900	2.06710500
C	-3.27604700	1.49465800	-0.06514100	C	-3.36001000	1.51926100	-0.01851200
C	3.27045000	1.52268000	-0.05619700	C	3.35859400	1.52707000	-0.02022300
H	-2.60675500	2.24034300	0.37434900	H	-2.69365100	2.26033700	0.43466600
H	2.59729100	2.25823700	0.39444200	H	2.68976500	2.26638000	0.43248300
C	-3.42479600	-1.41246300	-0.58422100	C	-3.51559500	-1.42517500	-0.43924200
C	3.44526300	-1.38235800	-0.58548400	C	3.52032700	-1.41666400	-0.43979800
C	-3.42466500	-2.74045700	0.16942700	C	-3.41334900	-2.73782000	0.33305800
C	3.45516900	-2.71318400	0.16308900	C	3.42309400	-2.72852700	0.33444200
O	0.00263600	0.51504900	-2.95011500	O	0.00487900	0.48298600	-3.16860300
H	4.45133300	-0.95589800	-0.51945100	H	4.53733700	-1.02869200	-0.32201100
H	-4.43438000	-0.99386000	-0.52065300	H	-4.53364200	-1.04051100	-0.31954100
C	3.11489600	-1.59989900	-2.06221800	C	3.25596900	-1.64543500	-1.92688300
C	-3.09203700	-1.63324100	-2.05999700	C	-3.25246400	-1.65127400	-1.92693700
H	3.08571700	-0.67005300	-2.63206200	H	3.33427400	-0.73088500	-2.51588200
H	-3.07004400	-0.70549400	-2.63352200	H	-3.33718500	-0.73662300	-2.51490100
H	2.15138700	-2.09815300	-2.18493500	H	2.26113000	-2.06359100	-2.09103400
H	-2.12464900	-2.12442700	-2.18062900	H	-2.25537700	-2.06341600	-2.09298800
H	3.87769700	-2.24096400	-2.51654500	H	3.98761300	-2.35752700	-2.32226600
H	-3.84961900	-2.28207400	-2.51203100	H	-3.98058100	-2.36725300	-2.32182500
C	-3.48190900	1.83531600	-1.53873300	C	-3.52806700	1.86277900	-1.49600700
C	3.46236100	1.87851800	-1.52794000	C	3.52483800	1.87051900	-1.49788500
H	-4.22059300	1.17483400	-2.00058900	H	-4.27449300	1.22193900	-1.97218700
H	4.20133200	1.22712200	-2.00196400	H	4.26988800	1.22880400	-1.97493700
H	-2.55873600	1.77127200	-2.11826300	H	-2.59412700	1.77174200	-2.05519100
H	2.53489300	1.81426000	-2.10048500	H	2.58991900	1.78066900	-2.05558600
H	-3.86073500	2.85835300	-1.62940300	H	-3.87650100	2.89557800	-1.59531100
H	3.83420100	2.90469100	-1.61201600	H	3.87457800	2.90284100	-1.59786100
C	-4.60308000	1.54376400	0.68864700	C	-4.69939900	1.56952400	0.71143700
C	4.60183900	1.57730800	0.68937700	C	4.69801300	1.58148400	0.70930600
H	-4.48339100	1.38755500	1.76215500	H	-4.60034900	1.39309600	1.78416600
H	4.49095800	1.40693600	1.76171500	H	4.59996100	1.40458400	1.78205000
H	-5.31649200	0.80447200	0.31413500	H	-5.41002600	0.84200800	0.31000700
H	5.32071900	0.85043000	0.30133100	H	5.41021400	0.85570200	0.30759600
H	-5.06018300	2.52983000	0.55224500	H	-5.14557400	2.56148000	0.58355300
H	5.04734700	2.56984900	0.56183300	H	5.14189100	2.57443400	0.58103800
H	0.00253900	0.50876700	2.28065800	H	-0.00209000	0.61277200	2.35566100

H -4.10975500 -3.43474500 -0.32855800	H -4.10168500 -3.46671600 -0.10711900
H 4.14573200 -3.40024400 -0.33733900	H 4.11251300 -3.45614900 -0.10613900
H -2.43800000 -3.20780900 0.17700800	H -2.40961300 -3.16452000 0.28073700
H 2.47211300 -3.18799100 0.16853800	H 2.42042800 -3.15799500 0.28463600
H -3.76348600 -2.63666500 1.20171000	H -3.68619900 -2.62769500 1.38399800
H 3.79285000 -2.61076400 1.19587700	H 3.69768300 -2.61624200 1.38469500
O -0.00429000 1.81214900 0.64672600	O -0.01773200 1.93655900 0.63666100
C 0.00372500 0.28916500 -1.80533600	C 0.00333900 0.27105800 -2.01268600
C 0.01247700 -1.80749400 -0.49773100	C 0.00510300 -1.92746600 -0.58190100
O 0.01712700 -2.94352500 -0.77328400	O 0.00541500 -3.07530800 -0.85174800
Mn 0.00507300 -0.11352600 -0.10261900	Re 0.00171200 -0.10176700 -0.16514200
C -0.02295200 2.90263200 -0.15067500	C -0.02013200 3.02562600 -0.18964600
H -0.88735400 2.93044500 -0.84014200	H -0.89579400 3.06496400 -0.85510100
O -0.11559000 4.07227500 0.70802200	O -0.10886000 4.24606600 0.56336100
H 0.89060200 3.02086500 -0.76418100	H 0.88691800 3.07583300 -0.81669300
H -0.07075400 4.85578400 0.14548400	H 0.68784600 4.30628500 1.10533200
Mn-TS(HOCH₂OH)-SMD(CH₃OH)	Re-TS(HOCH₂OH)-SMD(CH₃OH)
P -2.31679200 -0.09881500 -0.11599200	P 2.40303400 -0.07524600 0.20029100
P 2.31622100 -0.04663700 -0.11295700	P -2.41706300 -0.02425700 0.20267000
C -2.45425400 0.29084900 -1.92935600	C 2.47831400 0.41890200 1.99320600
C 2.43381700 0.43239900 -1.90564100	C -2.45889200 0.52317800 1.98056400
H -2.51682300 1.37977600 -2.00253300	H 2.56962200 1.50847500 2.00867600
H 2.43387200 1.52637900 -1.92490900	H -2.49905700 1.61647100 1.96042700
H -3.35765700 -0.12116200 -2.37876700	H 3.36061300 0.00812800 2.48773600
H 3.36184700 0.09330400 -2.37084500	H -3.35568800 0.17078000 2.49455000
C -1.19679100 -0.19436100 -2.63510800	C 1.19789300 0.00003900 2.70319700
C 1.20919700 -0.09246500 -2.63845900	C -1.19644700 0.07135400 2.70078900
H -1.17369400 0.23148400 -3.65210300	H 1.17097500 0.48649500 3.69094600
H 1.16827800 0.36607300 -3.63775400	H -1.15439200 0.57530700 3.67931700
H -1.22766600 -1.28459800 -2.76278800	H 1.21483700 -1.08360300 2.89746900
H 1.30583300 -1.17709100 -2.80039900	H -1.25964100 -1.00663100 2.91616000
C 3.29131800 1.32773700 0.72340100	N 0.01038900 0.36961600 1.93331600
C -3.25139000 1.33303100 0.65932900	C -3.38079900 1.35366100 -0.64190600
H 2.70228200 2.21534400 0.47326500	C 3.38442300 1.30527400 -0.61755600
H -2.64552500 2.18094000 0.33107400	H -2.84240700 2.23363600 -0.27802800
C 3.40839700 -1.56122500 0.11051900	H 2.88577000 2.18416200 -0.19954100
C -3.40829800 -1.59763100 0.19820800	C -3.51063800 -1.54191200 0.09026900
C 3.35554700 -2.53625200 -1.06430300	C 3.46086600 -1.61470600 0.05464400
C -3.37148800 -2.63277500 -0.92352000	C -3.27161200 -2.53281400 1.22689500
H -4.42670800 -1.19463800 0.24216400	C 3.18366300 -2.63087000 1.16052500
H 4.42475400 -1.15794500 0.15667000	O -0.00286600 -0.47014300 -3.24549500
C -3.09362700 -2.24083000 1.54888000	H 4.48776600 -1.25864000 0.18089100
C 3.12076400 -2.27792000 1.42754500	H -4.52814900 -1.15387900 0.19690000
H -3.11459200 -1.52694700 2.37137100	C 3.33645900 -2.25879200 -1.32477200
H 3.13895600 -1.60647600 2.28860000	C -3.39354000 -2.22308600 -1.27186100
H -2.10764300 -2.71598800 1.54470600	H 3.54317300 -1.55935800 -2.13640200
H 2.14657300 -2.76990600 1.41308900	H -3.60439800 -1.54461000 -2.09983600
H -3.83261400 -3.01845000 1.76566800	H 2.33846500 -2.67355500 -1.48468700
H 3.87809200 -3.05062800 1.59571100	H -2.39777200 -2.64339600 -1.42811200
C 3.33088100 1.21296200 2.24620500	H 4.05395300 -3.08161400 -1.40869700
C -3.25139300 1.31884800 2.18412000	H -4.11331400 -3.04613400 -1.33007600
H 3.97355400 0.39121000 2.57049200	C -3.27184300 1.34979400 -2.16320100
H -3.88213900 0.52314000 2.58633700	C 3.22374700 1.36988500 -2.13265100
H 2.33968800 1.06460400 2.67769500	H -3.83541400 0.52918600 -2.61279300
H -2.24522200 1.20171600 2.59728500	H 3.75994100 0.56405400 -2.63930900
H 3.74330300 2.13408900 2.66876000	H -2.23605600 1.27515000 -2.50052000
H -3.65108500 2.26559900 2.55981500	H 2.17482900 1.32239800 -2.43264500
C 4.69496200 1.53185300 0.15258000	H -3.68565800 2.28241600 -2.56044500
C -4.66861500 1.51981600 0.11578900	H 3.63418300 2.31509500 -2.50290600

H	4.69348200	1.64590100	-0.93604600	C	-4.83270600	1.47207400	-0.18574900
H	-4.69947700	1.55379300	-0.97522400	C	4.85269500	1.35313700	-0.20418100
H	5.36557000	0.70750300	0.40877600	H	-4.93406500	1.46130700	0.90217300
H	-5.34281800	0.72677500	0.45112400	H	4.98664200	1.30165400	0.87931500
H	5.12843400	2.44436400	0.57483500	H	-5.45229700	0.66973300	-0.59427200
H	-5.07661400	2.46578500	0.48679900	H	5.42918700	0.54339900	-0.65851200
H	4.03588600	-3.37118900	-0.86313500	H	-5.25185100	2.41776400	-0.54488200
H	-4.04407500	-3.45924600	-0.66867500	H	5.29593600	2.29486500	-0.54454500
H	2.36135200	-2.95585000	-1.20829300	H	0.16053100	1.69991000	1.24524400
H	-2.37531900	-3.05498300	-1.06155700	H	-3.95531400	-3.37998600	1.10948600
H	3.67369200	-2.07673200	-2.00293300	H	3.83767400	-3.49765700	1.01889800
H	-3.70757500	-2.22325200	-1.87620800	H	-2.25535900	-2.93006300	1.22120300
C	0.42060400	3.22005500	-0.17564800	H	2.15427100	-2.99247100	1.13910100
H	0.66448600	3.39274100	0.88246300	H	-3.46343100	-2.09291900	2.20739000
H	1.33729100	3.24755800	-0.77956100	H	3.38719900	-2.22953100	2.15511900
O	-0.36250000	4.30029500	-0.66933900	O	0.35453700	2.20304200	0.31153300
H	-1.11078800	4.43328400	-0.07095800	C	-0.00376600	-0.32890200	-2.07862900
N	-0.00746500	0.20747400	-1.89433500	C	-0.35871900	3.39142800	0.11962000
O	0.00210400	-0.40129900	3.05430100	H	-0.55187200	3.50863500	-0.95069300
H	-0.10394700	1.43835600	-1.26106200	H	-1.30060300	3.38229600	0.67422800
O	-0.24224900	2.00705900	-0.29923500	C	-0.04342400	-2.02018500	-0.13369500
C	0.00000800	-0.26721100	1.89403700	O	-0.05872000	-3.19899500	-0.11364100
C	0.01499300	-1.89349200	0.00764400	Re	-0.00342500	-0.17394200	-0.18598700
O	0.01147400	-3.05233100	-0.12239000	O	0.35119200	4.51003900	0.61426400
Mn	0.00188600	-0.17301200	0.14390300	H	1.09859600	4.67735100	0.02676700
Mn-TS3-H⁺-SMD(CH₃OH)				Re-TS3-H⁺-SMD(CH₃OH)			
O	-0.17470500	-3.11028600	-0.51719200	O	0.12119500	-3.21547300	0.28402700
P	-2.34178800	0.00138200	-0.09780400	P	2.43963100	0.04670100	0.16622700
P	2.26149600	-0.17868400	-0.07610600	P	-2.38234400	-0.11760200	0.16140200
C	-2.48851500	0.60943900	-1.84592500	C	2.49920100	0.72559500	1.89673300
C	2.42903500	0.57091900	-1.76520700	C	-2.44874000	0.73514300	1.81303200
H	-2.58162100	1.69658500	-1.79297700	H	2.59991800	1.80909500	1.79593400
H	2.49793800	1.65186200	-1.61464900	H	-2.50696600	1.80579100	1.59688400
H	-3.37846100	0.22883100	-2.34901600	H	3.37165800	0.36686700	2.44553800
H	3.33578300	0.25031700	-2.28062400	H	-3.34294500	0.46362600	2.37770100
C	-1.21817200	0.23328500	-2.59167000	C	1.21225600	0.39432600	2.63600700
C	1.18010000	0.24413600	-2.56381300	C	-1.18827200	0.44430700	2.61017200
H	-1.15451900	0.82506700	-3.51699300	H	1.16469500	1.00327400	3.55107600
H	1.15362800	0.87252400	-3.46687200	H	-1.16687000	1.10512400	3.48988000
H	-1.25189300	-0.82057100	-2.89741200	H	1.21937500	-0.65515500	2.95788700
H	1.20785800	-0.79748200	-2.90924700	H	-1.20892300	-0.58456600	2.99208600
N	-0.02819100	0.47408000	-1.75899200	N	0.02436900	0.65267600	1.80645100
C	3.18555800	1.06248800	0.98928200	C	-3.36289100	1.07053600	-0.91360500
C	-3.10099300	1.42967600	0.86331700	C	3.32003700	1.40736000	-0.78688300
H	2.60454900	1.97258900	0.81267500	H	-2.79579600	1.99636800	-0.76664300
H	-2.52113200	2.27461300	0.47701200	H	2.73973400	2.28530500	-0.48003400
C	3.32422700	-1.72894600	-0.05694400	C	-3.42509000	-1.66297000	0.32283600
C	-3.54955400	-1.42538000	0.07984700	C	3.57454200	-1.44433500	0.12874700
C	3.25184800	-2.52121400	-1.36001700	C	-3.14174600	-2.42578000	1.61453800
C	-3.54948200	-2.37053500	-1.11972500	C	3.40466100	-2.33901200	1.35422600
O	-0.10301100	-0.96951600	2.94389500	O	0.10239000	-0.85833300	-3.19739700
H	-4.53433300	-0.95133700	0.12934300	H	4.58599500	-1.02791900	0.15374300
H	4.34850900	-1.35963400	0.05372600	H	-4.45571300	-1.29705600	0.36819300
C	-3.31406400	-2.19583400	1.37738400	C	3.40508100	-2.23923800	-1.16360500
C	2.99991900	-2.61876600	1.14241400	C	-3.28218700	-2.56647200	-0.89958000
H	-3.32701200	-1.55211500	2.25843800	H	3.54177300	-1.62480900	-2.05482800
H	3.02475300	-2.07801700	2.08969400	H	-3.55245600	-2.05999400	-1.82715100
H	-2.35703800	-2.72234100	1.35881200	H	2.41636700	-2.69897300	-1.22261900
H	2.01447900	-3.07863900	1.04494900	H	-2.26096100	-2.93754100	-1.00601400

H -4.10122500 -2.94603000 1.50522400	H 4.14810000 -3.04253600 -1.19837000
H 3.73532900 -3.42759400 1.20537100	H -3.94286200 -3.43261500 -0.79173200
C 3.14285200 0.76261400 2.48391100	C -3.33172400 0.73896100 -2.40189000
C -2.87645500 1.36499400 2.37032300	C 3.20413700 1.27879800 -2.30103100
H 3.74127400 -0.11456700 2.74144200	H -3.95624200 -0.12489600 -2.64042400
H -3.41759600 0.53488700 2.83037000	H 3.79073600 0.44151400 -2.68597200
H 2.12630900 0.60272600 2.84654900	H -2.32012900 0.53728100 -2.75846100
H -1.82024800 1.26707000 2.62665700	H 2.16876200 1.14480000 -2.61974700
H 3.56000000 1.61195600 3.03471900	H -3.72301100 1.58820500 -2.97140800
H -3.24380900 2.28769800 2.83135700	H 3.58522200 2.18871000 -2.77574900
C 4.61703900 1.32151900 0.52490900	C -4.79058300 1.30800700 -0.42956400
C -4.57031100 1.68107800 0.53350400	C 4.76725200 1.61977400 -0.35162300
H 4.68016800 1.55567500 -0.53990300	H -4.83849100 1.56805200 0.63016100
H -4.76184100 1.71246000 -0.54187200	H 4.87249500 1.69809000 0.73293400
H 5.27157200 0.46949100 0.72646600	H -5.42508900 0.43380000 -0.59670600
H -5.22004500 0.92012100 0.97339300	H 5.41628600 0.81209900 -0.69966300
H 5.02454600 2.17770900 1.07257500	H -5.23086100 2.13888700 -0.99062700
H -4.87584800 2.64666700 0.94943200	H 5.14696900 2.54999200 -0.78648700
H 0.13038200 2.31003900 0.54066100	H -0.14918200 2.35385200 -0.59638400
H -0.05718800 1.80563100 -1.54212300	H 0.07667100 1.99538500 1.51966200
C 0.08115600 3.23551300 -0.07041900	C -0.07385100 3.31826600 -0.03439200
H 3.90852200 -3.39424300 -1.28479800	H -3.78608100 -3.30997200 1.65562200
H 2.24386900 -2.88819100 -1.56189800	H -2.10758100 -2.77051100 1.66990500
H 3.58359600 -1.93864700 -2.22141700	H -3.35252500 -1.82848200 2.50356400
H -4.30152300 -3.14964600 -0.95703900	H 4.08956800 -3.18928900 1.27290400
H -3.80541900 -1.86479200 -2.05218200	H 3.64065300 -1.81974900 2.28469700
H -2.58824700 -2.86936700 -1.25212300	H 2.39325600 -2.74085000 1.43311600
O -0.13701500 2.96488800 -1.39214700	O 0.17386400 3.11796900 1.28697700
C -0.12811800 -1.97442300 -0.25311800	C 0.09423100 -2.05196700 0.09634700
Mn -0.05819000 -0.29194200 0.09855400	Re 0.04168900 -0.23437400 -0.19042000
C -0.08188500 -0.65892000 1.82059700	C 0.07414200 -0.61256400 -2.04985000
H -0.71514500 3.87400900 0.33956000	H 0.71413600 3.91958600 -0.51251400
O 1.33657800 3.88497700 0.17567600	O -1.31915900 4.02175000 -0.18192400
H 1.29766600 4.75384800 -0.24330200	H -1.40531700 4.29231800 -1.10524400
3Mn⁺-HCH(OH)O⁻-SMD(CH₃OH)	3Re⁺-HCH(OH)O⁻-SMD(CH₃OH)
O 0.06776000 -3.04735100 -0.15250100	O 0.10675100 -3.18846800 0.36471700
P 2.33550900 -0.03240300 0.13178900	P 2.43485800 0.03180100 0.15508400
P -2.29149900 -0.10518400 0.13030500	P -2.38652200 -0.11806900 0.15779300
C 2.49490200 0.11247400 1.97813100	C 2.49104000 0.66892400 1.90289600
C -2.42064000 0.23672900 1.95034800	C -2.44776900 0.65514400 1.84967700
H 2.59729900 1.17766300 2.20073100	H 2.54220600 1.75856300 1.82974100
H -2.44379000 1.32503700 2.06008100	H -2.47647500 1.73698800 1.68738400
H 3.38261600 -0.39057400 2.36365200	H 3.38431000 0.33422200 2.43243100
H -3.33729300 -0.15892500 2.39041600	H -3.35167300 0.37974900 2.39561900
C 1.23464000 -0.43055400 2.62438000	C 1.23542300 0.26856200 2.65810200
C -1.19458100 -0.32185000 2.64547300	C -1.20661300 0.29767400 2.64752500
H 1.21176100 -0.16028900 3.68750800	H 1.20264300 0.79532000 3.61966700
H -1.16436300 0.01871700 3.68800300	H -1.19500800 0.86874900 3.58398600
H 1.20134600 -1.52084800 2.56122300	H 1.22743400 -0.80353400 2.86738200
H -1.21651300 -1.41398400 2.65761700	H -1.19851200 -0.76319300 2.90683800
N 0.03440500 0.10266300 1.94478000	N 0.02088100 0.59528500 1.87597800
C -3.27369600 1.31602700 -0.59693100	C -3.34734500 1.12958300 -0.86383200
C 3.26551300 1.49738600 -0.44000000	C 3.31841300 1.40633500 -0.77047400
H -2.70025600 2.17416300 -0.23556400	H -2.74973700 2.03453900 -0.70605000
H 2.76269000 2.28183700 0.13322800	H 2.72038300 2.27716200 -0.47834100
C -3.34809100 -1.62496800 -0.20333700	C -3.43986100 -1.66515000 0.23135700
C 3.43843600 -1.46594400 -0.38796000	C 3.56334400 -1.46356100 0.08375100
C -3.25056900 -2.69621400 0.87955800	C -3.23604400 -2.45437500 1.52171300
C 3.41819800 -2.65122600 0.57464500	C 3.43632600 -2.36282300 1.31117800

O	0.04090300	-0.17999900	-3.04578200	O	0.07286300	-0.91341300	-3.19161900
H	4.44815200	-1.04695200	-0.36724700	H	4.57478400	-1.04647500	0.07564900
H	-4.37313300	-1.24223900	-0.19679600	H	-4.47015600	-1.29593000	0.22152900
C	3.13698200	-1.91348700	-1.81681200	C	3.35278400	-2.25757000	-1.20331400
C	-3.06628400	-2.20947200	-1.58707400	C	-3.22415000	-2.54460200	-0.99779400
H	3.17178100	-1.08930600	-2.53129200	H	3.45467000	-1.64272400	-2.09864900
H	-3.12812400	-1.46261100	-2.38003600	H	-3.40371400	-2.01155800	-1.93249800
H	2.15390400	-2.38290200	-1.89237500	H	2.36557000	-2.72337200	-1.22799800
H	-2.07728600	-2.66830300	-1.63719900	H	-2.20831200	-2.94303300	-1.02921900
H	3.88052900	-2.65312300	-2.13118700	H	4.09861000	-3.05666300	-1.26372900
H	-3.80248500	-2.98845400	-1.81047300	H	-3.91472800	-3.39329900	-0.96361000
C	-3.26358500	1.36439300	-2.12186600	C	-3.34982600	0.82594600	-2.35872000
C	3.08673600	1.80484500	-1.92322900	C	3.23593300	1.26962900	-2.28666200
H	-3.88192200	0.57665900	-2.55913300	H	-3.99804300	-0.01983600	-2.59955200
H	3.59796100	1.07279400	-2.55285800	H	3.85053500	0.44510300	-2.65516400
H	-2.25733600	1.27636700	-2.53533000	H	-2.34956100	0.60902000	-2.73899200
H	2.03592000	1.82956800	-2.21853800	H	2.21079400	1.11039000	-2.62743800
H	-3.67702900	2.32150100	-2.45605400	H	-3.73304500	1.69384400	-2.90479600
H	3.51907700	2.78527800	-2.14773000	H	3.60583100	2.18622500	-2.75695100
C	-4.69668200	1.43338100	-0.05497400	C	-4.75927300	1.39754100	-0.35099200
C	4.74016000	1.52052700	-0.04333500	C	4.75356400	1.63671500	-0.30612100
H	-4.73544900	1.42902300	1.03664100	H	-4.78198200	1.63781700	0.71401800
H	4.89892000	1.27529000	1.00948000	H	4.83393300	1.73483900	0.77876800
H	-5.34479600	0.63370800	-0.42319500	H	-5.42231100	0.54614100	-0.52480800
H	5.33741600	0.83400200	-0.64855400	H	5.41699200	0.82912300	-0.62589500
H	-5.13130500	2.38027600	-0.39216600	H	-5.18317000	2.25212600	-0.88842100
H	5.14017200	2.52624800	-0.20808700	H	5.13491900	2.56260000	-0.74859800
H	-0.15499300	1.72196900	-0.12500300	H	-0.08471400	2.37833900	-0.45635400
H	0.08752800	1.14777400	1.99544200	H	0.03673800	1.64697200	1.71660100
C	0.10933700	2.81861500	0.30559400	C	0.02006200	3.37933400	0.06323600
H	-3.92109900	-3.52331600	0.62341600	H	-3.89224900	-3.33062400	1.51141100
H	-2.24428000	-3.10915300	0.96665300	H	-2.21076200	-2.81443400	1.62467900
H	-3.55596800	-2.32490000	1.85948300	H	-3.48769900	-1.87146600	2.40966300
H	4.12798000	-3.40551600	0.21928900	H	4.12811900	-3.20483600	1.20685900
H	3.72211800	-2.37430600	1.58564400	H	3.69293900	-1.84542500	2.23714300
H	2.43868200	-3.12744500	0.62877100	H	2.43216000	-2.77677500	1.41525600
O	0.26175400	2.83953200	1.59669600	O	0.12812900	3.28637600	1.38255400
C	0.05407000	-1.88340400	-0.13031500	C	0.08125900	-2.03306900	0.14477600
Mn	0.02196300	-0.14951500	-0.12809500	Re	0.03210000	-0.22549700	-0.20680000
C	0.02980000	-0.14585000	-1.88276000	C	0.05400000	-0.64691700	-2.05133000
H	0.98112200	3.10857700	-0.30472600	H	0.87172600	3.89085500	-0.43193200
O	-0.99471000	3.63355300	-0.12180400	O	-1.17797900	4.13811500	-0.30284300
H	-0.97312600	3.69539800	-1.08634000	H	-1.17786700	4.24897200	-1.26296200
Mn-TS3-H-SMD(CH₃OH)				Re-TS3-H-SMD(CH₃OH)			
O	0.07006300	-3.10130800	-0.16269900	O	0.07271100	-3.23695700	-0.15919900
P	2.31137100	-0.04105000	0.12593500	P	2.41651600	0.02647100	0.19381900
P	-2.27111300	-0.11087200	0.13081100	P	-2.37444200	-0.08615600	0.18094800
C	2.48645000	0.11239100	1.97288100	C	2.47809000	0.32027600	2.03461200
C	-2.41542100	0.20430700	1.95754500	C	-2.44487300	0.25501900	2.01114500
H	2.56861700	1.17963200	2.19610700	H	2.49760700	1.40386800	2.17969800
H	-2.43804900	1.29066500	2.08615000	H	-2.47751700	1.34306900	2.12161500
H	3.38729600	-0.37133700	2.35306200	H	3.38663400	-0.08594400	2.48228300
H	-3.33492200	-0.19737700	2.38640200	H	-3.34914700	-0.14704200	2.47060000
C	1.24180700	-0.45501800	2.62840600	C	1.24537200	-0.26090600	2.70402800
C	-1.19429100	-0.36772600	2.65085800	C	-1.20539200	-0.28672200	2.69919400
H	1.22716400	-0.20275700	3.69646800	H	1.21025600	0.04953400	3.75524900
H	-1.17193400	-0.05409900	3.70234500	H	-1.18778900	0.03649700	3.74696500
H	1.21670900	-1.54394400	2.54414500	H	1.25902700	-1.35223300	2.67861200
H	-1.21043900	-1.45958200	2.63231700	H	-1.19019200	-1.37824000	2.68606700

N	0.03418500	0.07626700	1.96454000	N	0.01602900	0.19163000	2.01287900
C	-3.25370400	1.32883600	-0.56672200	C	-3.34876000	1.36055600	-0.50302400
C	3.22701200	1.49665700	-0.45123800	C	3.32527500	1.53816200	-0.45470500
H	-2.73996400	2.17292800	-0.09984100	H	-2.76396800	2.20278300	-0.12193300
H	2.73955500	2.27125000	0.14855900	H	2.80930200	2.34135400	0.08087600
C	-3.35500100	-1.61195600	-0.21157700	C	-3.46392100	-1.58911000	-0.10416800
C	3.44443300	-1.45778900	-0.37855200	C	3.58052200	-1.41418300	-0.11154400
C	-3.24142300	-2.70815100	0.84448500	C	-3.30136000	-2.66529600	0.96554500
C	3.42257600	-2.64448000	0.58228500	C	3.39663400	-2.55397900	0.88584500
O	0.03190500	-0.20512100	-3.04514200	O	0.05848000	-0.30919800	-3.25976400
H	4.45060700	-1.03105100	-0.34676700	H	4.58022900	-0.99662500	0.03935200
H	-4.37844500	-1.22748700	-0.17662200	H	-4.48510200	-1.20132600	-0.03797200
C	3.16148900	-1.90997700	-1.80986500	C	3.47623700	-1.92030800	-1.54786400
C	-3.10117200	-2.16868200	-1.61180700	C	-3.25802100	-2.17392300	-1.50048000
H	3.19353700	-1.08559400	-2.52456600	H	3.64087300	-1.13106400	-2.28331900
H	-3.18972200	-1.40692300	-2.38842400	H	-3.34814100	-1.42527500	-2.28917800
H	2.18268500	-2.38783900	-1.89254500	H	2.49689000	-2.36321800	-1.74411700
H	-2.10716000	-2.61318200	-1.69314600	H	-2.27732700	-2.64580900	-1.59482300
H	3.91401000	-2.64314200	-2.11866200	H	4.23105700	-2.69438400	-1.71995900
H	-3.83250700	-2.95268700	-1.83456300	H	-4.01380700	-2.94347000	-1.68858000
C	-3.12540300	1.49594600	-2.07778300	C	-3.33258500	1.44069500	-2.02612000
C	2.99901100	1.82510300	-1.92318300	C	3.13287800	1.77657100	-1.94906400
H	-3.65583500	0.71188800	-2.62376900	H	-3.96888900	0.67731800	-2.48057600
H	3.49136000	1.10374800	-2.57991900	H	3.65366100	1.02915800	-2.55216200
H	-2.08486000	1.49313100	-2.40658000	H	-2.32521100	1.33067500	-2.43271500
H	1.93777000	1.84636500	-2.18017600	H	2.07924600	1.76763100	-2.23602300
H	-3.56673100	2.45226800	-2.37759800	H	-3.71739200	2.41484500	-2.34465900
H	3.41873900	2.81058000	-2.15032100	H	3.54424200	2.75496900	-2.21768100
C	-4.71711500	1.37020100	-0.13246000	C	-4.76929500	1.48032800	0.04324100
C	4.71285300	1.52674000	-0.09995700	C	4.79964600	1.60172500	-0.06346400
H	-4.84329300	1.24604500	0.94580300	H	-4.80652400	1.44529700	1.13458200
H	4.90462200	1.26674200	0.94399100	H	4.95992000	1.42281300	1.00269800
H	-5.31562100	0.60596100	-0.63507900	H	-5.42552800	0.69754100	-0.34603000
H	5.29611500	0.85246300	-0.73212200	H	5.40036000	0.88184700	-0.62494300
H	-5.14554500	2.34165100	-0.40103400	H	-5.19480600	2.44062100	-0.26636300
H	5.10228500	2.53717700	-0.26210600	H	5.19179000	2.59815800	-0.29125400
H	-0.06909300	1.51567200	-0.17280700	H	-0.04721700	1.69097600	-0.18712200
H	0.07555300	1.10172000	2.03692800	H	0.00643900	1.22262000	2.06459300
C	0.13256700	3.01404900	0.39038600	C	0.07523200	3.09174600	0.36366800
H	-3.91835400	-3.52858500	0.58289000	H	-3.97272400	-3.49994500	0.73775200
H	-2.23478200	-3.12468700	0.90415100	H	-2.28577500	-3.06409000	0.99617600
H	-3.52796700	-2.35859900	1.83817200	H	-3.56030400	-2.30551000	1.96294400
H	4.13750300	-3.39697600	0.23290200	H	4.12956500	-3.33829300	0.66931800
H	3.71690500	-2.36754800	1.59627400	H	3.55852200	-2.23684300	1.91757300
H	2.44393400	-3.12354400	0.62813100	H	2.40651500	-3.00587600	0.81531300
O	0.25301500	2.95230800	1.62661800	O	0.03670000	3.05051600	1.61318800
C	0.05403100	-1.93367600	-0.11045000	C	0.06070900	-2.06326700	-0.14710200
Mn	0.01949100	-0.18912400	-0.13486700	Re	0.02662700	-0.17776100	-0.20209700
C	0.02372700	-0.18768700	-1.87646200	C	0.04348900	-0.25698800	-2.08603500
H	0.99317500	3.13714000	-0.27395800	H	1.01741500	3.26162200	-0.17088900
O	-0.98677600	3.64484500	-0.09590400	O	-0.98435000	3.72421500	-0.26133200
H	-0.92358300	3.71266100	-1.05923200	H	-0.81011500	3.77694000	-1.21172700
Mn-TS4-H⁺-SMD(CH₃OH)				Re-TS4-H⁺-SMD(CH₃OH)			
O	-0.02234400	-3.12045400	0.15017600	O	0.07187700	-3.16266100	-0.10807100
P	2.31332500	-0.07634000	0.10217900	P	2.41376600	-0.03134100	0.19911300
C	-1.21242100	-0.11075000	2.62992500	P	-2.38783200	-0.10555700	0.17674400
H	-1.17491500	0.31697400	3.64018300	C	2.48028500	0.50592600	1.97871600
H	-1.24186700	-1.19676600	2.74237300	C	-2.48885000	0.43191800	1.95257100
N	0.00632200	0.25710400	1.88546900	H	2.61172700	1.59053900	1.97821500

H	0.01823500	1.60714500	1.73411800	H	-2.65643800	1.51163100	1.95071200
O	0.02541700	2.81935700	1.51506800	H	-3.33533500	-0.02738900	2.46445400
C	-0.01174700	-1.96348500	0.04780800	C	1.17880800	0.13476600	2.67647200
P	-2.30514900	-0.06104800	0.12122100	C	-1.18209600	0.10131900	2.66847900
C	2.46097300	0.34812600	1.90805400	H	1.12855800	0.66439100	3.64077300
C	-2.45517700	0.38481600	1.91542000	H	-1.15856300	0.63818200	3.63013700
H	2.53174500	1.43784700	1.96165500	H	1.17287000	-0.93750800	2.91120900
H	-2.50805700	1.47537000	1.96816800	H	-1.14549400	-0.96729900	2.90640300
H	3.36466200	-0.05916400	2.36383500	C	-3.45904200	-1.59113500	0.11201000
H	-3.36407100	-0.01011600	2.37197800	C	-3.19753200	-2.48701100	1.32496200
C	1.20981900	-0.12033100	2.63449000	O	0.03820900	-0.43008800	-3.26062700
H	1.18759800	0.32524700	3.64004300	H	-4.45509800	-1.31918600	0.26730500
H	1.23445300	-1.20871200	2.77436000	C	-3.34678800	-2.31938400	-1.29329400
C	-3.14509300	1.40933200	-0.70566900	H	-3.63967100	-1.64722500	-2.10513200
C	3.15081300	1.40698700	-0.69748900	H	-2.33557700	-2.68239300	-1.50439500
H	-2.62563900	2.24736500	-0.22916100	H	-4.02036200	-3.18388800	-1.31782600
H	2.54767400	2.23244200	-0.30424300	H	-3.83813900	-3.37044500	1.26824000
C	-3.45594200	-1.51846200	-0.15099500	H	-2.16228800	-2.83254900	1.36558400
C	3.45440200	-1.53223300	-0.21354700	H	-3.42681400	-1.98602500	2.26535900
C	-3.38045100	-2.56194000	0.96101400	C	0.03079400	-0.31146500	-2.09495600
C	3.42685100	-2.56812900	0.90735000	C	0.04949200	-1.98650700	-0.14603500
O	-0.02609700	-0.68235600	-2.99551900	Re	0.01616300	-0.14880400	-0.20330200
H	4.45780400	-1.09700400	-0.24397000	N	-0.00380500	0.46807800	1.86947500
H	-4.45914700	-1.08310200	-0.12730400	H	-0.02082700	1.72393900	1.66386700
C	-3.23772900	-2.15832500	-1.52059600	O	-0.03521300	3.00672500	1.43622700
H	-3.30762800	-1.43711300	-2.33666300	H	3.33825900	0.07936300	2.50108500
H	-2.26215600	-2.64597800	-1.58475900	C	-3.36432300	1.26527700	-0.67258800
H	-4.00114700	-2.92421200	-1.69120400	C	3.35565900	1.37147900	-0.63017400
C	-2.89977700	1.50681200	-2.20695300	H	-2.87034700	2.16071200	-0.28115600
C	3.05058400	1.43728200	-2.21842700	H	2.79012800	2.23704100	-0.26609600
H	-3.38577800	0.69710900	-2.75600400	C	3.50683700	-1.54740100	0.07080400
H	3.67107800	0.66640500	-2.68125400	C	3.26143500	-2.54992400	1.19876700
H	-1.83606300	1.49189100	-2.44964800	H	4.52231900	-1.15856900	0.18648100
H	2.02540000	1.30743000	-2.56922300	C	3.39314100	-2.21305300	-1.29888200
H	-3.31155700	2.44898400	-2.58286800	H	3.61773600	-1.52783900	-2.11541100
H	3.40606800	2.40476800	-2.58710400	H	2.39165700	-2.62139800	-1.46447900
C	-4.62905700	1.53445200	-0.37102500	H	4.10310200	-3.04440900	-1.35762600
C	4.59062400	1.61509600	-0.23444600	C	-3.22043200	1.28446000	-2.18872300
H	-4.82605700	1.44093100	0.69968700	C	3.26849700	1.37367700	-2.15236900
H	4.68903000	1.59816100	0.85310200	H	-3.70553200	0.42724000	-2.66101600
H	-5.22824100	0.78606200	-0.89573800	H	3.84705100	0.56049600	-2.59548200
H	5.26297500	0.85997000	-0.64990200	H	-2.17258400	1.29223100	-2.50128600
H	-4.99032000	2.51851000	-0.68688300	H	2.23700100	1.28918600	-2.50535200
H	4.94616200	2.59093500	-0.58103700	H	-3.69337400	2.18654700	-2.59023700
H	-0.15507700	2.27011400	-0.43651200	H	3.67436400	2.31347800	-2.53925400
H	-4.10872900	-3.35303400	0.75409700	C	-4.83150700	1.31699200	-0.25417200
H	-2.39811500	-3.03199600	1.02208100	C	4.79889700	1.51619400	-0.15732300
H	-3.62440200	-2.14699700	1.94045700	H	-4.95946500	1.30027800	0.83185000
H	4.12577900	-3.37502500	0.66374300	H	4.88838500	1.51653400	0.93146400
H	3.73442200	-2.15342100	1.86871300	H	-5.40330200	0.48763000	-0.67983900
H	2.43971100	-3.01777400	1.02693800	H	5.43320400	0.71639600	-0.55242200
C	-0.01429800	-0.46384900	-1.85210600	H	-5.28530600	2.24403000	-0.62076500
C	-0.05124900	3.11771200	0.27295500	H	5.21113200	2.46203200	-0.52243500
O	-0.02673100	4.25924200	-0.18666500	H	-0.47102400	2.39970000	-0.44595900
Mn	-0.00067600	-0.25205600	-0.10239400	H	3.95811500	-3.38611000	1.08606700
H	2.19802200	-2.68867000	-1.56647800	H	3.43408900	-2.11475400	2.18607500
H	3.93204000	-2.93913300	-1.77475400	H	2.25139100	-2.95880900	1.17355600
C	3.16705500	-2.18464100	-1.56496400	C	-0.24918000	3.27381700	0.20889700
H	3.17507600	-1.47008300	-2.38952500	O	-0.24171300	4.39624800	-0.30230300
3Mn⁺-OOCH⁻-SMD(CH₃OH)				3Re⁺-OOCH⁻-SMD(CH₃OH)			

O	-0.01563800	-3.06025500	-0.38397000	O	-0.02839000	-3.16994900	0.20643500
P	2.30011800	-0.07348600	0.15658700	P	2.40205700	-0.05932800	0.17526200
P	-2.31237700	-0.05309700	0.16164800	P	-2.41604200	-0.02425500	0.17030400
C	2.45054800	-0.07290400	2.00964100	C	2.46599900	0.48401400	1.95447200
C	-2.45889400	-0.04062400	2.01520900	C	-2.47532300	0.50051500	1.95567000
H	2.50953300	0.97470200	2.31815800	H	2.51484600	1.57667600	1.94102700
H	-2.50250900	1.00914400	2.31953100	H	-2.51609000	1.59347700	1.95468600
H	3.35805300	-0.56918400	2.35620200	H	3.36223100	0.12489500	2.46263300
H	-3.37257900	-0.52277700	2.36573700	H	-3.37405400	0.14245300	2.46000600
C	1.21471000	-0.71612500	2.60882600	C	1.21730700	0.03590400	2.69137600
C	-1.23042500	-0.69834700	2.61404700	C	-1.22935800	0.03570100	2.68811900
H	1.19436700	-0.55666500	3.69353600	H	1.19458200	0.48366000	3.69156300
H	-1.20483800	-0.53554600	3.69815600	H	-1.20389600	0.47394500	3.69247600
H	1.20727700	-1.79400600	2.43275700	H	1.19939600	-1.04908500	2.81204200
H	-1.23724900	-1.77677200	2.44122500	H	-1.21903400	-1.05052700	2.79834000
N	-0.00515400	-0.14806100	1.99446500	N	-0.00454700	0.42699700	1.94928800
C	-3.16605500	1.56091900	-0.28736700	C	-3.30356400	1.40158500	-0.67024200
C	3.17147700	1.53174300	-0.29002200	C	3.32148800	1.34169900	-0.67560900
H	-2.60524900	2.27823600	0.32137300	H	-2.69018600	2.25029700	-0.34427200
H	2.58931400	2.26308600	0.28047000	H	2.73236600	2.20754500	-0.35238000
C	-3.45487300	-1.40757100	-0.46033800	C	-3.53081300	-1.51973700	0.00556700
C	3.42601500	-1.43703700	-0.47962000	C	3.49625900	-1.57183700	0.02923600
C	-3.43426900	-2.66660800	0.40237000	C	-3.41128900	-2.48738800	1.18053300
C	3.41504500	-2.69221400	0.38902000	C	3.35667300	-2.52964700	1.20991600
O	-0.00519400	-0.01795800	-3.02015300	O	-0.01075200	-0.76693100	-3.21171000
H	4.42994300	-1.00545200	-0.42817600	H	4.51438100	-1.17053000	0.04036600
H	-4.45573000	-0.97205600	-0.38934600	H	-4.54366700	-1.10517400	0.01198400
C	3.12082600	-1.77976900	-1.93669000	C	3.27118200	-2.29591700	-1.29607300
C	-3.17413700	-1.74220300	-1.92385200	C	-3.30536700	-2.23887800	-1.32259900
H	3.11643300	-0.90292300	-2.58596200	H	3.39338500	-1.64069900	-2.15955400
H	-3.18327800	-0.86133400	-2.56776400	H	-3.40664300	-1.57610300	-2.18313900
H	2.15355200	-2.27729200	-2.03493200	H	2.27233000	-2.73443000	-1.34679600
H	-2.20674200	-2.23549700	-2.04094900	H	-2.31421300	-2.69555200	-1.36576700
H	3.88437300	-2.46661500	-2.31572500	H	3.99713600	-3.10950400	-1.39260900
H	-3.94177700	-2.42928900	-2.29399800	H	-4.04473400	-3.03868700	-1.43174300
C	-3.00437400	1.95803000	-1.75079900	C	-3.24368000	1.33827700	-2.19280300
C	3.06820500	1.89789300	-1.76701900	C	3.25583500	1.27581900	-2.19790300
H	-3.57477400	1.30294700	-2.41344500	H	-3.88165500	0.54579200	-2.59085200
H	3.67290700	1.23519000	-2.39072600	H	3.87709200	0.47048500	-2.59647200
H	-1.96122300	1.94545400	-2.07129100	H	-2.22726500	1.17462000	-2.55816700
H	2.04024900	1.86976400	-2.13222200	H	2.23549800	1.13143500	-2.56024200
H	-3.38268900	2.97515700	-1.89413000	H	-3.60033200	2.28441100	-2.61189400
H	3.44407700	2.91523600	-1.91479400	H	3.62955800	2.21403800	-2.61984700
C	-4.62756000	1.63000700	0.14852600	C	-4.72945400	1.62122700	-0.17455100
C	4.61677500	1.60730900	0.19645000	C	4.75362100	1.53149700	-0.18493300
H	-4.77210600	1.33827100	1.19145800	H	-4.79153300	1.67689200	0.91448700
H	4.72214000	1.35069300	1.25296100	H	4.82002600	1.59177600	0.90361200
H	-5.26896300	1.00209700	-0.47482000	H	-5.40151000	0.82914500	-0.51481400
H	5.27617300	0.95501000	-0.38148200	H	5.40808600	0.72405300	-0.52311000
H	-4.98462300	2.65963300	0.04488800	H	-5.11293300	2.56564600	-0.57397400
H	4.98456200	2.63072000	0.07081100	H	5.15581300	2.46561300	-0.59020300
H	-0.20783300	1.70052100	-0.03158100	H	0.09498900	2.44251300	-0.39094600
H	0.00299500	0.86677100	2.17411600	H	-0.00779300	1.46211400	1.88223400
H	-4.16531000	-3.37881300	0.00606700	H	-4.09849700	-3.32428900	1.02035800
H	-2.46078700	-3.15891800	0.39006300	H	-2.40612500	-2.90261800	1.27075200
H	-3.70665000	-2.46683300	1.44003000	H	-3.68012800	-2.02589400	2.13220500
H	4.13207200	-3.41165300	-0.01965800	H	4.03881000	-3.37311300	1.06314000
H	3.71100900	-2.49007000	1.41967800	H	3.61941900	-2.06267600	2.16063400
H	2.43787800	-3.17752700	0.39983500	H	2.34730400	-2.93611900	1.29275000

O 0.06484900 2.78661900 1.67491900	O -0.03079100 3.30069000 1.43637400
C -0.00458000 -0.05474500 -1.85980800	C -0.00990600 -0.52871700 -2.06615800
C 0.00755600 2.74734100 0.43614600	C 0.09147700 3.40333700 0.19112400
O 0.09959800 3.63663600 -0.41527900	O 0.21206400 4.44672100 -0.48062900
C -0.00960000 -1.90458700 -0.25813700	C -0.02102100 -2.00450900 0.05347500
Mn -0.00637200 -0.17726600 -0.10617900	Re -0.00803700 -0.18151500 -0.20403300
Mn-TS4-H-SMD(CH₃OH)	Re-TS4-H-SMD(CH₃OH)
O -0.00072600 -3.17208800 -0.35207000	O 0.00124600 -3.28639700 -0.25419400
P 2.26672900 -0.07426200 0.15138800	P 2.38088000 -0.01876500 0.20750300
P -2.26695700 -0.07358700 0.15130400	P -2.38059500 -0.02000700 0.20824900
C 2.43906800 -0.05068400 2.00664100	C 2.45482400 0.09713900 2.06905000
C -2.43921800 -0.04969700 2.00655000	C -2.45530500 0.09179800 2.06998000
H 2.46604400 1.00041100 2.30982000	H 2.46436700 1.16396600 2.31280700
H -2.46560000 1.00145900 2.30957600	H -2.46809000 1.15799200 2.31643800
H 3.36511300 -0.51414800 2.35029300	H 3.37036600 -0.33610500 2.47398000
H -3.36547700 -0.51260900 2.35034100	H -3.36964500 -0.34524500 2.47353600
C 1.22611200 -0.72595200 2.61871400	C 1.23165400 -0.55312000 2.69054900
C -1.22657000 -0.72551200 2.61862500	C -1.23056000 -0.55681700 2.69013400
H 1.21228200 -0.57298000 3.70546800	H 1.21046400 -0.35882000 3.76958900
H -1.21272800 -0.57266700 3.70539700	H -1.20946500 -0.36421600 3.76948100
H 1.23847500 -1.80231100 2.43367000	H 1.23832600 -1.63473400 2.54298500
H -1.23936900 -1.80183900 2.43344300	H -1.23506800 -1.63821800 2.54075800
N -0.00011000 -0.17692100 2.00999800	N -0.00015400 -0.02295500 2.06334300
C -3.10882600 1.54635900 -0.30386900	C -3.24220700 1.57500200 -0.28251400
C 3.10893900 1.54562700 -0.30346800	C 3.24208000 1.57554800 -0.28594400
H -2.52911500 2.25681700 0.29501800	H -2.62333000 2.31622700 0.23475100
H 2.52943300 2.25601400 0.29570900	H 2.62316200 2.31764100 0.22999400
C -3.45942200 -1.40077800 -0.44699000	C -3.56324800 -1.39022100 -0.29098500
C 3.45895300 -1.40161100 -0.44697800	C 3.56410000 -1.38969900 -0.28801000
C -3.44298200 -2.66087200 0.41421600	C -3.50869900 -2.59612700 0.64289200
C 3.44145600 -2.66224100 0.41341600	C 3.50905000 -2.59346800 0.64861300
O 0.00000300 -0.08467000 -3.02475400	O -0.00083900 -0.17835800 -3.24648300
H 4.45305100 -0.95310900 -0.36163800	H 4.56151500 -0.94651100 -0.21416300
H -4.45338900 -0.95183100 -0.36252600	H -4.56077100 -0.94736100 -0.21667500
C 3.20717600 -1.74659100 -1.91354400	C 3.32664000 -1.82108000 -1.73403100
C -3.20690700 -1.74667200 -1.91321700	C -3.32498200 -1.81836100 -1.73784000
H 3.22267500 -0.86965000 -2.56292300	H 3.33537400 -0.98360200 -2.43382100
H -3.22140700 -0.87003200 -2.56303100	H -3.33253100 -0.97934600 -2.43581300
H 2.24234000 -2.24201000 -2.04393400	H 2.36777700 -2.33413100 -1.83851500
H -2.24232000 -2.24279900 -2.04274800	H -2.36645900 -2.33199400 -1.84278300
H 3.98219900 -2.43376700 -2.26888700	H 4.11240900 -2.51878300 -2.04156500
H -3.98217500 -2.43348600 -2.26872500	H -4.11103100 -2.51477200 -2.04759400
C -2.94820600 1.93229000 -1.77095300	C -3.16965200 1.86587400 -1.77750200
C 2.94824500 1.93210800 -1.77040000	C 3.16957900 1.86418400 -1.78135600
H -3.54890000 1.29444500 -2.42401700	H -3.81589900 1.19642900 -2.35058000
H 3.54908700 1.29465900 -2.42371100	H 3.81325200 1.19179100 -2.35387000
H -1.90957600 1.87705600 -2.10152800	H -2.15295000 1.77408100 -2.16368000
H 1.90963500 1.87677500 -2.10101600	H 2.15231500 1.77531500 -2.16676100
H -3.29104300 2.96153300 -1.91917100	H -3.50994100 2.88854300 -1.96897300
H 3.29085700 2.96148400 -1.91820800	H 3.51317200 2.88543600 -1.97454100
C -4.56717100 1.65239700 0.13537900	C -4.67084800 1.70804700 0.23833500
C 4.56735100 1.65120600 0.13566200	C 4.67067700 1.70960300 0.23484400
H -4.71413700 1.37998800 1.18333700	H -4.75097700 1.50863600 1.30954900
H 4.71439700 1.37826500 1.18347100	H 4.75110400 1.51021900 1.30603900
H -5.22288400 1.02572800 -0.47459000	H -5.35872000 1.03924200 -0.28532800
H 5.22287000 1.02470800 -0.47469200	H 5.35901800 1.04133100 -0.28889700
H -4.90820300 2.68607300 0.01568100	H -5.02438100 2.73029800 0.06878100
H 4.90856000 2.68487800 0.01643000	H 5.02339900 2.73213600 0.06531400
H 0.00001200 1.38216000 -0.06488200	H 0.00361200 1.59165900 -0.10864900

H	0.00006300	0.82560700	2.19380600	H	-0.00168400	0.98520800	2.22331400
H	-4.17700000	-3.37309100	0.02255900	H	-4.21634900	-3.35406900	0.29122700
H	-2.47016000	-3.15493800	0.39855800	H	-2.51862400	-3.05598800	0.65535200
H	-3.70943500	-2.46070800	1.45360500	H	-3.78520700	-2.34575700	1.66878200
H	4.17673800	-3.37376500	0.02286800	H	4.21495600	-3.35331400	0.29755600
H	3.70553600	-2.46263500	1.45351300	H	3.78752800	-2.34126400	1.67352400
H	2.46895000	-3.15683800	0.39529800	H	2.51827800	-3.05173900	0.66357400
O	0.00120800	2.97356500	1.70068400	O	-0.00110600	3.16645000	1.59176700
C	-0.00005300	-0.14833500	-1.85674700	C	-0.00039200	-0.19103200	-2.07044600
C	0.00139100	3.12972300	0.53511000	C	-0.00171900	3.27425000	0.41828800
O	0.00183400	3.68607100	-0.49784800	O	-0.00308000	3.82020300	-0.62304700
C	-0.00045000	-2.01013000	-0.21067000	C	0.00044500	-2.11332400	-0.20188700
Mn	-0.00012400	-0.26174000	-0.12219900	Re	0.00012200	-0.21243100	-0.18789600
Mn-TS(HCOOH)-SMD(CH₃OH)				Re-TS(HCOOH)-SMD(CH₃OH)			
P	-2.31046900	-0.02456100	0.12011600	P	-2.40630600	-0.02455200	0.18906900
P	2.30673200	-0.01761000	0.10377700	P	2.40974600	-0.03225600	0.19773800
C	-2.44716400	-0.40646000	1.93425700	C	-2.46489600	-0.57821000	1.96306300
C	2.44919800	-0.39909100	1.91619300	C	2.46443500	-0.59364500	1.97015400
H	-2.50088300	-1.49502700	2.02467000	H	-2.51470200	-1.67036300	1.93637700
H	2.49708000	-1.48907400	1.99476100	H	2.51495900	-1.68574400	1.94322200
H	-3.35295900	0.00527300	2.38282600	H	-3.36386500	-0.22079800	2.46869100
H	3.35913700	0.00157900	2.36543300	H	3.36192300	-0.23544900	2.47819700
C	-1.19147300	0.11159200	2.61832300	C	-1.20158700	-0.14565000	2.69219900
C	1.19718600	0.11000700	2.61236800	C	1.20034600	-0.15935700	2.69787300
H	-1.17162200	-0.25501400	3.65795600	H	-1.15814900	-0.67229200	3.65803200
H	1.18746500	-0.26704000	3.64843700	H	1.15005500	-0.69292300	3.65958400
H	-1.23324400	1.20948400	2.68689700	H	-1.25328900	0.92727600	2.93129400
H	1.23390100	1.20741200	2.69212300	H	1.25837800	0.91127100	2.94557900
C	3.20997700	-1.47268700	-0.67268800	N	-0.00061100	-0.44459300	1.90961900
C	-3.20453400	-1.49363800	-0.64757000	C	3.33823700	-1.42174300	-0.66236800
H	2.58393700	-2.31660300	-0.36757200	C	-3.34320300	-1.41257900	-0.66446400
H	-2.66481000	-2.33208400	-0.19555900	H	2.75936700	-2.29150700	-0.33210600
C	3.42769700	1.45347300	-0.24381300	H	-2.72485400	-2.27747600	-0.39949000
C	-3.45165200	1.43981300	-0.17706800	C	3.51319200	1.47787300	0.09083400
C	3.46150200	2.47399600	0.89165900	C	-3.50408100	1.48707600	0.05616400
C	-3.38111500	2.50454300	0.91547500	C	3.28844900	2.45542700	1.24181100
O	-0.03434100	0.64286400	-3.02223900	C	-3.32816400	2.45251900	1.22549500
H	-4.45947300	1.01480900	-0.15769000	O	0.00464000	0.50915500	-3.24347800
H	4.43164400	1.02944600	-0.34093500	H	-4.52493400	1.09379100	0.09503300
C	-3.20779600	2.06226600	-1.55049400	H	4.53077200	1.08476200	0.17938100
C	3.06235500	2.12768100	-1.56577300	C	-3.30894900	2.20178700	-1.27977600
H	-3.30367800	1.34131700	-2.36404800	C	3.37515200	2.17700000	-1.25979100
H	2.97213400	1.42014700	-2.39154600	H	-3.42091800	1.53435600	-2.13531600
H	-2.21042100	2.50400900	-1.61169800	H	3.60610500	1.51856300	-2.09847300
H	2.11730600	2.66828700	-1.48603100	H	-2.32157000	2.66343200	-1.34442800
H	-3.93545800	2.86088200	-1.72811200	H	2.36548900	2.56760600	-1.40707700
H	3.83816300	2.85222800	-1.83408300	H	-4.05470700	2.99703100	-1.38037700
C	3.22664000	-1.42992900	-2.19773100	H	4.06821400	3.02339100	-1.30498800
C	-3.04192500	-1.59796200	-2.16024200	C	3.26468200	-1.37048400	-2.18436600
H	3.57605100	-2.39020900	-2.59053800	C	-3.36443100	-1.30328300	-2.18573200
H	-1.99726700	-1.53275900	-2.46741300	H	3.62559900	-2.31739300	-2.59887700
H	3.90876000	-0.66114900	-2.56975800	H	-2.37746300	-1.08966500	-2.60140000
H	-3.43153200	-2.56120600	-2.50589900	H	3.89271100	-0.57672200	-2.59544200
H	2.23718800	-1.23938300	-2.61874500	H	-3.70783900	-2.25033500	-2.61429000
H	-3.60060800	-0.81787200	-2.68266000	H	2.24437200	-1.21891600	-2.54177300
C	4.61113400	-1.70450400	-0.11241100	H	-4.05391400	-0.52669800	-2.52531300
C	-4.67068500	-1.61214900	-0.23890000	C	4.77443400	-1.59802500	-0.17720500
H	4.62939400	-1.72651100	0.97918500	C	-4.74435800	-1.64226700	-0.10518200
H	-4.81871000	-1.49671200	0.83744000	H	4.84709900	-1.64411600	0.91179800

H 5.31671500 -0.94037300 -0.44898000	H -4.74695200 -1.76651600 0.97982800
H -5.29452900 -0.87360100 -0.74878500	H 5.42258300 -0.79105000 -0.52834300
H 4.99004600 -2.66953100 -0.46544400	H -5.42122300 -0.82155400 -0.35622800
H -5.04876300 -2.60139300 -0.51766400	H 5.18127800 -2.53454500 -0.57275500
H 4.10184800 3.31346200 0.60049500	H -5.16652800 -2.55404300 -0.54056300
H -4.12512300 3.27976000 0.70365600	H -0.00258400 -1.89510400 1.66149000
H 2.47241100 2.88003100 1.11044100	H 3.97471500 3.30100200 1.12910000
H -2.40596900 2.99144200 0.95493800	H -3.98503000 3.31588900 1.07759400
H 3.87285600 2.05906200 1.81350300	H 2.27363200 2.85643500 1.24829600
H -3.60515500 2.10517500 1.90608700	H -2.30578000 2.82796200 1.29738400
O 0.00237800 -2.06067800 -0.55326300	H 3.48533100 2.00372400 2.21578900
C -0.01827800 0.39875200 -1.88188600	H -3.59529000 2.00029800 2.18228000
C 0.00043200 1.82652100 0.11701100	O 0.00082900 -2.40021500 -0.74709900
O 0.00955700 2.98193300 0.28741900	C 0.00412500 0.35616300 -2.07992100
Mn -0.00431400 0.11799000 -0.15104900	C 0.00681800 1.97809500 -0.05135000
C 0.00208200 -2.97580200 0.27886600	O 0.00941300 3.15647400 0.00653100
H 0.00860500 -4.01863700 -0.06626500	Re 0.00290600 0.14020500 -0.19200800
N 0.00101000 -0.32580000 1.90022700	C -0.00275400 -3.23819800 0.15808100
H -0.00667900 -1.53937800 1.79781800	H -0.00420100 -4.30961500 -0.09038500
O -0.00414600 -2.82104000 1.55127600	O -0.00597000 -2.99916800 1.42488600
2Mn-OCH-SMD(CH₃OH)	2Re-OCH-SMD(CH₃OH)
P -2.31109700 -0.01677300 0.11685600	P -2.40433400 -0.06093600 0.17774300
P 2.31115100 -0.01626400 0.11705800	P 2.40434700 -0.06095500 0.17781200
C -2.44568900 -0.34599300 1.94277100	C -2.46251200 -0.47830100 1.99410900
C 2.44595100 -0.34372800 1.94327500	C 2.46242000 -0.47837400 1.99417000
H -2.46667800 -1.43294700 2.06338200	H -2.48372200 -1.56995500 2.06159100
H 2.46806000 -1.43055800 2.06478900	H 2.48354800 -1.57003500 2.06160700
H -3.36525700 0.04849200 2.37706800	H -3.36995600 -0.10699900 2.47261800
H 3.36507900 0.05204700 2.37733200	H 3.36986600 -0.10716100 2.47274200
C -1.22258000 0.22143300 2.63988200	C -1.22771600 0.05258100 2.70284900
C 1.22221000 0.22300300 2.63983200	C 1.22762600 0.05255300 2.70287600
H -1.20703500 -0.09439400 3.69087600	H -1.20905400 -0.30972000 3.73778500
H 1.20681200 -0.09223300 3.69100600	H 1.20893000 -0.30973400 3.73781600
H -1.23458700 1.31402400 2.62485000	H -1.23075300 1.14422700 2.73325000
H 1.23318300 1.31560300 2.62416300	H 1.23069500 1.14420000 2.73326800
N 0.00010100 -0.23456000 1.95487500	N -0.00004100 -0.38108800 2.00218100
C 3.20147700 -1.50518400 -0.60480800	C 3.29703900 -1.52449300 -0.58355400
C -3.20131400 -1.50508700 -0.60639100	C -3.29692400 -1.52454300 -0.58360200
H 2.59856300 -2.33290000 -0.21971000	H 2.66735900 -2.35991500 -0.26092200
H -2.59841700 -2.33307800 -0.22185900	H -2.66728600 -2.35992100 -0.26075800
C 3.44547000 1.43902900 -0.24580800	C 3.53524900 1.41371100 -0.07671100
C -3.44581300 1.43867600 -0.24409700	C -3.53527200 1.41369300 -0.07683500
C 3.44655800 2.50464500 0.84742400	C 3.46208500 2.42738800 1.06206500
C -3.44666400 2.50321100 0.85018400	C -3.46232600 2.42727900 1.06203800
O 0.00018100 0.58790300 -3.02916600	O 0.00012300 0.78471600 -3.18655100
H -4.44960100 1.00550200 -0.28651000	H -4.54566700 0.99393600 -0.09281800
H 4.44934400 1.00606600 -0.28825300	H 4.54567300 0.99401800 -0.09252900
C -3.13292000 2.05994300 -1.60452300	C -3.26632100 2.08753000 -1.42133500
C 3.13173000 2.05883100 -1.60668500	C 3.26645600 2.08743000 -1.42130400
H -3.13328000 1.32637000 -2.41232300	H -3.29941200 1.38839900 -2.25852500
H 3.13248600 1.32450200 -2.41378800	H 3.29960300 1.38822800 -2.25843300
H -2.15979700 2.55597100 -1.60245300	H -2.28895400 2.57561900 -1.43034600
H 2.15818500 2.55403200 -1.60482900	H 2.28910400 2.57554000 -1.43044900
H -3.88872400 2.81507400 -1.84402300	H -4.02452100 2.85634500 -1.60163100
H 3.88686600 2.81435100 -1.84706700	H 4.02469400 2.85620900 -1.60159900
C 3.14951200 -1.55776100 -2.12842900	C 3.29542000 -1.49700700 -2.10884100
C -3.14907700 -1.55646000 -2.13002700	C -3.29506200 -1.49725700 -2.10889300
H 3.78242200 -0.79072100 -2.58154400	H 3.96809900 -0.72945600 -2.49927800
H -3.78180000 -0.78899000 -2.58267100	H -3.96770900 -0.72978400 -2.49953800

H 2.13449200 -1.43349300 -2.51039600	H 2.29843600 -1.31795400 -2.51755400
H -2.13397200 -1.43201400 -2.51169600	H -2.29802100 -1.31821300 -2.51747300
H 3.51866900 -2.52862700 -2.47435000	H 3.64486100 -2.46095000 -2.49221600
H -3.51826500 -2.52701600 -2.47678200	H -3.64440100 -2.46126400 -2.49219800
C 4.62794500 -1.68776200 -0.09220100	C 4.70117200 -1.74816000 -0.02929400
C -4.62787200 -1.68797300 -0.09416600	C -4.70114200 -1.74814700 -0.02952400
H 4.68903600 -1.66667600 0.99820000	H 4.71906300 -1.79052500 1.06195500
H -4.68912200 -1.66773800 0.99623700	H -4.71921000 -1.79032700 1.06173100
H 5.30560000 -0.92596000 -0.48631000	H 5.39572500 -0.96809700 -0.35164300
H -5.30540500 -0.92579600 -0.48777000	H -5.39565600 -0.96815100 -0.35211900
H 5.00937000 -2.65981700 -0.42223400	H 5.09100700 -2.70173700 -0.40027400
H -5.00933400 -2.65973300 -0.42502200	H -5.09089800 -2.70179500 -0.40040500
H 0.00076100 -1.26293100 1.97368400	H -0.00006400 -1.41020800 1.98282500
H 4.14724000 3.29885600 0.56922900	H 4.13654000 3.26117400 0.84128900
H -4.14746800 3.29766200 0.57296900	H -4.13680000 3.26104100 0.84123400
H 2.46596400 2.96649600 0.97364400	H 2.45859100 2.84115700 1.17753800
H -2.46606900 2.96500400 0.97663000	H -2.45887600 2.84109600 1.17769400
H 3.76959000 2.11394900 1.81389600	H 3.77266000 2.00550200 2.01939600
H -3.76942700 2.11154000 1.81634800	H -3.77301500 2.00529600 2.01928900
O 0.00006900 -1.96823300 -0.49732900	O 0.00000600 -2.05396600 -0.63323900
C 0.00003700 0.37817700 -1.88461500	C 0.00002100 0.51572600 -2.04533900
C -0.00015700 1.84743800 0.06997800	C -0.00001700 1.97197900 0.11507100
O -0.00021600 3.00814700 0.18731700	O -0.00011000 3.13531100 0.28838500
Mn 0.00001200 0.12335900 -0.14780000	Re -0.00000200 0.13316000 -0.19707800
C 0.00034000 -3.01201600 0.21142700	C -0.00012700 -3.10736600 0.07161700
H 0.00041800 -3.95896800 -0.36473700	H 0.00015100 -4.04401300 -0.51726500
O 0.00064500 -3.09306600 1.45718700	O -0.00012200 -3.19286200 1.31256000
1Mn-TS(HOCH₂OH-H-H)-SMD(CH₃OH)	1Re-TS(HOCH₂OH-H-H)-SMD(CH₃OH)
O 0.12652700 -3.19810900 -0.47565100	O 0.13293800 -3.26566400 0.49570600
P -2.26043600 -0.22906700 -0.08384000	P 2.42534300 -0.00170800 0.15403600
P 2.31228500 -0.06577700 -0.09241200	P -2.38207400 -0.17184300 0.15619200
C -2.43064000 0.29073200 -1.85948800	C 2.44952100 0.63299300 1.90429800
C 2.45208300 0.42399700 -1.88368100	C -2.47228300 0.39848500 1.92684400
H -2.47545700 1.38362700 -1.85990800	H 2.40727000 1.72394300 1.82838000
H 2.45098500 1.51693900 -1.90983000	H -2.55339100 1.48805900 1.89481200
H -3.34605000 -0.07361900 -2.32337500	H 3.37261200 0.37472900 2.42547000
H 3.38325700 0.08618600 -2.34167000	H -3.35922700 0.01959600 2.43644100
C -1.20157000 -0.16357300 -2.62798800	C 1.23788600 0.13490500 2.67244700
C 1.24549100 -0.10544900 -2.63159400	C -1.21148700 0.00364800 2.67630500
H -1.20313000 0.27040900 -3.63507700	H 1.19966300 0.61672700 3.65670000
H 1.21343200 0.31656100 -3.64452600	H -1.20960700 0.46715700 3.66998800
H -1.18706100 -1.25053200 -2.73680400	H 1.28641100 -0.94423200 2.83090800
H 1.28771600 -1.19279100 -2.72782700	H -1.15496700 -1.07846800 2.81209700
N 0.01230400 0.24538300 -1.90113800	N -0.00710000 0.43050800 1.92918200
C 3.09194900 1.41056700 0.76892500	C -3.31240600 1.19123900 -0.73764900
C -3.13145000 1.18083700 0.80441100	C 3.26671700 1.40019100 -0.76701600
H 2.44860300 2.22352200 0.41710600	H -2.71514800 2.06856600 -0.46453700
H -2.53343900 2.03635200 0.47109300	H 2.59579900 2.23599100 -0.53753600
C 3.52378900 -1.48171600 0.16039000	C -3.45676600 -1.70201100 0.01842000
C -3.38116800 -1.72074200 0.14084600	C 3.60342600 -1.45761400 0.06468000
C 3.58027800 -2.45396100 -1.01619100	C -3.35056000 -2.62406000 1.23043100
C -3.36813100 -2.67938600 -1.04805700	C 3.54802500 -2.34976300 1.30190600
O 0.07144000 -1.05924300 2.96819100	O 0.06172500 -1.10851400 -3.15403700
H -4.38667100 -1.30265700 0.22188500	H 4.59855400 -1.00467400 0.01624400
H 4.50176300 -0.99712400 0.23969600	H -4.48092200 -1.31882900 -0.02640200
C -3.06309500 -2.47040900 1.43550600	C 3.37558400 -2.27467200 -1.20586700
C 3.24337300 -2.22771500 1.46159500	C -3.16292000 -2.46511600 -1.27131500
H -3.06331400 -1.82044600 2.31167500	H 3.41651200 -1.66771900 -2.11148400
H 3.20001800 -1.56454900 2.32989900	H -3.24793400 -1.83932000 -2.16088900

H	-2.08589600	-2.95642900	1.38098400	H	2.40782000	-2.78041300	-1.18467500
H	2.29754300	-2.77317600	1.41038600	H	-2.15739800	-2.89128900	-1.25781100
H	-3.81190200	-3.24811500	1.60118100	H	4.15036800	-3.04387700	-1.28686700
H	4.03718900	-2.95693000	1.64512300	H	-3.87423600	-3.29050400	-1.37677600
C	2.99258700	1.35605400	2.28954900	C	-3.27752700	1.05218100	-2.25638700
C	-3.03252500	1.10571900	2.32480600	C	3.27759100	1.20674400	-2.27990200
H	3.64116200	0.58618900	2.71362500	H	-3.91147200	0.23234200	-2.60286000
H	-3.63544500	0.29131700	2.72895100	H	3.99509000	0.44035800	-2.58285900
H	1.97308400	1.17037900	2.63219700	H	-2.26590600	0.88579800	-2.63380000
H	-2.00334000	0.97442900	2.66556900	H	2.29562000	0.92766400	-2.66771600
H	3.30948000	2.31564200	2.71213300	H	-3.65611800	1.97132100	-2.71463400
H	-3.40830500	2.03572700	2.75811800	H	3.57558300	2.14130500	-2.76544700
C	4.52187800	1.70594200	0.32061500	C	-4.73607500	1.39989500	-0.23051900
C	-4.57146000	1.39787800	0.35434500	C	4.65805000	1.74119000	-0.24183600
H	4.62011900	1.75187400	-0.76620200	H	-4.78222500	1.51453400	0.85465000
H	-4.66980100	1.45210500	-0.73204900	H	4.66927900	1.91820800	0.83584100
H	5.22958100	0.96390700	0.69784800	H	-5.39376300	0.57434800	-0.51478500
H	-5.23383800	0.60825200	0.71505900	H	5.38080500	0.95254200	-0.46661300
H	4.83128200	2.67780900	0.71716500	H	-5.15064000	2.31099300	-0.67401500
H	-4.94311900	2.34240100	0.76601900	H	5.01517500	2.65480800	-0.72807100
H	-0.07666100	1.22281200	0.78593200	H	0.09790800	1.46785400	-0.87078200
H	-0.01005200	1.27437200	-1.80351100	H	-0.06538800	1.45456100	1.80661600
H	4.32960000	-3.22341700	-0.80154400	H	-4.00050600	-3.49111400	1.07460500
H	2.62769900	-2.96420900	-1.17191800	H	-2.33570000	-2.99935600	1.37270200
H	3.86968900	-1.97066800	-1.94910300	H	-3.67181500	-2.14136600	2.15483400
H	-4.06011500	-3.50289600	-0.84690500	H	4.27493300	-3.16045000	1.18844900
H	-3.69288900	-2.20216600	-1.97441600	H	3.80088900	-1.81249100	2.21762700
H	-2.38289100	-3.11534100	-1.21404900	H	2.56553400	-2.80814300	1.43051300
H	0.00057900	1.68720900	0.07680400	H	-0.24503500	1.80975800	-0.17106800
O	0.19699200	2.89084400	-0.95480700	O	-0.47588400	3.02752700	0.88198500
C	0.09223100	-2.05622400	-0.25889000	C	0.16219600	4.06988400	0.30930900
C	0.05856700	-0.76074900	1.84405600	H	0.78115800	4.63370800	1.03307900
Mn	0.03442700	-0.35336400	0.13877600	H	0.81313900	3.77731900	-0.53699900
C	-0.64730400	3.93927300	-0.80470000	C	0.09055900	-2.12324700	0.25295900
H	-0.48744600	4.69823400	-1.59875400	C	0.04800800	-0.78938000	-2.02807400
H	-1.72378800	3.66694000	-0.81351600	Re	0.02722400	-0.29671900	-0.20121400
O	-0.49875900	4.62136400	0.48144900	O	-0.74410300	5.02676600	-0.31023200
H	0.42440900	4.91566400	0.53469400	H	-1.33250000	5.33978500	0.38842000
1Mn-TS(HCOOH-H-H)-SMD(CH₃OH)				1Re-TS(HCOOH-H-H)-SMD(CH₃OH)			
O	0.00507600	-3.07426900	-0.91801100	O	0.09272800	-3.05615800	-1.01451600
P	-2.27836700	-0.08064400	-0.06090300	P	-2.38047000	-0.04290400	-0.11724600
P	2.27976400	-0.07852400	-0.06035600	P	2.42030600	0.05658100	-0.09618600
C	-2.43807300	0.70889700	-1.73958400	C	-2.44046500	0.85475400	-1.74936200
C	2.44077900	0.70467300	-1.74183800	C	2.46793700	0.93915800	-1.73740900
H	-2.45641800	1.79084400	-1.57870300	H	-2.45510400	1.92310400	-1.51233000
H	2.46228400	1.78707500	-1.58487300	H	2.44722600	2.00981200	-1.51449300
H	-3.36452200	0.43643100	-2.24663400	H	-3.34992500	0.63352300	-2.31019300
H	3.36634500	0.42780700	-2.24807500	H	3.38937700	0.73902400	-2.28626000
C	-1.22263200	0.33995300	-2.56855300	C	-1.20728100	0.53640700	-2.57711900
C	1.22406900	0.33625300	-2.56917100	C	1.25261800	0.57175800	-2.57091300
H	-1.20513100	0.92479700	-3.49696100	H	-1.20352400	1.14703600	-3.48824900
H	1.20694100	0.91937700	-3.49865800	H	1.23264100	1.17493000	-3.48671300
H	-1.23682000	-0.71741200	-2.84242600	H	-1.19361200	-0.51321000	-2.87671300
H	1.23599800	-0.72169100	-2.84106500	H	1.27664100	-0.48022200	-2.86157600
N	0.00128100	0.59751300	-1.78493500	N	0.01691100	0.80423000	-1.79422400
C	3.06539500	1.23241400	1.03293600	C	3.28649100	1.28027200	1.03075700
C	-3.06963100	1.22370100	1.03626000	C	-3.34238700	1.11144100	1.00509000
H	2.44432800	2.10192400	0.79183800	H	2.61117000	2.14147300	0.97260500
H	-2.45231600	2.09641800	0.79742300	H	-2.71849800	2.01075400	0.97741200

C	3.47774900	-1.52555300	-0.03911200	C	3.58756400	-1.40687400	-0.24342500
C	-3.47292100	-1.53070200	-0.04923000	C	-3.46574700	-1.56559200	-0.29482700
C	3.48845500	-2.31960200	-1.34317100	C	3.54739800	-2.07009300	-1.61740800
C	-3.47662600	-2.31908400	-1.35664700	C	-3.38852300	-2.21152600	-1.67560800
O	0.00026200	-1.49725300	2.79342200	O	0.00186700	-1.60008000	2.96554800
H	-4.46172000	-1.07854000	0.07333700	H	-4.48586300	-1.19480900	-0.15422300
H	4.46508700	-1.07061200	0.08518400	H	4.58664400	-0.98365400	-0.10032100
C	-3.21121500	-2.45615700	1.13737500	C	-3.16958300	-2.59220700	0.79722300
C	3.21388100	-2.44695500	1.15020100	C	3.33257100	-2.43339300	0.85864000
H	-3.21838200	-1.93028200	2.09344900	H	-3.19654200	-2.16373100	1.80029200
H	3.21148400	-1.91671000	2.10384500	H	3.34531600	-1.99420300	1.85741600
H	-2.24878400	-2.96391100	1.04049600	H	-2.18904500	-3.05166100	0.65392400
H	2.25513400	-2.96085000	1.04930800	H	2.36902700	-2.92909000	0.72177000
H	-3.98818400	-3.22650900	1.17929000	H	-3.91820600	-3.39011500	0.75761600
H	3.99509500	-3.21248000	1.20085000	H	4.11021900	-3.20322800	0.82487000
C	2.92010000	0.95913900	2.52634700	C	3.33556100	0.81652400	2.48311900
C	-2.92292700	0.94716500	2.52894800	C	-3.39652900	0.62317500	2.44955300
H	3.54619900	0.12396800	2.84929700	H	4.04727500	-0.00140200	2.62028600
H	-3.54592000	0.10895900	2.85005500	H	-4.05703700	-0.24060400	2.55959600
H	1.88806300	0.74190600	2.80742100	H	2.35942900	0.48448500	2.84327000
H	-1.89008200	0.73289800	2.80929900	H	-2.40925200	0.35082300	2.82968500
H	3.23887600	1.84116000	3.09114900	H	3.66325000	1.64335800	3.12097800
H	-3.24460800	1.82668000	3.09600900	H	-3.79183100	1.41819600	3.08971400
C	4.51066500	1.56632400	0.67209600	C	4.66466000	1.71662400	0.54157400
C	-4.51629000	1.55248100	0.67629100	C	-4.73181900	1.47807600	0.49110900
H	4.64356300	1.76774000	-0.39347100	H	4.64709800	2.09171000	-0.48395700
H	-4.64965300	1.75731900	-0.38858200	H	-4.71260000	1.87002000	-0.52818100
H	5.19673400	0.76369300	0.95504100	H	5.39374200	0.90387000	0.59488900
H	-5.19896600	0.74580000	0.95593300	H	-5.41684800	0.62652200	0.51585300
H	4.82266700	2.46396400	1.21605800	H	5.03588400	2.52541700	1.17937900
H	-4.83246300	2.44668800	1.22349700	H	-5.16095600	2.25526800	1.13202000
H	0.01143900	1.11659800	0.92978200	H	0.26065400	1.30197700	1.17481800
H	0.00299800	1.60464100	-1.57931300	H	0.00628400	1.80741700	-1.56033000
H	4.23411900	-3.11794900	-1.26861000	H	4.24840900	-2.91108000	-1.62838500
H	2.52482800	-2.79208100	-1.54234800	H	2.55820400	-2.46836500	-1.85047700
H	3.75549700	-1.70722000	-2.20641000	H	3.84313700	-1.39229300	-2.41959600
H	-4.21815400	-3.12173800	-1.28731700	H	-4.06172900	-3.07470300	-1.70238200
H	-3.74508200	-1.70418800	-2.21762700	H	-3.69889800	-1.53502200	-2.47344300
H	-2.51005100	-2.78542900	-1.55580600	H	-2.38486600	-2.57578500	-1.90312300
H	-0.01187100	2.00701900	0.69327000	H	-0.17040000	2.08878000	0.87440400
O	-0.03028900	3.33747300	0.76212300	O	-0.57722400	3.35375300	0.90322300
C	0.00263100	-1.96908600	-0.54551500	C	0.05122600	-1.97015700	-0.57660600
C	0.00052600	-1.02850700	1.72655700	C	0.01519000	-1.07735500	1.91542100
Mn	0.00089000	-0.35248500	0.11455600	Re	0.02950800	-0.25863500	0.21736100
C	-0.01047000	4.00398300	-0.32762900	C	-0.36743600	4.08226700	-0.12437600
H	-0.01770200	5.10008800	-0.18332500	H	-0.60821400	5.15115600	0.02309600
O	0.01447300	3.55090500	-1.47771500	O	0.06183200	3.71096000	-1.22382700
1Mn-OCH₃-SMD(CH₃OH)				1Re-OCH₃-SMD(CH₃OH)			
O	-0.00238600	-2.89407700	-0.25018800	O	-0.00028900	-3.07029400	-0.39872500
P	2.29351800	0.07813600	0.16495800	P	2.39247700	0.09018700	0.23602300
P	-2.29682200	0.07963600	0.16699700	P	-2.39293200	0.08869600	0.23755900
C	2.42787800	0.02110800	2.01623100	C	2.44131500	0.24011800	2.08769600
C	-2.43112900	0.01166200	2.01787400	C	-2.44309800	0.22203900	2.09037000
H	2.43710900	1.06182100	2.35383100	H	2.43738300	1.31448000	2.29552700
H	-2.44494600	1.05096800	2.35960400	H	-2.44608900	1.29456900	2.30730700
H	3.35187300	-0.44868700	2.36091200	H	3.35526800	-0.17679400	2.51625600
H	-3.35333300	-0.46359600	2.35980600	H	-3.35431200	-0.20454400	2.51509000
C	1.18321500	-0.67217200	2.55420600	C	1.18731400	-0.38922000	2.68068900
C	-1.18366700	-0.67853000	2.55331600	C	-1.18462400	-0.40312200	2.67836600

H	1.15411200	-0.53364200	3.65232900	H	1.14080200	-0.11285200	3.75039500
H	-1.15453500	-0.54251000	3.65173600	H	-1.13948400	-0.13380000	3.74990600
H	1.28655000	-1.77031500	2.41023300	H	1.29333700	-1.49495800	2.67431000
H	-1.28308900	-1.77673400	2.40686500	H	-1.28248900	-1.50956400	2.66427400
N	-0.00149500	-0.12233000	1.94103500	N	-0.00072800	0.06423300	1.99202900
C	-3.22921400	1.66961700	-0.22745900	C	-3.32109300	1.63581300	-0.29155700
C	3.22397400	1.66356200	-0.24543900	C	3.31875100	1.63340900	-0.30702700
H	-2.61952600	2.41470200	0.29125500	H	-2.66696100	2.42458200	0.09277900
H	2.60389700	2.41524800	0.25090200	H	2.66278400	2.42443900	0.06963700
C	-3.44479900	-1.26910500	-0.48794600	C	-3.53250100	-1.32695200	-0.24409300
C	3.43926600	-1.27646900	-0.48259000	C	3.53355100	-1.32948600	-0.22967700
C	-3.47244400	-2.53227400	0.36926500	C	-3.47122500	-2.50530900	0.72462100
C	3.47173400	-2.53153900	0.38633500	C	3.46675400	-2.50028300	0.74771500
O	-0.00276100	0.02685800	-3.05244100	O	-0.00362500	-0.01342000	-3.25463300
H	4.44065800	-0.83500600	-0.46262700	H	4.54303500	-0.90844700	-0.18447300
H	-4.44623500	-0.82858900	-0.45864200	H	-4.54206300	-0.90591600	-0.20077500
C	3.10755300	-1.64008600	-1.92929300	C	3.27269500	-1.81067500	-1.65630300
C	-3.11993300	-1.61847700	-1.93956400	C	-3.26425600	-1.79658400	-1.67315800
H	3.06837900	-0.76931200	-2.58588400	H	3.26416500	-0.99811800	-2.38449700
H	-3.08394400	-0.74117900	-2.58767500	H	-3.25363200	-0.97831700	-2.39495800
H	2.14560600	-2.15340000	-1.99801600	H	2.31552100	-2.33203500	-1.72617400
H	-2.15817200	-2.13088100	-2.01746800	H	-2.30569900	-2.31544700	-1.74258200
H	3.87189200	-2.31759400	-2.32546000	H	4.05622300	-2.51554600	-1.95462100
H	-3.88595400	-2.29220900	-2.33887100	H	-4.04510400	-2.50045900	-1.98072800
C	-3.22176300	2.01445500	-1.71322400	C	-3.39615800	1.79557900	-1.80691900
C	3.23377400	1.98001700	-1.73765200	C	3.39588500	1.78043200	-1.82357300
H	-3.86677000	1.34416500	-2.28793200	H	-4.09679700	1.08549500	-2.25386200
H	3.89122900	1.30369200	-2.29085800	H	4.09929300	1.06877900	-2.26361700
H	-2.21702400	1.96910700	-2.13827800	H	-2.42152500	1.65947600	-2.28000900
H	2.23521900	1.91941400	-2.17508900	H	2.42240700	1.63801400	-2.29698900
H	-3.59971500	3.03191400	-1.86100700	H	-3.75106500	2.80129500	-2.05528300
H	3.60671200	2.99714700	-1.89961300	H	3.74835700	2.78509200	-2.07954200
C	-4.64144200	1.73447000	0.34715700	C	-4.69633700	1.79867700	0.34955900
C	4.62933500	1.74311500	0.34403700	C	4.69298300	1.80516100	0.33419000
H	-4.66829700	1.51005400	1.41589200	H	-4.66205300	1.73268800	1.43932900
H	4.64375000	1.54558300	1.41827000	H	4.65759700	1.74999900	1.42452900
H	-5.32500800	1.04819800	-0.16027600	H	-5.40854500	1.05249500	-0.01360200
H	5.31856900	1.04404300	-0.13783600	H	5.40694800	1.05674300	-0.02083200
H	-5.04516000	2.74445800	0.21552800	H	-5.10397700	2.78277100	0.09442000
H	5.03499900	2.74938600	0.19176600	H	5.09903400	2.78742400	0.06966500
H	-0.06604400	2.29048900	2.07184000	H	-0.17387500	2.51900000	1.87375200
C	0.03251300	2.90993000	1.16446500	C	0.00357600	3.05609400	0.93040700
H	-4.18041800	-3.24730400	-0.06432800	H	-4.15485800	-3.28994500	0.38292700
H	-2.49776500	-3.02207400	0.40828800	H	-2.47073500	-2.94064700	0.76949400
H	-3.79620600	-2.33578600	1.39279100	H	-3.77099300	-2.23089200	1.73765200
H	4.17515800	-3.25193100	-0.04580300	H	4.15167000	-3.28786700	0.41548600
H	3.80358200	-2.32596000	1.40548100	H	3.76144100	-2.21843600	1.76017200
H	2.49661600	-3.01949300	0.43762400	H	2.46575500	-2.93466400	0.79052100
O	0.00584800	2.16376200	-0.00126000	O	-0.00078100	2.21920500	-0.18122200
H	0.97270800	3.49121500	1.28868100	H	0.96523800	3.59455100	1.05498800
C	-0.00266300	-1.71870000	-0.21302400	C	-0.00073900	-1.88729900	-0.29673000
Mn	-0.00063900	-0.00166300	-0.12964600	Re	0.00020300	-0.02810000	-0.17567400
C	-0.00160400	0.08387400	-1.87774200	C	-0.00161200	0.02534800	-2.07191700
H	-0.77961200	3.66681400	1.20400000	H	-0.76883300	3.84558200	0.85243100
1Mn-HCH₂O⁻-SMD(CH₃OH)				1Re-HCH₂O⁻-SMD(CH₃OH)			
N	0.02226700	-0.22061400	1.91866000	N	0.02801500	-0.16765700	1.93742800
P	2.31924600	0.04086700	0.20904300	P	2.43202500	0.02796900	0.28068300
P	-2.26149600	-0.03937800	0.17016300	P	-2.37828600	-0.11133200	0.24558200
H	-0.13314000	1.90153000	0.23497400	H	-0.21730600	2.60577500	0.10640400

C	0.04733100	3.02290600	0.45140000	C	-0.13122900	3.70112000	0.33750500
C	2.45600100	-0.08049400	2.05440000	C	2.47125500	0.11844900	2.13436100
C	-2.40624000	-0.04245800	2.01510900	C	-2.42003400	0.12643200	2.08532700
H	2.47380900	0.95178800	2.41726300	H	2.48500200	1.18488900	2.37735600
H	-2.38972800	1.01126600	2.31495200	H	-2.42932900	1.21013000	2.23831100
H	3.37359500	-0.56991400	2.38882000	H	3.37748900	-0.32958600	2.54782700
H	-3.33904200	-0.47861100	2.37376700	H	-3.32837300	-0.28525400	2.53176200
C	1.20202700	-0.76482100	2.57022400	C	1.21443500	-0.50857600	2.71319100
C	-1.17060700	-0.72953700	2.57013900	C	-1.16838600	-0.45862900	2.71716900
H	1.14136800	-0.60937300	3.66244400	H	1.09746000	-0.15177500	3.74814500
H	-1.12322100	-0.54147700	3.65731300	H	-1.06298400	-0.03673600	3.72897100
H	1.28685000	-1.85744100	2.43634800	H	1.33857800	-1.60220100	2.78869700
H	-1.26781200	-1.82755400	2.46717500	H	-1.29269200	-1.54495000	2.86105600
C	-3.15767900	1.52196200	-0.31626100	C	-3.40417500	1.35002500	-0.33887800
C	3.19953200	1.66565100	-0.13972100	C	3.30015300	1.63435700	-0.17139200
H	-2.49529400	2.30913100	0.07335000	H	-2.88575400	2.18071800	0.15600700
H	2.55262800	2.37590300	0.39064000	H	2.65612100	2.35956900	0.34047600
C	-3.37266800	-1.41611200	-0.47927000	C	-3.40345400	-1.64694100	-0.07515100
C	3.46804600	-1.25030800	-0.54684200	C	3.59480400	-1.35809200	-0.19645400
H	-4.36561700	-0.95910600	-0.52341900	H	-4.42255800	-1.37323700	0.21621800
H	4.46094300	-0.79394600	-0.51132700	H	4.59322800	-0.99849400	0.07271800
C	0.01948500	0.23892600	-1.79438700	C	0.04302500	0.38140500	-1.98605500
O	0.01273800	0.37932700	-2.95934400	O	0.04878300	0.63692800	-3.13584900
C	3.11945600	-1.52310400	-2.00804300	C	3.55776400	-1.63448400	-1.69716500
C	-2.97474600	-1.84803400	-1.89151800	C	-3.40516000	-2.03824000	-1.55007900
H	2.16404200	-2.04287500	-2.09753500	H	3.85281800	-0.76748300	-2.28973800
H	-2.89610900	-1.01126700	-2.58620300	H	-3.82115900	-1.25699300	-2.18778700
H	3.88695300	-2.16217400	-2.45645200	H	2.56023600	-1.93805700	-2.02245400
H	-2.01977700	-2.37369500	-1.89062900	H	-2.39795500	-2.26331300	-1.90736600
H	3.06060800	-0.60992800	-2.60510900	H	4.24965200	-2.44824400	-1.93749400
H	-3.72875300	-2.53870600	-2.28561400	H	-4.01579900	-2.93634300	-1.68932700
C	3.52689800	-2.55673500	0.24356000	C	3.31342100	-2.62636100	0.60560700
C	-3.45142100	-2.63189600	0.43991100	C	-2.95800400	-2.81035400	0.80740300
H	2.55677600	-3.05328800	0.28523500	H	2.30127500	-2.99885000	0.43454800
H	-2.48330800	-3.13190000	0.53946400	H	-1.90855000	-3.06648300	0.64651100
H	3.88449200	-2.41582900	1.26289400	H	3.44611800	-2.47567900	1.67859200
H	-3.80801100	-2.38042200	1.44005800	H	-3.09814000	-2.59783500	1.86872100
H	4.22203200	-3.24449300	-0.25193000	H	4.01074800	-3.41183900	0.29646200
H	-4.15126600	-3.35902100	0.01905600	H	-3.55557300	-3.69613100	0.56830100
C	-3.25614600	1.70591700	-1.82926200	C	-3.34342100	1.60877900	-1.84006600
C	3.22365800	2.03294400	-1.61879300	C	3.28331700	1.97279900	-1.65828600
H	-3.94279000	0.99338000	-2.28714200	H	-3.88252800	0.85013700	-2.41188000
H	3.92344100	1.40049100	-2.17289500	H	3.98265300	1.35321600	-2.22430000
H	-2.28661400	1.61824300	-2.32562200	H	-2.31746900	1.64775900	-2.20817100
H	2.24296500	1.95031000	-2.08827100	H	2.29181000	1.85747700	-2.09820200
H	-3.64388000	2.70964400	-2.04179500	H	-3.81026700	2.57459900	-2.05916700
H	3.55937100	3.06897200	-1.74195500	H	3.58933600	3.01482200	-1.79694800
C	-4.53508500	1.65927500	0.32671600	C	-4.84588400	1.32047500	0.16085800
C	4.59860300	1.75880000	0.46569400	C	4.70913000	1.75743000	0.40234100
H	-4.50809500	1.54763900	1.41535200	H	-4.91528200	1.14311000	1.23664900
H	4.61133100	1.53361400	1.53350300	H	4.74751100	1.55284300	1.47461400
H	-5.24411400	0.93055800	-0.07201500	H	-5.43465300	0.55369600	-0.34977500
H	5.30642000	1.09283600	-0.03182500	H	5.40867400	1.08289300	-0.09858200
H	-4.93832200	2.65761200	0.11228900	H	-5.32299800	2.28471500	-0.04261700
H	4.97943100	2.77897600	0.34297100	H	5.07730200	2.77740400	0.25057200
H	0.84877900	2.99532700	1.22923700	H	0.71876700	3.76524600	1.05430700
H	0.54016500	3.38187400	-0.48276900	H	0.25115200	4.15017700	-0.60747100
O	-1.06489600	3.70581800	0.80976900	O	-1.29344100	4.27561900	0.80160800
C	0.06668500	-1.79948000	-0.32347700	C	0.10212900	-1.85156700	-0.78447000
O	0.09667200	-2.96468900	-0.42489800	O	0.14330100	-2.97085100	-1.16557500

Mn 0.02767500 -0.09880600 -0.07219900	Re 0.03778700 -0.12409800 -0.14325300
1Mn-TS(HCH₂O)-SMD(CH₃OH)	1Re-TS(HCH₂O)-SMD(CH₃OH)
N 0.02573700 -0.43922800 2.00136500	N 0.01793900 -0.26692600 2.04680600
P 2.27748300 0.02259300 0.22925600	P 2.38603600 0.05855700 0.28732500
P -2.23297400 -0.13012200 0.21802000	P -2.35908700 -0.07938300 0.28238500
H 0.01398200 1.50399800 0.17422200	H -0.07754700 1.69140900 0.09522300
C -0.00555500 3.57581600 0.51315000	C 0.02639500 3.53799500 0.51416100
C 2.44447600 -0.25698700 2.05885000	C 2.45631900 -0.08626000 2.13972500
C -2.39773400 -0.46089200 2.03850500	C -2.42812100 -0.23712700 2.13439700
H 2.42221800 0.73207500 2.52712000	H 2.43929400 0.93734300 2.52689700
H -2.45951300 0.51715600 2.52611000	H -2.47883900 0.78316400 2.52696100
H 3.38785100 -0.73557300 2.33048900	H 3.38072900 -0.55721600 2.48124200
H -3.30146100 -1.01866700 2.29196000	H -3.32155900 -0.76910100 2.46901000
C 1.22805700 -1.04999900 2.50582900	C 1.21820500 -0.82797400 2.62307700
C -1.12380200 -1.15943300 2.48335200	C -1.14729000 -0.90135500 2.61938500
H 1.21926700 -1.08992800 3.61273000	H 1.18692100 -0.76475000 3.72653300
H -1.12086600 -1.21861500 3.58938300	H -1.12229100 -0.83776100 3.72298200
H 1.34644600 -2.10796700 2.17932900	H 1.33259900 -1.90987500 2.39460300
H -1.14755000 -2.21695500 2.13572100	H -1.19355300 -1.98777100 2.38922000
C -3.17379300 1.49050300 0.05377600	C -3.28077000 1.53503200 0.00651100
C 3.12439700 1.69334200 0.03087000	C 3.23935100 1.70941800 -0.00275100
H -2.58033600 2.13953400 0.70536700	H -2.69850800 2.20859800 0.64441300
H 2.46653500 2.32667300 0.62922600	H 2.58140900 2.38322400 0.55681600
C -3.36445600 -1.38096200 -0.63318200	C -3.49240000 -1.41756000 -0.39503800
C 3.50196200 -1.16407800 -0.58383000	C 3.59409100 -1.21720700 -0.38748600
H -4.37626400 -0.97984000 -0.51720000	H -4.50991400 -1.06734900 -0.19560800
H 4.48187300 -0.69081900 -0.46699800	H 4.58718100 -0.78414700 -0.23078200
C 0.01237800 0.25446900 -1.78001600	C 0.02210700 0.22387700 -2.01376200
O -0.00284300 0.51413000 -2.92874400	O 0.02779800 0.41552600 -3.18127100
C 3.21797200 -1.31698200 -2.07702300	C 3.38922400 -1.43653900 -1.88493200
C -3.06014200 -1.48271500 -2.12724500	C -3.31400100 -1.57584800 -1.90332500
H 2.25802700 -1.80950600 -2.24770700	H 2.42638000 -1.91240400 -2.08598000
H -3.08407900 -0.51394800 -2.62972900	H -3.48453200 -0.64562700 -2.44755000
H 3.99454300 -1.93506700 -2.54101400	H 4.17336600 -2.09592000 -2.27226100
H -2.07599300 -1.92382800 -2.30338200	H -2.30612500 -1.92354900 -2.14413900
H 3.20001500 -0.36108200 -2.60349000	H 3.42714500 -0.50836500 -2.45702300
H -3.80228800 -2.12512900 -2.61384600	H -4.02413500 -2.31708000 -2.28524400
C 3.56888800 -2.53476400 0.08590000	C 3.53570800 -2.54557800 0.36112100
C -3.34220200 -2.76623800 0.00921100	C -3.30759500 -2.75793700 0.31061300
H 2.61530000 -3.06328500 0.03257900	H 2.55193400 -3.01275200 0.28215400
H -2.34795000 -3.21614200 -0.01767400	H -2.29764100 -3.15016600 0.17661500
H 3.86728200 -2.47524600 1.13412300	H 3.77926000 -2.44021900 1.41974400
H -3.68180900 -2.75188500 1.04655300	H -3.51152300 -2.69814900 1.38122800
H 4.31310300 -3.15229100 -0.42921200	H 4.26328100 -3.23890800 -0.07458000
H -4.01556800 -3.43123900 -0.54305400	H -4.00309200 -3.48957200 -0.11462900
C -3.13453100 2.08767300 -1.34877900	C -3.19026000 2.06576200 -1.41984600
C 3.11907700 2.22188700 -1.39975700	C 3.22864700 2.14648300 -1.46390600
H -3.75982800 1.52379200 -2.04625300	H -3.80226800 1.48197500 -2.11201200
H 3.84668800 1.69537000 -2.02323500	H 3.95935600 1.58846100 -2.05500100
H -2.12050600 2.12364100 -1.75187700	H -2.16241000 2.06620400 -1.78929300
H 2.13953200 2.13136600 -1.87237400	H 2.24686400 2.01333300 -1.92354200
H -3.51849700 3.11286700 -1.32656100	H -3.55725800 3.09680000 -1.45328000
H 3.39572800 3.28153300 -1.40694300	H 3.49472400 3.20610400 -1.53829800
C -4.60092400 1.45682500 0.59499500	C -4.72152200 1.52703600 0.50930700
C 4.52560900 1.77491300 0.63147200	C 4.63882700 1.81288900 0.59616000
H -4.65394500 1.05262200 1.60848200	H -4.80596200 1.14286000 1.52877900
H 4.55222200 1.45579700 1.67555800	H 4.66435000 1.52706900 1.65015000
H -5.26651400 0.86624600 -0.04066400	H -5.37334400 0.92919500 -0.13354500
H 5.24785400 1.17248300 0.07378800	H 5.35937600 1.19146500 0.05753500

H -5.00644000	2.47419400	0.62594300	H -5.11756300	2.54824500	0.50987500
H 4.87955700	2.81126100	0.59637300	H 4.99235400	2.84741900	0.52877000
H 0.46792100	3.23404800	1.44590100	H 0.40323500	3.17535600	1.48253200
H 0.62593800	3.59472600	-0.38684000	H 0.75829400	3.57995200	-0.30539200
O -1.11010500	4.10430900	0.51516800	O -1.05488800	4.12000100	0.42854200
C 0.08995100	-1.86400300	-0.43408800	C 0.07704700	-1.97621700	-0.53540900
O 0.13936800	-3.00026400	-0.73512500	O 0.10784100	-3.10621200	-0.88077200
Mn 0.02962300	-0.15602000	-0.09735800	Re 0.01867200	-0.12019300	-0.15448600
2Mn-SMD(CH₃OH)			2Re-SMD(CH₃OH)		
P -2.23333700	0.08161300	-0.33198700	P -2.36001700	0.03988400	-0.38423800
P 2.23333100	0.08162600	-0.33203100	P 2.36000900	0.03987000	-0.38422400
C -2.41476300	-0.97898200	-1.84978000	C -2.43445500	-1.06628000	-1.88111700
C 2.41473200	-0.97893700	-1.84984700	C 2.43443800	-1.06631700	-1.88108900
H -2.41973600	-0.30152300	-2.70933100	H -2.43228200	-0.40388800	-2.75235900
H 2.41966700	-0.30146200	-2.70938600	H 2.43228400	-0.40394100	-2.75234300
H -3.34982100	-1.54353700	-1.86377400	H -3.35366100	-1.65560600	-1.91346500
H 3.34980100	-1.54347300	-1.86387800	H 3.35363300	-1.65566100	-1.91342100
C -1.18171100	-1.86702800	-1.91882400	C -1.18503800	-1.93592300	-1.91089500
C 1.18169400	-1.86700400	-1.91887100	C 1.18500700	-1.93594300	-1.91086700
H -1.18133700	-2.39791100	-2.89167800	H -1.16452300	-2.47729000	-2.87558600
H 1.18130000	-2.39787100	-2.89173300	H 1.16449400	-2.47732300	-2.87555000
H -1.26869100	-2.66846500	-1.14945300	H -1.27432300	-2.72622300	-1.13269300
H 1.26870900	-2.66845400	-1.14951600	H 1.27427100	-2.72623200	-1.13265200
N -0.00001300	-1.06414300	-1.76315600	N -0.00001100	-1.12989800	-1.75183200
C 3.01798800	1.69614100	-0.91184500	C 3.18261300	1.60403600	-1.03071500
C -3.01800000	1.69611800	-0.91182700	C -3.18262100	1.60406100	-1.03069500
H 2.36520600	1.94334400	-1.75715500	H 2.52349700	1.84495400	-1.87289300
H -2.36511500	1.94340200	-1.75703200	H -2.52361000	1.84489600	-1.87297900
C 3.49091500	-0.60371300	0.89890700	C 3.58882100	-0.67021100	0.85254400
C -3.49090700	-0.60368500	0.89899100	C -3.58883300	-0.67020600	0.85251500
C 3.52857300	-2.12952300	0.93327300	C 3.53487400	-2.19340700	0.92742300
C -3.52864500	-2.12949500	0.93333100	C -3.53491900	-2.19340500	0.92734500
H -4.46771100	-0.25195300	0.55234600	H -4.57830000	-0.38201200	0.48432300
H 4.46772300	-0.25203500	0.55221600	H 4.57829100	-0.38205300	0.48433500
C -3.24692700	-0.05427300	2.30305300	C -3.38312600	-0.06290200	2.23843200
C 3.24702100	-0.05426400	2.30296900	C 3.38315000	-0.06285900	2.23844500
H -3.21029800	1.03593800	2.33066100	H -3.41483900	1.02795300	2.23138900
H 3.21045700	1.03595000	2.33055800	H 3.41489800	1.02799500	2.23137200
H -2.30522200	-0.42904700	2.71224700	H -2.41944000	-0.36482400	2.65617900
H 2.30531000	-0.42897600	2.71220700	H 2.41945900	-0.36473700	2.65620900
H -4.05069700	-0.37585000	2.97448900	H -4.16701700	-0.41400700	2.91803600
H 4.05079800	-0.37587500	2.97438100	H 4.16703400	-0.41397000	2.91805500
C 2.91409000	2.83269000	0.10010300	C 3.13224700	2.77319400	-0.05299300
C -2.91431500	2.83261900	0.10019900	C -3.13204400	2.77326900	-0.05304500
H 3.59470200	2.68693500	0.94289700	H 3.82140800	2.63138800	0.78332500
H -3.59506100	2.68678300	0.94287100	H -3.82109800	2.63155600	0.78337800
H 1.90151700	2.94126900	0.49374200	H 2.12890600	2.92435800	0.35139900
H -1.90181400	2.94121800	0.49401700	H -2.12863600	2.92438900	0.35120200
H 3.18907400	3.78025600	-0.37575400	H 3.42882400	3.69555700	-0.56354300
H -3.18926100	3.78020000	-0.37564900	H -3.42862800	3.69562400	-0.56360500
C 4.44594500	1.56300200	-1.43424000	C 4.59468200	1.39514700	-1.57039700
C -4.44587400	1.56293600	-1.43443900	C -4.59478200	1.39522500	-1.57015800
H 4.55135000	0.75944400	-2.16674000	H 4.65331100	0.56591300	-2.27945600
H -4.55113800	0.75939300	-2.16697700	H -4.65356700	0.56596500	-2.27917300
H 5.15921800	1.38000600	-0.62577300	H 5.31256500	1.20694000	-0.76740500
H -5.15925800	1.37989100	-0.62608300	H -5.31255600	1.20709500	-0.76705000
H 4.74917000	2.49476600	-1.92433600	H 4.92672500	2.29822500	-2.09371300
H -4.74906400	2.49470100	-1.92455400	H -4.92685200	2.29830000	-2.09346300
H -0.00002400	1.39262300	-0.83923700	H -0.00001500	1.52255800	-0.99275500

H 4.27698100 -2.45889600 1.66264300	H 4.26318900 -2.54693600 1.66530100
H 2.56889700 -2.55169800 1.23836400	H 2.55126900 -2.54757700 1.24367800
H 3.80061000 -2.56500000 -0.02984200	H 3.77846000 -2.66854900 -0.02443000
H -4.27703200 -2.45884100 1.66273600	H -4.26325100 -2.54694200 1.66520100
H -3.80075900 -2.56493800 -0.02977700	H -3.77850000 -2.66851300 -0.02452600
H -2.56897700 -2.55172800 1.23836200	H -2.55132400 -2.54760100 1.24360200
Mn 0.00000300 0.04653500 0.06910600	Re -0.00000700 0.11336100 0.09766000
C 0.00002500 1.08005800 1.45916000	C -0.00002100 1.30681200 1.56085800
C 0.00001000 -1.38659400 1.07073400	C -0.00000600 -1.35475300 1.31622600
O 0.00003800 1.76830100 2.41697100	O 0.00007600 2.03896400 2.49260200
O 0.00015300 -2.28979200 1.82819600	O 0.00001700 -2.18472200 2.15869900
1Mn-OCH₂OH-SMD(CH₃OH)	1Re-OCH₂OH-SMD(CH₃OH)
O 0.01814000 2.86418000 0.65684500	O 0.01600500 3.05652800 0.59895500
P -2.30638800 -0.00766300 0.08951400	P -2.40696400 -0.04042300 0.16436400
P 2.30076700 -0.05879700 0.08978100	P 2.39654300 -0.09087700 0.15890900
C -2.47660700 -0.42793100 1.89314600	C -2.48911600 -0.57826700 1.94379900
C 2.41700900 -0.69306400 1.83120600	C 2.43640100 -0.81501300 1.87072900
H -2.61565600 -1.51004500 1.94659400	H -2.61350100 -1.66372900 1.92862000
H 2.41168200 -1.78464500 1.75871200	H 2.43470800 -1.90117200 1.74028700
H -3.34900400 0.03672400 2.35511200	H -3.35311500 -0.15864200 2.46227600
H 3.34294000 -0.40006300 2.33064000	H 3.34744900 -0.55001000 2.41158600
C -1.18347000 -0.04074100 2.59765000	C -1.18529700 -0.21959000 2.64636800
C 1.18445800 -0.22800700 2.59307500	C 1.18747600 -0.39180600 2.63315000
H -1.19587300 -0.46607600 3.61718600	H -1.18321300 -0.70124300 3.63948600
H 1.17179800 -0.72261300 3.58106600	H 1.16450500 -0.93829000 3.59192100
H -1.15028800 1.05542800 2.73438400	H -1.15663800 0.86793000 2.83926300
H 1.27188900 0.85332700 2.80499800	H 1.26845700 0.67718900 2.89920700
N -0.03086000 -0.52574400 1.85483200	N -0.02747600 -0.65193700 1.87306600
C 3.28884000 -1.32968600 -0.88690300	C 3.39871000 -1.32479700 -0.84648700
C -3.27113300 -1.39687900 -0.73518100	C -3.36084700 -1.40884800 -0.70234100
H 2.64999400 -2.21447300 -0.82804800	H 2.74967900 -2.20521500 -0.84395300
H -2.67013300 -2.27059500 -0.46504900	H -2.75826300 -2.28664300 -0.44721000
C 3.40929400 1.46759300 -0.00217100	C 3.48997700 1.44172900 0.18683200
C -3.39632700 1.50785200 -0.20265900	C -3.50398900 1.47810600 0.00440200
C 3.45144600 2.29448500 1.28082800	C 3.40931900 2.22390200 1.49488600
C -3.45384700 2.47834400 0.97517500	C -3.43888400 2.40921300 1.21288800
O 0.02166600 0.95452200 -2.96108900	O 0.02478100 1.05644800 -3.12844600
H -4.40352000 1.10428500 -0.34553900	H -4.52281600 1.08381200 -0.06019700
H 4.41465700 1.06755000 -0.16825400	H 4.50998200 1.05579700 0.08827500
C -2.99638300 2.24592800 -1.47958600	C -3.20073900 2.24651700 -1.28056900
C 3.05094300 2.35278600 -1.19646000	C 3.20238900 2.35469800 -1.00439100
H -2.94783200 1.58851900 -2.34912600	H -3.24804600 1.61690000 -2.17053700
H 2.99593200 1.79772300 -2.13392600	H 3.22884500 1.82760000 -1.95875500
H -2.02260600 2.72884900 -1.37075900	H -2.20623900 2.69669400 -1.24392400
H 2.09185000 2.85358000 -1.04981000	H 2.22294900 2.82734600 -0.91135100
H -3.73141900 3.02824100 -1.69776800	H -3.92917400 3.05452800 -1.40651000
H 3.81297200 3.13032600 -1.31822800	H 3.95340700 3.15103000 -1.04489500
C 3.43528100 -0.96360900 -2.36121300	C 3.58802400 -0.89575800 -2.29846500
C -3.28053100 -1.28804600 -2.25702100	C -3.36160400 -1.26606000 -2.22115700
H 4.11757600 -0.12150000 -2.50469000	H 4.29856200 -0.06999900 -2.38784100
H -3.90083800 -0.45526900 -2.59953300	H -4.00492500 -0.44587700 -2.55044000
H 2.47746000 -0.71201400 -2.82204800	H 2.64802800 -0.59255400 -2.76495100
H -2.27654000 -1.15736700 -2.66691600	H -2.35830000 -1.09356300 -2.61748800
H 3.85247700 -1.81446800 -2.91007600	H 3.99050600 -1.73353700 -2.87722000
H -3.69875000 -2.20268400 -2.69068000	H -3.74707400 -2.18353000 -2.67818600
C 4.64115500 -1.67871000 -0.27137100	C 4.73072700 -1.70957100 -0.20898700
C -4.68189400 -1.59751200 -0.18923900	C -4.77181600 -1.62431900 -0.16311000
H 4.55433500 -2.01933200 0.76248200	H 4.61386200 -2.09602900 0.80552500
H -4.69986100 -1.69623400 0.89833000	H -4.79134900 -1.73868600 0.92307900

H	5.33553800	-0.83402400	-0.29248600	H	5.42638700	-0.86659100	-0.17373200
H	-5.35056900	-0.77787900	-0.46673900	H	-5.44132300	-0.80206300	-0.42998200
H	5.10470200	-2.48949300	-0.84406800	H	5.20715500	-2.49540700	-0.80501100
H	-5.10945400	-2.51561600	-0.60710100	H	-5.19508400	-2.53737300	-0.59552900
H	1.32906000	-3.08120000	0.30269200	H	1.34966700	-3.09721000	0.18926900
C	0.24935800	-3.02208400	0.03922300	C	0.27276000	-3.08687500	-0.07442600
H	4.13932900	3.13591700	1.14317700	H	4.09341700	3.07797600	1.44605700
H	2.47406600	2.71053200	1.53222200	H	2.40680100	2.61887900	1.67075300
H	3.80901300	1.72044100	2.13766100	H	3.69915500	1.62479100	2.36010200
H	-4.11079800	3.31634300	0.71745400	H	-4.09960400	3.26558700	1.04083700
H	-3.85830100	2.01953400	1.87879100	H	-3.77010000	1.92588900	2.13347600
H	-2.47388400	2.89573600	1.21327100	H	-2.43285500	2.80068500	1.37398800
O	-0.02366200	-1.97518500	-0.79160800	O	-0.04740700	-2.02318600	-0.87549500
C	0.00947000	1.74038400	0.31960800	C	0.00847500	1.91049100	0.30148900
Mn	0.00226800	0.08409200	-0.17201500	Re	-0.00026400	0.11497700	-0.20371000
C	0.01143700	0.56853400	-1.85515400	C	0.01464100	0.66597400	-2.01492500
H	0.00124300	-3.98779400	-0.44709000	H	0.06445900	-4.03895300	-0.59589300
O	-0.48088200	-2.99026200	1.26230800	O	-0.46485100	-3.13194000	1.14439800
H	-0.28289700	-1.99872500	1.60090300	H	-0.28578200	-2.18769200	1.54384900
1Mn-HCH(OH)O-SMD(CH₃OH)				1Re-HCH(OH)O-SMD(CH₃OH)			
N	-0.01050400	-0.63954600	1.85556600	N	-0.02951500	-0.38344900	1.92141300
P	2.26993600	-0.34247600	0.19224900	P	2.36607300	-0.33691600	0.23958900
P	-2.30233100	-0.24208700	0.24610500	P	-2.43559500	-0.09349300	0.29371300
H	-0.02916600	2.94620800	0.36191000	H	0.22914900	2.97177300	0.23098600
C	-0.02361100	4.02794200	0.62643300	C	0.31181600	4.00837500	0.63406100
C	2.41980700	-0.35961400	2.03811400	C	2.43014400	-0.16775800	2.08538900
C	-2.42917200	-0.29429300	2.09410400	C	-2.45851500	0.01913200	2.14556400
H	2.44209300	0.68916400	2.34690600	H	2.49622400	0.90671500	2.27998500
H	-2.42769600	0.74651700	2.42891800	H	-2.43642300	1.08726900	2.37995700
H	3.34179400	-0.83217000	2.38334800	H	3.32012100	-0.64005300	2.50787200
H	-3.35569500	-0.75727000	2.43985000	H	-3.37659200	-0.39631000	2.56712800
C	1.18127900	-1.02095500	2.60791400	C	1.15738200	-0.71272900	2.70703100
C	-1.19666700	-0.99516500	2.63029900	C	-1.22307800	-0.64673100	2.72267400
H	1.07115800	-0.72218300	3.66128500	H	1.05788700	-0.29057900	3.71811300
H	-1.05555200	-0.71140100	3.68403100	H	-1.07185000	-0.27068500	3.74526900
H	1.30226400	-2.11642800	2.61911100	H	1.23948900	-1.80227700	2.84655600
H	-1.34753800	-2.08694900	2.63222300	H	-1.38993700	-1.73096600	2.82385000
C	-3.08621500	1.43893200	-0.09642900	C	-3.29935500	1.51319000	-0.16653900
C	3.13743700	1.28155800	-0.20957500	C	3.41322000	1.13229800	-0.29001200
H	-2.47134700	2.08145800	0.54380900	H	-2.66029500	2.24016600	0.34876600
H	2.50376300	1.99712300	0.32784100	H	2.88849100	1.95149600	0.21657800
C	-3.52925500	-1.51814800	-0.37624800	C	-3.62074800	-1.48071700	-0.12556400
C	3.41086700	-1.69518300	-0.43149900	C	3.35851700	-1.87980900	-0.14372400
H	-4.51591800	-1.11560300	-0.12637900	H	-4.59893900	-1.13359400	0.22267800
H	4.42514400	-1.32775400	-0.24576600	H	4.38025400	-1.65215500	0.17730900
C	-0.03600700	0.15382200	-1.68895500	C	-0.02280900	0.41113800	-1.90427700
O	-0.04509300	0.47927700	-2.81324900	O	-0.00482700	0.82740600	-3.00552700
C	3.24107600	-1.92715200	-1.93095800	C	3.37126600	-2.19904500	-1.63540100
C	-3.44454900	-1.69572300	-1.89026900	C	-3.69590600	-1.73780200	-1.62784300
H	3.41709300	-1.02510300	-2.51801300	H	3.84161700	-1.41141600	-2.22528900
H	-3.61888400	-0.76391300	-2.43023700	H	-4.07866600	-0.87759800	-2.17839100
H	2.23813900	-2.28889800	-2.16658000	H	2.36090700	-2.35104900	-2.02156600
H	-2.47002700	-2.08353700	-2.19624200	H	-2.71779100	-1.99308500	-2.04170300
H	3.95496400	-2.68551000	-2.26909100	H	3.93586800	-3.12108300	-1.80811100
H	-4.20333100	-2.41351900	-2.21906400	H	-4.36972600	-2.57847900	-1.82245900
C	3.23012000	-2.99807800	0.34419700	C	2.85981100	-3.06952100	0.67270100
C	-3.37290000	-2.85582000	0.34385700	C	-3.26900200	-2.75528100	0.63779200
H	2.22196100	-3.40330800	0.23174800	H	1.81210900	-3.29615900	0.46186900
H	-2.39200200	-3.30295800	0.17066400	H	-2.26743900	-3.11416800	0.39046300

H	3.43396200	-2.87877000	1.40985800	H	2.96386600	-2.90454500	1.74654600
H	-3.52116300	-2.76548200	1.42154100	H	-3.32514200	-2.61841500	1.71928500
H	3.92899100	-3.74820800	-0.04065400	H	3.44844100	-3.95677300	0.41786700
H	-4.12444000	-3.55824500	-0.03165100	H	-3.97843400	-3.54509100	0.37018200
C	-2.94838400	1.95507200	-1.52389300	C	-3.27743500	1.85579800	-1.65223200
C	3.13516700	1.67727300	-1.68229900	C	3.39608400	1.43149100	-1.78461600
H	-3.52526500	1.36025000	-2.23589500	H	-3.95778000	1.22442300	-2.22769600
H	3.82017800	1.06179900	-2.27045100	H	3.95846200	0.69159100	-2.35827300
H	-1.91180700	1.97813600	-1.85745100	H	-2.28094500	1.76561500	-2.08483900
H	2.14481700	1.61322000	-2.13242700	H	2.38345900	1.47584400	-2.18589800
H	-3.33002900	2.97995800	-1.57375000	H	-3.60432600	2.89182700	-1.78817500
H	3.47283700	2.71456700	-1.77602300	H	3.86487900	2.40481700	-1.96250900
C	-4.53316800	1.53974300	0.38124100	C	-4.71109900	1.63206500	0.40187900
C	4.54869400	1.37393500	0.36660000	C	4.84119200	1.07571200	0.24551000
H	-4.66919100	1.17920500	1.40353300	H	-4.75407600	1.42554900	1.47361100
H	4.58775100	1.13941300	1.43226600	H	4.87945700	0.87531900	1.31843400
H	-5.21226300	0.98240000	-0.26941500	H	-5.40718000	0.95753000	-0.10367300
H	5.24302100	0.70936800	-0.15477800	H	5.43329300	0.31186200	-0.26552300
H	-4.85082500	2.58733100	0.35944700	H	-5.07971300	2.65182400	0.25041200
H	4.92344000	2.39537000	0.24374900	H	5.33428800	2.03811900	0.07417300
H	-0.91862200	4.21984400	1.25613400	H	-0.56100200	4.17198700	1.30148900
O	1.12708000	4.44314900	1.15548600	O	1.49441700	4.27455400	1.18869600
O	-0.39675700	4.73540100	-0.62109400	O	-0.02627700	4.89690000	-0.50155800
H	0.33663000	4.59166600	-1.23260700	H	0.69974600	4.80308700	-1.13139100
C	-0.07502300	-2.06863400	-0.71760800	C	-0.15826000	-1.95195500	-0.96544100
O	-0.10879800	-3.16541300	-1.12872800	O	-0.22942200	-3.02956300	-1.44634400
Mn	-0.02752800	-0.48787600	-0.04901900	Re	-0.04870400	-0.30191400	-0.13942900
Mn-TS(HCH(OH)O)-SMD(CH₃OH)				Re-TS(HCH(OH)O)-SMD(CH₃OH)			
N	0.00356100	0.19381300	-1.89617800	N	-0.03683000	-0.32868500	2.02471400
P	-2.28001200	-0.06231200	-0.11137800	P	2.34558500	-0.19136300	0.25816100
P	2.28685700	-0.05851000	-0.11936100	P	-2.41693600	-0.01112000	0.29459400
H	-0.04821700	1.59349400	0.26221400	H	0.05678000	1.66895300	0.14708900
C	-0.12287100	2.95212500	-0.64263100	C	0.10053700	3.24894500	0.51297200
C	-2.42891700	0.32975000	-1.91940400	C	2.41152000	-0.28650100	2.11167700
C	2.43471600	0.30738800	-1.93288200	C	-2.47908100	-0.14978100	2.14728700
H	-2.44091700	1.42109700	-1.99355900	H	2.45487200	0.74830900	2.46546100
H	2.45682800	1.39771000	-2.02243000	H	-2.47440000	0.87502000	2.53092600
H	-3.35310000	-0.04557000	-2.36410200	H	3.30644300	-0.80238900	2.46697000
H	3.35434200	-0.08218100	-2.37457000	H	-3.39594500	-0.63337800	2.49220100
C	-1.18569700	-0.21055400	-2.61246600	C	1.13305500	-0.93647500	2.61953600
C	1.18414000	-0.22870400	-2.61538100	C	-1.23172600	-0.87600800	2.62953200
H	-1.16569000	0.17469600	-3.64935000	H	1.10684900	-0.83060200	3.71937300
H	1.16222600	0.14796200	-3.65533200	H	-1.18429400	-0.78541500	3.72993600
H	-1.27373400	-1.31239600	-2.71611400	H	1.18081700	-2.02987700	2.43139800
H	1.26228000	-1.33215800	-2.71019800	H	-1.34480000	-1.96254100	2.42934600
C	3.28095700	1.33904400	0.65393700	C	-3.30585800	1.62404700	0.00948100
C	-3.26149600	1.32606100	0.69162000	C	3.35174600	1.35914100	-0.08500500
H	2.69273000	2.20882200	0.35279300	H	-2.76033500	2.27543900	0.70084000
H	-2.65357300	2.19530000	0.42564500	H	2.76217700	2.10995000	0.45134100
C	3.38289000	-1.56434400	0.19822500	C	-3.60523200	-1.31737900	-0.35083000
C	-3.37968000	-1.56944400	0.18386000	C	3.41841000	-1.59871900	-0.37836800
H	4.39812800	-1.16030400	0.25883500	H	-4.60331800	-0.93720500	-0.11367500
H	-4.39417800	-1.16379000	0.24974000	H	4.44962100	-1.27244700	-0.21022800
C	0.00373800	-0.25160100	1.88475600	C	-0.04598000	0.23619500	-2.00593600
O	0.00693100	-0.35863400	3.05666200	O	-0.05112500	0.46423800	-3.16573300
C	-3.05604800	-2.25130600	1.51338900	C	3.21601100	-1.81985200	-1.87571300
C	3.05740000	-2.22548300	1.53742300	C	-3.48978200	-1.47146800	-1.86512100
H	-3.06252000	-1.55843900	2.35625400	H	3.40557100	-0.92091000	-2.46359600
H	3.06623100	-1.51958400	2.36952200	H	-3.65971900	-0.53296500	-2.39559900

H -2.07639400 -2.73213100 1.48700500	H 2.19790400 -2.15027100 -2.09212600
H 2.07644200 -2.70412100 1.51874600	H -2.50254400 -1.84277400 -2.15170400
H -3.80001200 -3.02840100 1.72017400	H 3.90195100 -2.59685200 -2.22975200
H 3.79942100 -3.00122200 1.75586700	H -4.23357100 -2.19169400 -2.22226600
C -3.36700600 -2.58399600 -0.95704400	C 3.20717300 -2.89969000 0.39106100
C 3.36947400 -2.59465500 -0.92847100	C -3.44263700 -2.66436800 0.34763000
H -2.37567300 -3.01101500 -1.11775000	H 2.18257800 -3.26525200 0.29859600
H 2.37813000 -3.02332100 -1.08403600	H -2.45494300 -3.09616400 0.17845500
H -3.71013400 -2.15513300 -1.90030200	H 3.43953500 -2.79892600 1.45271000
H 3.71384800 -2.17923600 -1.87728400	H -3.60566300 -2.59628900 1.42474800
H -4.04287200 -3.41115200 -0.71250000	H 3.86869500 -3.67167600 -0.01671000
H 4.04469600 -3.41862600 -0.67172200	H -4.18132500 -3.36808200 -0.05114900
C 3.30303900 1.30212100 2.17932500	C -3.13184600 2.18685000 -1.39638000
C -3.31276700 1.24136600 2.21431100	C 3.38995900 1.75187600 -1.55851500
H 3.92981600 0.49110500 2.55954000	H -3.69678600 1.61565100 -2.13710800
H -3.96107400 0.43094500 2.55810700	H 4.05540800 1.10220800 -2.13266700
H 2.30324200 1.18838500 2.60348500	H -2.08433900 2.19753600 -1.70379900
H -2.32356300 1.09791300 2.65362800	H 2.40034300 1.71891800 -2.01912800
H 3.72067800 2.23890500 2.56393500	H -3.50172800 3.21710500 -1.43048400
H -3.72086200 2.17368000 2.61954300	H 3.77336500 2.77267500 -1.66045700
C 4.69103600 1.50641200 0.09220800	C -4.77108600 1.62536100 0.43615900
C -4.65853700 1.53161500 0.11102300	C 4.75303200 1.34171600 0.51930400
H 4.70462700 1.56206300 -0.99877700	H -4.91559700 1.20856500 1.43599300
H -4.65009300 1.63096000 -0.97673300	H 4.74627600 1.08493400 1.58083700
H 5.35735300 0.69518600 0.39870700	H -5.39779500 1.06310200 -0.26110400
H -5.33914400 0.71603600 0.37180800	H 5.41162100 0.63814300 0.00317700
H 5.12670600 2.43773500 0.47086300	H -5.14812000 2.65352500 0.45203000
H -5.09179500 2.45207600 0.51802600	H 5.20590900 2.33464700 0.42519900
H -0.00507100 2.24268100 -1.48286400	H -0.99071700 3.28594200 0.47400800
O -1.17648800 3.57585700 -0.39732100	O 0.73156200 3.37411700 1.57484300
O 1.07639800 3.58131000 -0.35162200	O 0.59825600 3.75174700 -0.66830200
H 0.87445400 4.30711200 0.25885600	H 1.55334400 3.87479300 -0.55993900
C 0.00547100 -1.89057700 -0.03315200	C -0.11118900 -2.00241600 -0.59975900
O 0.00226500 -3.06013500 -0.14062500	O -0.14651200 -3.12330400 -0.97287700
Mn 0.00107700 -0.16831800 0.14640200	Re -0.04340900 -0.16886500 -0.15601300
1Mn-OOCH-SMD(CH₃OH)	1Re-OOCH-SMD(CH₃OH)
O -0.00031200 -3.03753900 -0.03092700	O -0.00005300 -3.17686300 -0.37985700
P 2.29550900 -0.02903400 0.16122100	P 2.39458500 -0.00216500 0.23096300
P -2.29563600 -0.02874300 0.16120300	P -2.39433800 -0.00257000 0.23106400
C 2.43055100 0.06736100 2.00906800	C 2.44218200 0.25720800 2.07001400
C -2.43066100 0.06777600 2.00904000	C -2.44248300 0.25503800 2.07034000
H 2.43985800 1.13337200 2.25628100	H 2.44496600 1.34137000 2.21861400
H -2.43977800 1.13380400 2.25618600	H -2.44662900 1.33903400 2.21998000
H 3.35393400 -0.37047500 2.39373600	H 3.35466800 -0.14062700 2.51952400
H -3.35412300 -0.36986100 2.39374600	H -3.35455200 -0.14432500 2.51932100
C 1.18332900 -0.57542900 2.59841400	C 1.18666400 -0.33388300 2.69594500
C -1.18355200 -0.57519800 2.59842200	C -1.18635200 -0.33533200 2.69578700
H 1.15466200 -0.35405000 3.68194700	H 1.13181400 0.01292400 3.74366100
H -1.15486000 -0.35378500 3.68194800	H -1.13171100 0.01085500 3.74371400
H 1.27567400 -1.68102600 2.53380900	H 1.29191100 -1.43652300 2.76124200
H -1.27607900 -1.68078300 2.53385800	H -1.29064400 -1.43811100 2.76036800
N -0.00006300 -0.06453600 1.94384000	N -0.00003500 0.07100600 1.97176600
C -3.18573200 1.53752100 -0.37958900	C -3.30543900 1.51861100 -0.39197400
C 3.18585800 1.53711900 -0.37947300	C 3.30496000 1.51878100 -0.39346900
H -2.56377100 2.31586500 0.07210700	H -2.68415700 2.32167700 0.01763700
H 2.56412600 2.31555500 0.07238400	H 2.68180200 2.32174600 0.01348000
C -3.44586900 -1.41312100 -0.39801600	C -3.53831000 -1.44715500 -0.12686300
C 3.44556700 -1.41352900 -0.39810200	C 3.53906000 -1.44669400 -0.12534100
C -3.49922900 -2.59802400 0.56394400	C -3.38557800 -2.58483900 0.87914100

C	3.49874300	-2.59854300	0.56373300	C	3.38613400	-2.58355100	0.88154800
O	-0.00001200	-0.29780600	-3.04031600	O	-0.00066700	-0.17573400	-3.25430800
H	4.44190500	-0.96100200	-0.42014500	H	4.54812100	-1.03556700	-0.02097200
H	-4.44214400	-0.96046100	-0.42014600	H	-4.54750200	-1.03637200	-0.02253400
C	3.10369900	-1.88543000	-1.81047800	C	3.37050700	-1.96667200	-1.55175800
C	-3.10400400	-1.88523700	-1.81032000	C	-3.36909500	-1.96586700	-1.55364900
H	3.06741800	-1.06702200	-2.53124300	H	3.45018700	-1.17875100	-2.30193500
H	-3.06761000	-1.06692100	-2.53118200	H	-3.44877900	-1.17732000	-2.30317600
H	2.13893700	-2.39732500	-1.83659600	H	2.40439100	-2.45929700	-1.68263800
H	-2.13929400	-2.39724100	-1.83635000	H	-2.40276900	-2.45805200	-1.68461100
H	3.86362800	-2.59500600	-2.15516100	H	4.14949800	-2.70607400	-1.76563200
H	-3.86400100	-2.59477200	-2.15493800	H	-4.14776300	-2.70534800	-1.76842400
C	-3.16911400	1.74758100	-1.89067800	C	-3.29748000	1.65875000	-1.91058100
C	3.16910400	1.74732900	-1.89053800	C	3.29919200	1.65595800	-1.91237700
H	-3.82115600	1.03571500	-2.40363400	H	-3.96389300	0.93627800	-2.38829000
H	3.82090000	1.03534400	-2.40364400	H	3.96813800	0.93418500	-2.38760500
H	-2.16509500	1.65351600	-2.30946800	H	-2.29713900	1.52977200	-2.32778600
H	2.16500800	1.65355000	-2.30920900	H	2.29984700	1.52378800	-2.33097300
H	-3.53621400	2.75174600	-2.12740700	H	-3.64917600	2.65763000	-2.18856200
H	3.53642300	2.75142400	-2.12722100	H	3.64893100	2.65514500	-2.19171600
C	-4.59906200	1.68571600	0.17915200	C	-4.71521400	1.67995200	0.17128700
C	4.59929500	1.68491800	0.17909700	C	4.71366800	1.68274800	0.17162800
H	-4.63702700	1.56491300	1.26419000	H	-4.74447100	1.60539600	1.26085800
H	4.63740000	1.56388200	1.26410400	H	4.74121600	1.61107800	1.26142500
H	-5.29456700	0.96908100	-0.26615800	H	-5.40547500	0.93801600	-0.23913900
H	5.29458700	0.96823400	-0.26646900	H	5.40519700	0.94027800	-0.23570700
H	-4.97829100	2.68707800	-0.05154000	H	-5.10468500	2.66702000	-0.09949500
H	4.97869000	2.68625200	-0.05144300	H	5.10279500	2.66942000	-0.10110400
H	0.00002800	2.46837100	1.76302800	H	-0.01671100	2.58266300	1.69724600
C	0.00059500	2.88808200	0.74108700	C	-0.00502900	3.00651800	0.67805700
H	-4.20390700	-3.34257200	0.17790300	H	-4.08131800	-3.39010600	0.62005100
H	-2.52939400	-3.08898800	0.66440600	H	-2.37862000	-3.00636900	0.86545700
H	-3.84196200	-2.31312800	1.56020900	H	-3.61339100	-2.27393300	1.90005300
H	4.20335200	-3.34313100	0.17764300	H	4.08207700	-3.38895800	0.62344100
H	3.84146300	-2.31379500	1.56004400	H	3.61346200	-2.27172300	1.90228600
H	2.52884800	-3.08940800	0.66409600	H	2.37921600	-3.00519300	0.86777900
O	0.00011500	2.05058000	-0.20079100	O	0.00359000	2.16646800	-0.27064800
C	-0.00018900	-1.86599800	-0.07929700	C	-0.00011200	-1.99745600	-0.28063200
Mn	-0.00008300	-0.14681900	-0.12184100	Re	0.00010500	-0.14559900	-0.17581600
C	-0.00010500	-0.17747500	-1.87363700	C	-0.00028300	-0.12679500	-2.07534700
O	0.00164800	4.13344100	0.60230600	O	-0.00064300	4.24566900	0.53319800
1Mn-HCOO⁻-SMD(CH₃OH)				1Re-HCOO⁻-SMD(CH₃OH)			
N	-0.01914900	-0.66486200	1.85727600	N	-0.00006200	-0.30326300	1.92366700
P	-2.29824700	-0.23304900	0.22176600	P	-2.41272900	-0.18689700	0.26824100
P	2.27368100	-0.34185400	0.23423100	P	2.41272600	-0.18701400	0.26847400
H	0.18388500	3.20796200	0.12262000	H	-0.00001800	2.98067800	0.08574900
C	0.19760900	4.31388900	0.26023900	C	0.00010200	4.07159000	0.32473500
C	2.41820300	-0.45380900	2.07894000	C	2.45163800	-0.00607100	2.11424400
C	-2.42730200	-0.25717500	2.06891900	C	-2.45177700	-0.00589800	2.11401400
H	2.48326900	0.57525500	2.44288900	H	2.48719400	1.07029000	2.30600600
H	-2.38151900	0.78847500	2.38589000	H	-2.48729000	1.07046800	2.30574600
H	3.32012500	-0.97943000	2.39853700	H	3.34987500	-0.45190000	2.54794800
H	-3.37157200	-0.67498900	2.42415400	H	-3.35007000	-0.45167400	2.54766400
C	1.15415200	-1.09879500	2.61242100	C	1.18900000	-0.58569200	2.72520900
C	-1.22224900	-0.99419400	2.61686200	C	-1.18922500	-0.58557900	2.72510700
H	1.03756100	-0.83089900	3.67318500	H	1.06410000	-0.15919600	3.73163000
H	-1.08593200	-0.71813500	3.67336900	H	-1.06438600	-0.15905900	3.73152700
H	1.24639800	-2.19690300	2.58995600	H	1.30462100	-1.67094000	2.87419300
H	-1.40205000	-2.08148500	2.61313800	H	-1.30492800	-1.67081300	2.87412600

C	-3.08058800	1.43803200	-0.16147300	C	-3.41932400	1.31279800	-0.25762600
C	3.12315300	1.31531400	-0.06758700	C	3.41944700	1.31265700	-0.25722100
H	-2.37957300	2.11907000	0.33574600	H	-2.88059100	2.11338400	0.26299600
H	2.54841600	1.96314500	0.60430400	H	2.88109400	2.11315500	0.26393000
C	-3.51631900	-1.51646200	-0.40265700	C	-3.46434500	-1.69505600	-0.08923700
C	3.43836800	-1.64779400	-0.44228800	C	3.46416500	-1.69529600	-0.08904400
H	-4.50725800	-1.09149800	-0.21165400	H	-4.46727700	-1.43407400	0.26367500
H	4.44438300	-1.29251300	-0.19898000	H	4.46702100	-1.43466100	0.26434100
C	0.00460200	0.18372400	-1.67231200	C	0.00026200	0.47846900	-1.90055800
O	0.01769900	0.52963400	-2.79029900	O	0.00040700	0.90141000	-2.99918000
C	3.31926100	-1.77763900	-1.95875600	C	3.53422200	-2.00578200	-1.58104200
C	-3.36773200	-1.75259100	-1.90427700	C	-3.53389300	-2.00600700	-1.58116500
H	3.52602900	-0.83953600	-2.47605900	H	4.00148800	-1.20120400	-2.15022200
H	-3.45984800	-0.83465200	-2.48545900	H	-4.00067000	-1.20147700	-2.15081400
H	2.32174900	-2.11101300	-2.25419500	H	2.54202400	-2.18264900	-2.00154000
H	-2.40311000	-2.20430100	-2.14460200	H	-2.54158100	-2.18331300	-2.00121600
H	4.03755200	-2.51969500	-2.32266800	H	4.13005400	-2.91042700	-1.73999100
H	-4.14866400	-2.43967300	-2.24645900	H	-4.12994600	-2.91051600	-1.74005200
C	3.23712200	-2.99791200	0.24222500	C	2.97984800	-2.90250000	0.71004100
C	-3.40734500	-2.83055800	0.36719500	C	-2.98062600	-2.90209400	0.71044400
H	2.23370300	-3.39486000	0.07708000	H	1.94231200	-3.15343400	0.47848900
H	-2.42133800	-3.28764400	0.25570600	H	-1.94301700	-3.15322700	0.47948100
H	3.41108900	-2.94685100	1.31864200	H	3.05924900	-2.74104900	1.78657200
H	-3.60691500	-2.70534600	1.43288000	H	-3.06056000	-2.74030200	1.78688400
H	3.94828000	-3.72155700	-0.16979100	H	3.59560000	-3.77308800	0.46204000
H	-4.14363300	-3.54116900	-0.02285200	H	-3.59637500	-3.77266500	0.46237900
C	-3.12229500	1.81413800	-1.63941300	C	-3.37434400	1.62803600	-1.74827200
C	2.98285400	1.88047400	-1.47563100	C	3.37398700	1.62853500	-1.74772700
H	-3.88026700	1.24281300	-2.18069800	H	-3.92615100	0.89553800	-2.34126600
H	3.52830200	1.28811100	-2.21402200	H	3.92558100	0.89626000	-2.34119300
H	-2.16435500	1.67222500	-2.13920600	H	-2.35378400	1.67562200	-2.12848800
H	1.94216100	1.94584600	-1.79101200	H	2.35332100	1.67635400	-2.12762800
H	-3.38857200	2.87183800	-1.73366600	H	-3.83771000	2.60426100	-1.92432000
H	3.39793800	2.89296200	-1.50015100	H	3.83735800	2.60480700	-1.92349800
C	-4.45758100	1.62857000	0.47180600	C	-4.85505000	1.28483600	0.25905500
C	4.58068200	1.33318700	0.38704000	C	4.85537000	1.28418600	0.25888700
H	-4.46575600	1.42228500	1.54378300	H	-4.91350100	1.07181800	1.32884000
H	4.71506200	0.92601900	1.39187500	H	4.91419600	1.07086400	1.32858900
H	-5.21153000	0.99548600	-0.00373400	H	-5.45844200	0.54247300	-0.27004100
H	5.22280700	0.77100200	-0.29630900	H	5.45836100	0.54181800	-0.27065500
H	-4.77575900	2.66759600	0.33740600	H	-5.32230200	2.26107400	0.09351900
H	4.94553400	2.36543500	0.40008800	H	5.32280200	2.26035100	0.09342200
O	-0.91891000	4.87776000	0.35937000	O	-1.12298000	4.61739800	0.44464100
O	1.32651000	4.85924100	0.30037900	O	1.12326700	4.61740400	0.44378400
C	-0.05226100	-2.05636100	-0.73245000	C	-0.00002300	-1.88777600	-0.97994100
O	-0.07771700	-3.14903000	-1.15485400	O	-0.00003700	-2.96231800	-1.47258700
Mn	-0.01554900	-0.48443500	-0.04320800	Re	0.00001300	-0.24124400	-0.13810500
Mn-TS(HCO₂)-SMD(CH₃OH)				Re-TS(HCO₂)-SMD(CH₃OH)			
N	0.00057400	-0.42339400	-2.00019800	N	0.00064000	-0.33208100	-2.04168700
P	2.25277200	-0.11044600	-0.20792400	P	2.37168400	-0.07491300	-0.28090200
P	-2.25222000	-0.10970700	-0.20737200	P	-2.37161500	-0.07250400	-0.28145400
H	-0.00321800	1.38908200	-0.08887900	H	0.00099900	1.59183100	-0.09649000
C	-0.00211100	3.33806800	-0.41542800	C	0.00262200	3.45014900	-0.36238800
C	-2.42109600	-0.32186600	-2.04627700	C	-2.44041800	-0.21295700	-2.13445300
C	2.42226100	-0.33130800	-2.04582800	C	2.44208000	-0.21998300	-2.13352600
H	-2.43591600	0.68584400	-2.47278300	H	-2.44862200	0.81189200	-2.51833000
H	2.44096500	0.67442300	-2.47682200	H	2.45446200	0.80404500	-2.51942400
H	-3.34905300	-0.82133500	-2.33294600	H	-3.35318100	-0.70600000	-2.47637900
H	3.34858200	-0.83524500	-2.32983400	H	3.35359600	-0.71668400	-2.47340700

C	-1.17988600	-1.05208600	-2.53286400	C	-1.18414900	-0.92178400	-2.62111900
C	1.17857300	-1.05876800	-2.53030000	C	1.18399700	-0.92504200	-2.62071700
H	-1.17303000	-1.03656000	-3.64046200	H	-1.15425300	-0.85176700	-3.72423300
H	1.17219800	-1.04700600	-3.63793300	H	1.15471400	-0.85467200	-3.72383300
H	-1.26153800	-2.12868800	-2.26012300	H	-1.27117700	-2.00755400	-2.39844100
H	1.25576900	-2.13473300	-2.25357200	H	1.26791400	-2.01110200	-2.39836100
C	3.12870200	1.54263300	0.04267000	C	3.24841700	1.56587700	0.00609000
C	-3.12873900	1.54211000	0.05037200	C	-3.24871400	1.56745300	0.01056500
H	2.49087700	2.20745900	-0.54968000	H	2.61044200	2.24102000	-0.57498800
H	-2.49225500	2.20888400	-0.54121800	H	-2.61071600	2.24470500	-0.56808300
C	3.44991000	-1.34509500	0.57249100	C	3.55339400	-1.37195600	0.39702000
C	-3.44972200	-1.34896100	0.56508200	C	-3.55353400	-1.37207700	0.39104000
H	4.44092400	-0.89107500	0.47383000	H	4.55693600	-0.96999800	0.22543100
H	-4.44118600	-0.89622800	0.46501200	H	-4.55726700	-0.96965600	0.22142400
C	0.00014900	0.06354800	1.81862100	C	-0.00183000	0.14979000	2.01670700
O	-0.00004900	0.25941500	2.97985500	O	-0.00336100	0.35101200	3.18272600
C	-3.15972300	-1.54817300	2.05182500	C	-3.35325500	-1.57247100	1.89150400
C	3.15578700	-1.53928900	2.05911300	C	3.35398200	-1.56603000	1.89847700
H	-3.13879300	-0.60978100	2.60844600	H	-3.44574400	-0.64419100	2.45702800
H	3.13395800	-0.59905800	2.61263400	H	3.45258200	-0.63611600	2.46041600
H	-2.19876000	-2.04540300	2.20220800	H	-2.36735900	-1.99376600	2.10304000
H	2.19411300	-2.03544300	2.20850500	H	2.36626500	-1.98171400	2.11294500
H	-3.93400000	-2.18069100	2.49980700	H	-4.10479800	-2.27050200	2.27560600
H	3.92857100	-2.17077400	2.51112500	H	4.10245400	-2.26665400	2.28385600
C	-3.48031500	-2.69674700	-0.15178300	C	-3.44736700	-2.70358000	-0.34657100
C	3.48500900	-2.69560700	-0.13911700	C	3.44690600	-2.70661600	-0.33497300
H	-2.51133900	-3.19849800	-0.11799100	H	-2.45309900	-3.14374900	-0.24593100
H	2.51681800	-3.19894500	-0.10641500	H	2.45181300	-3.14496700	-0.23457500
H	-3.78268700	-2.60999800	-1.19695200	H	-3.67343300	-2.61137700	-1.41030600
H	3.79053600	-2.61251700	-1.18365600	H	3.67556400	-2.61960300	-1.39864900
H	-4.20482500	-3.35318500	0.34293900	H	-4.16480800	-3.41261900	0.08051400
H	4.20908300	-3.34886900	0.36040900	H	4.16240100	-3.41473800	0.09683000
C	3.11214000	2.03338700	1.48657300	C	3.21765100	2.02596200	1.45988500
C	-3.11010600	2.02921600	1.49545200	C	-3.21937900	2.02286700	1.46577700
H	3.80114600	1.45958200	2.11201400	H	3.93292900	1.47069600	2.07210500
H	-3.79601500	1.45215500	2.12127700	H	-3.92779500	1.45859100	2.07764700
H	2.11806600	1.97466900	1.93280600	H	2.22687900	1.91024200	1.90413300
H	-2.11477500	1.97228000	1.93906100	H	-2.22677800	1.91560600	1.90788800
H	3.43402600	3.07940400	1.52835600	H	3.49217800	3.08416700	1.52146700
H	-3.43472700	3.07426300	1.54045500	H	-3.50461600	3.07802500	1.53122200
C	4.53918200	1.60999000	-0.53703500	C	4.65977000	1.63522600	-0.56885600
C	-4.54009200	1.61029700	-0.52701300	C	-4.65995900	1.63774800	-0.56449600
H	4.58044700	1.28082900	-1.57758000	H	4.69852400	1.33140300	-1.61747600
H	-4.58249600	1.28492400	-1.56872000	H	-4.69924500	1.33268800	-1.61273600
H	5.24702700	1.00663500	0.03799700	H	5.35924000	1.01007100	-0.00723900
H	-5.24658800	1.00421700	0.04680000	H	-5.35987900	1.01389800	-0.00198900
H	4.90058300	2.64380200	-0.50603300	H	5.03073700	2.66428500	-0.51194600
H	-4.90234600	2.64366900	-0.49172800	H	-5.02987600	2.66722800	-0.50877200
O	0.00044500	3.70488900	0.69675700	O	-0.00326600	3.80915900	0.75478900
O	-0.00404300	3.32612400	-1.58647600	O	0.00939900	3.48704600	-1.53534800
C	0.00093600	-1.98075200	0.36921700	C	-0.00073000	-2.06052100	0.53432000
O	0.00123900	-3.13114900	0.61625800	O	-0.00115300	-3.19357200	0.87076000
Mn	0.00006600	-0.25599400	0.11418700	Re	-0.00017800	-0.20038200	0.15904100
2Mn...H₂O-SMD(CH₃OH)				2Re...H₂O-SMD(CH₃OH)			
O	-0.00213700	3.02901300	-0.77372400	O	-0.00030100	3.06878700	-0.37287300
P	2.22118700	-0.15858900	-0.07120100	P	-2.39693300	-0.10438900	0.22750900
P	-2.21981700	-0.15918100	-0.06763800	P	2.39686300	-0.10423300	0.22746700
C	2.42712000	-0.74176500	-1.83060100	C	-2.44517700	-0.48660300	2.04359400
C	-2.42568200	-0.75102000	-1.82412900	C	2.44510800	-0.48662000	2.04351700

H	2.47130200	-1.83382000	-1.80465200	H	-2.45228700	-1.57832600	2.11832400
H	-2.46365400	-1.84308600	-1.79324700	H	2.45213700	-1.57834800	2.11813700
H	3.35310100	-0.38102400	-2.28367900	H	-3.35412400	-0.11337500	2.52051700
H	-3.35423800	-0.39745900	-2.27754400	H	3.35408100	-0.11349200	2.52047200
C	1.19061700	-0.30038500	-2.60226900	C	-1.18752700	0.05232500	2.70632600
C	-1.19276600	-0.30607400	-2.59948700	C	1.18747200	0.05227000	2.70631500
H	1.18677800	-0.79662200	-3.59100200	H	-1.11522600	-0.38910800	3.71495800
H	-1.18952000	-0.80371100	-3.58752600	H	1.11520400	-0.38922200	3.71492400
H	1.25725400	0.78530800	-2.81171700	H	-1.29232900	1.14209700	2.87000400
H	-1.26416900	0.77902000	-2.81010100	H	1.29226000	1.14203200	2.87004900
N	0.00056900	-0.63633300	-1.85004700	N	-0.00004300	-0.26919600	1.93536600
C	-2.94403200	-1.61761400	0.88606000	C	3.29715200	-1.58917300	-0.49296700
C	2.94409100	-1.62261200	0.87544800	C	-3.29685600	-1.58960500	-0.49286100
H	-2.33642900	-2.43435400	0.47898800	H	2.66842400	-2.40649500	-0.12116500
H	2.33653600	-2.43683300	0.46325200	H	-2.66786800	-2.40675200	-0.12110300
C	-3.52418200	1.19342700	0.10807300	C	3.53426900	1.36317400	-0.03259500
C	3.52708400	1.19158200	0.10963200	C	-3.53465500	1.36272100	-0.03290900
C	-3.48879300	2.19733700	-1.04120900	C	3.33837000	2.44570500	1.02550000
C	3.48221500	2.20651800	-1.02948300	C	-3.33929800	2.44533900	1.02519600
O	0.00248500	1.10275300	2.88660900	O	0.00016200	0.10270500	-3.24931500
H	4.49306200	0.67865600	0.06294600	H	-4.54454000	0.95552700	0.08019700
H	-4.49059300	0.68043100	0.07413600	H	4.54423400	0.95624100	0.08075600
C	3.40967900	1.90524500	1.45367900	C	-3.39840500	1.94839800	-1.43724000
C	-3.39570900	1.91975200	1.44430400	C	3.39824100	1.94885600	-1.43694400
H	3.51913900	1.22705800	2.30161000	H	-3.53020000	1.20205600	-2.22184800
H	-3.49685100	1.24918200	2.29947500	H	3.53102400	1.20266000	-2.22152600
H	2.44176700	2.40536400	1.54794300	H	-2.42191100	2.41677200	-1.58016100
H	-2.42760100	2.42152100	1.52536400	H	2.42143700	2.41645000	-1.58033100
H	4.18761100	2.67159600	1.54128500	H	-4.16009400	2.72101700	-1.58554600
H	-4.17361900	2.68615200	1.53180500	H	4.15938900	2.72209100	-1.58481900
C	-2.69519600	-1.57508800	2.39046100	C	3.27776500	-1.64887400	-2.01660700
C	2.69400100	-1.58897300	2.37992200	C	-3.27759900	-1.64920700	-2.01650700
H	-3.30346000	-0.81459600	2.88674600	H	3.95271900	-0.91313800	-2.46062000
H	3.30310300	-0.83289400	2.88176700	H	-3.95284900	-0.91365400	-2.46037900
H	-1.64706400	-1.37785500	2.62268600	H	2.27719600	-1.48457400	-2.42152800
H	1.64597400	-1.39120800	2.61228200	H	-2.27714400	-1.48451500	-2.42153900
H	-2.95927600	-2.54070100	2.83536900	H	3.61259200	-2.63708100	-2.34816500
H	2.95579100	-2.55790800	2.81893700	H	-3.61214000	-2.63749300	-2.34811500
C	-4.40795600	-1.92124900	0.58034300	C	4.70959600	-1.78479400	0.05122500
C	4.40820500	-1.92459600	0.56916600	C	-4.70919800	-1.78560900	0.05143700
H	-4.61545700	-1.95663500	-0.49219100	H	4.74418100	-1.77255400	1.14304200
H	4.61635400	-1.95429400	-0.50341000	H	-4.74365800	-1.77351500	1.14325800
H	-5.07828200	-1.18426900	1.03099400	H	5.39690800	-1.01976500	-0.32007800
H	5.07810600	-1.18985400	1.02407200	H	-5.39671000	-1.02067100	-0.31968600
H	-4.67733100	-2.89784700	0.99722100	H	5.09734700	-2.75473300	-0.27761900
H	4.67751400	-2.90335300	0.98099900	H	-5.09678600	-2.75558200	-0.27749800
H	0.00037600	-1.26772100	0.66405900	H	0.00005600	-2.22919700	-0.60103100
H	-4.30578100	2.91732500	-0.92048600	H	4.03277900	3.26988700	0.83104200
H	-2.55550100	2.76264400	-1.05670100	H	2.32727000	2.85711200	1.00175500
H	-3.61481700	1.72518600	-2.01729700	H	3.53788100	2.08266400	2.03514600
H	4.30256100	2.92304800	-0.91099100	H	-4.03358500	3.26952400	0.83031100
H	3.59588100	1.74312500	-2.01143200	H	-3.53934700	2.08237300	2.03476100
H	2.55048200	2.77441500	-1.02906000	H	-2.32817600	2.85672100	1.00195400
H	0.00339400	-2.22521000	-1.62965300	H	0.00162200	-2.90062300	-0.07826400
O	-0.01341800	-3.27299200	-1.56109200	O	0.00118400	-4.17000400	0.78010400
C	-0.00089400	1.88780500	-0.47744100	C	-0.00018200	1.88918200	-0.28304400
C	0.00179200	0.75282900	1.76095600	C	0.00007100	0.04360300	-2.07217400
Mn	0.00067600	0.23848100	0.10648500	Re	-0.00003100	0.04769200	-0.16817100
H	-0.01690700	-3.45084200	-0.61534000	H	0.00068700	-3.78464400	1.66311800
Mn-TS(H⁺ transfer, H₂ formation)-SMD(CH₃OH)				Re-TS(H⁺ transfer, H₂ formation)-SMD(CH₃OH)			

O	0.00071300	-2.92741200	0.26853500	O	0.00051200	-2.53205800	-1.88007400
P	2.27052000	0.15179400	0.12805300	P	-2.36740200	0.24024900	-0.00654500
P	-2.27019100	0.15158400	0.12849500	P	2.36742000	0.24086200	-0.00670100
C	2.42914800	0.42172400	1.95718700	C	-2.44869000	1.56932100	-1.30727400
C	-2.42844500	0.42285400	1.95745800	C	2.44827200	1.57009200	-1.30729000
H	2.44055600	1.50551700	2.10229100	H	-2.47423500	2.52166600	-0.77042200
H	-2.44029000	1.50662900	2.10260700	H	2.47344000	2.52242400	-0.77040000
H	3.35499800	0.01715700	2.37008600	H	-3.35860500	1.50447500	-1.90677900
H	-3.35423500	0.01821800	2.37047300	H	3.35821100	1.50561700	-1.90677700
C	1.18683400	-0.15798000	2.61651900	C	-1.19579600	1.51163500	-2.17080000
C	-1.18625500	-0.15681400	2.61704800	C	1.19538400	1.51197800	-2.17080800
H	1.16583100	0.16693200	3.67302300	H	-1.18364600	2.39776600	-2.82907100
H	-1.16489600	0.16919100	3.67321100	H	1.18294100	2.39806200	-2.82914900
H	1.26875800	-1.26403500	2.65306500	H	-1.24033500	0.63427200	-2.83885300
H	-1.26882600	-1.26278900	2.65479900	H	1.24024000	0.63459200	-2.83880400
N	0.00034800	0.29771500	1.92498500	N	-0.00019400	1.48587200	-1.33732200
C	-3.07797500	1.70237900	-0.56642200	C	3.20770900	1.08980300	1.44616100
C	3.07762600	1.70351400	-0.56557900	C	-3.20780300	1.08940100	1.44616600
H	-2.42766700	2.48115500	-0.15218300	H	2.54973900	1.95548000	1.58323200
H	2.42827200	2.48162900	-0.14854100	H	-2.54881400	1.95414100	1.58424700
C	-3.45895800	-1.23739900	-0.31973500	C	3.57485500	-1.09739500	-0.54505100
C	3.45919900	-1.23683100	-0.32173800	C	-3.57451700	-1.09833100	-0.54476100
C	-3.53341900	-2.34083300	0.73334800	C	3.51856300	-1.37327900	-2.04498700
C	3.53617700	-2.33918700	0.73235100	C	-3.51865100	-1.37371600	-2.04480000
O	0.00012800	-0.46421200	-3.02856200	O	0.00031000	-2.28685300	2.39272300
H	4.44365000	-0.76210600	-0.38083200	H	-4.56970100	-0.71137500	-0.30436900
H	-4.44382400	-0.76321100	-0.37645100	H	4.56998000	-0.70996800	-0.30512200
C	3.12971500	-1.83231800	-1.68948200	C	-3.34691200	-2.38987900	0.23863000
C	-3.13168200	-1.83157900	-1.68859700	C	3.34814500	-2.38884100	0.23878500
H	3.07150100	-1.07765000	-2.47520900	H	-3.39104400	-2.24431500	1.31930200
H	-3.07571900	-1.07628200	-2.47387300	H	3.39261400	-2.24296000	1.31940700
H	2.17815600	-2.36956700	-1.66970700	H	-2.37207700	-2.82224400	0.00039000
H	-2.17959100	-2.36799500	-1.67106400	H	2.37342900	-2.82172700	0.00100200
H	3.90779700	-2.54814600	-1.97549500	H	-4.11381400	-3.12468300	-0.02850800
H	-3.90964100	-2.54794000	-1.97361300	H	4.11528800	-3.12336600	-0.02842500
C	-3.01654600	1.79442500	-2.08727300	C	3.17525500	0.27060200	2.73219100
C	3.01314600	1.79807600	-2.08610400	C	-3.17755500	0.26950900	2.73183100
H	-3.68868400	1.07568100	-2.56331600	H	3.86852800	-0.57334600	2.69093100
H	3.67833300	1.07476500	-2.56499000	H	-3.87228000	-0.57319400	2.68969400
H	-2.00842400	1.62381300	-2.46989800	H	2.17663900	-0.11682600	2.94603000
H	2.00267100	1.63580000	-2.46613200	H	-2.17975600	-0.11973700	2.94614400
H	-3.32871000	2.79318500	-2.40980300	H	3.47818300	0.89740100	3.57748800
H	3.33225700	2.79481200	-2.40809900	H	-3.47997500	0.89640100	3.57724100
C	-4.49601000	1.94678300	-0.05806400	C	4.61701200	1.59741800	1.15385000
C	4.49663900	1.94648100	-0.05929200	C	-4.61614600	1.59915500	1.15295900
H	-4.56393300	1.89923500	1.03092100	H	4.66716300	2.20052000	0.24441200
H	4.56624300	1.89760700	1.02953600	H	-4.66472600	2.20269400	0.24371100
H	-5.20852000	1.22956700	-0.47483700	H	5.33243500	0.77629200	1.05704700
H	5.20808100	1.22932400	-0.47799500	H	-5.33265200	0.77908500	1.05527600
H	-4.82823100	2.94485200	-0.36351700	H	4.95979600	2.22653700	1.98228800
H	4.82897300	2.94468200	-0.36416500	H	-4.95868200	2.22842100	1.98138400
H	-0.00312900	1.61429200	-0.62174200	H	-0.00019800	1.09512100	1.35956700
H	-4.25373500	-3.09901200	0.40784900	H	4.23243100	-2.16564800	-2.29435900
H	-2.57275700	-2.84166000	0.86873500	H	2.52916600	-1.71648900	-2.35510800
H	-3.86725400	-1.97302600	1.70506200	H	3.78104100	-0.49970600	-2.64463300
H	4.25152600	-3.10056200	0.40339300	H	-4.23219900	-2.16637800	-2.29417500
H	3.87747500	-1.97104200	1.70134300	H	-3.78179200	-0.50005900	-2.64402000
H	2.57455900	-2.83628500	0.87469400	H	-2.52920000	-1.71634200	-2.35541400
H	0.00027600	1.99296700	0.12842700	H	-0.00038100	2.79507200	-0.64711000

O -0.00104200 3.11305600 1.34115200	O -0.00065600 3.80577600 -0.22760100
C 0.00057400 -1.76958100 0.11306600	C 0.00032500 -1.60207800 -1.15318500
C 0.00012800 -0.26576600 -1.87433700	C 0.00020300 -1.47718200 1.52934900
Mn 0.00014700 -0.05135500 -0.13923100	Re 0.00005700 -0.20042200 0.14268100
H -0.00064200 2.23434600 1.77851500	H 0.00040500 3.67200200 0.72539100
2Mn-...K⁺-SMD(CH₃OH)	2Re-...K⁺-SMD(CH₃OH)
O -0.00008900 -2.90197300 -1.17796800	O 0.00000400 -2.90861600 -1.36356000
P -2.24250000 0.04453200 -0.03826400	P -2.37296900 0.11969700 -0.07391200
P 2.24250400 0.04454500 -0.03828200	P 2.37297600 0.11968600 -0.07393100
C -2.43624900 0.91917300 -1.67421600	C -2.45538700 1.18072200 -1.60423200
C 2.43623600 0.91913600 -1.67426000	C 2.45539400 1.18077800 -1.60420400
H -2.52859800 1.99067700 -1.46702300	H -2.53574100 2.22051600 -1.26902500
H 2.52860700 1.99063900 -1.46708000	H 2.53573600 2.22056100 -1.26895900
H -3.34666000 0.62714400 -2.20134600	H -3.35032900 0.97808500 -2.19582100
H 3.34663100 0.62708400 -2.20140500	H 3.35034700 0.97817900 -2.19579200
C -1.18011900 0.63910800 -2.48696600	C -1.18216200 0.98225600 -2.41569800
C 1.18008900 0.63908600 -2.48698500	C 1.18217800 0.98231900 -2.41568700
H -1.18877900 1.28482200 -3.38706100	H -1.17603200 1.72204200 -3.23768100
H 1.18874500 1.28479700 -3.38708300	H 1.17603200 1.72212600 -3.23765200
H -1.23383200 -0.40087900 -2.87573800	H -1.22671100 -0.00907300 -2.91283400
H 1.23377900 -0.40090300 -2.87575400	H 1.22675700 -0.00899600 -2.91285000
N -0.00000600 0.87325300 -1.68750500	N 0.00000000 1.12447200 -1.58875900
C 3.06888800 1.27134000 1.13697200	C 3.27149100 1.18864500 1.18902500
C -3.06885400 1.27130800 1.13704600	C -3.27145000 1.18871800 1.18900900
H 2.47736800 2.17538800 0.94863700	H 2.63198600 2.07928100 1.21121500
H -2.47719700 2.17529600 0.94886200	H -2.63201500 2.07941000 1.21105900
C 3.46721600 -1.38934600 -0.10533800	C 3.54746900 -1.32236800 -0.36851500
C -3.46720800 -1.38935900 -0.10537400	C -3.54752100 -1.32232500 -0.36841000
C 3.46907700 -2.11908600 -1.44594300	C 3.50430200 -1.84947600 -1.80062600
C -3.46906300 -2.11907700 -1.44599500	C -3.50458400 -1.84935300 -1.80055700
O -0.00004900 -1.58824400 2.71320500	O -0.00001100 -1.89203700 2.76941600
H -4.45476500 -0.93894700 0.03193900	H -4.55059600 -0.92418900 -0.18670200
H 4.45476900 -0.93891100 0.03196300	H 4.55057800 -0.92425300 -0.18695200
C -3.22373300 -2.37893200 1.03224700	C -3.28629900 -2.45442700 0.62394800
C 3.22378400 -2.37889200 1.03231600	C 3.28632200 -2.45441700 0.62392000
H -3.24044500 -1.90592400 2.01554300	H -3.28724200 -2.11795800 1.66212800
H 3.24032200 -1.90582800 2.01558600	H 3.28742400 -2.11790400 1.66208400
H -2.25953400 -2.88001400 0.91904300	H -2.32252700 -2.93145600 0.43040200
H 2.25969000 -2.88016000 0.91905600	H 2.32249600 -2.93140100 0.43053000
H -4.00110200 -3.15057900 1.02446100	H -4.06331000 -3.21950200 0.52229800
H 4.00128900 -3.15040500 1.02464900	H 4.06327600 -3.21953800 0.52219000
C 2.89934500 0.92632400 2.61269100	C 3.27232600 0.59224100 2.59248200
C -2.89951700 0.92612700 2.61275000	C -3.27211900 0.59244600 2.59252200
H 3.50292100 0.06162900 2.89873300	H 3.95047800 -0.26167900 2.66522500
H -3.50327000 0.06151100 2.89865600	H -3.95020600 -0.26151600 2.66540500
H 1.85828100 0.71512600 2.86382200	H 2.27625400 0.26563800 2.89964600
H -1.85851700 0.71472200 2.86396800	H -2.27599800 0.26594000 2.89962500
H 3.22795400 1.76882900 3.23052200	H 3.61631600 1.34149200 3.31297900
H -3.22803900 1.76863400 3.23062500	H -3.61609100 1.34174200 3.31298200
C 4.52446600 1.59404100 0.81046700	C 4.67373400 1.62085600 0.77107200
C -4.52434500 1.59426700 0.81041400	C -4.67377100 1.62076000 0.77114300
H 4.67597700 1.83068100 -0.24550800	H 4.69866900 2.04923600 -0.23331500
H -4.67569600 1.83104600 -0.24555300	H -4.69883400 2.04907500 -0.23326800
H 5.19074000 0.76765100 1.07139000	H 5.38113100 0.78815900 0.80245700
H -5.19077400 0.76795100 1.07117300	H -5.38108000 0.78799200 0.80264000
H 4.84899000 2.46383300 1.39174200	H 5.04519800 2.38362000 1.46355400
H -4.84880100 2.46404500 1.39174700	H -5.04525600 2.38353000 1.46360800
H 0.00000300 1.13462200 0.92252800	H 0.00004900 1.25540800 1.16435500
H 4.20488900 -2.93004800 -1.41413400	H 4.19475400 -2.69458900 -1.89392100

H 2.49899300 -2.56770100 -1.66627900	H 2.51011300 -2.20939600 -2.07335400
H 3.74114500 -1.46894400 -2.27906400	H 3.80895400 -1.09984700 -2.53331900
H -4.20492300 -2.92999800 -1.41422000	H -4.19504300 -2.69446800 -1.89378400
H -3.74106600 -1.46891300 -2.27911900	H -3.80936800 -1.09968600 -2.53315700
H -2.49899900 -2.56774500 -1.66629700	H -2.51044100 -2.20924700 -2.07347400
C 0.00000600 -1.82065000 -0.71373100	C -0.00000200 -1.85710000 -0.82825200
C 0.00003600 -1.05326000 1.66440500	C 0.00000400 -1.24619200 1.77833500
Mn 0.00000600 -0.27937600 0.11341000	K 0.00001500 3.49127500 -0.15808600
K 0.00002700 3.32258600 -0.47691600	Re 0.00000500 -0.24017200 0.18015400
1Mn-OCH₃...K⁺-SMD(CH₃OH)	1Re-OCH₃...K⁺-SMD(CH₃OH)
N -0.00776400 -0.67408600 -1.73463700	N -0.00577600 0.77705700 -1.75867600
P 2.31262400 0.06914500 -0.08521800	P -2.39714300 -0.03364800 -0.15442600
P -2.30375000 0.09666100 -0.08182700	P 2.40174500 -0.01227400 -0.15722900
C 0.00681500 -2.05085700 2.25227100	C 0.01304900 2.10985400 2.30176800
C 2.43296900 -0.77060700 -1.73800800	C -2.46286400 0.83631400 -1.79884400
C -2.44881600 -0.68689600 -1.76077500	C 2.45068800 0.88386600 -1.78731200
H 2.47465300 -1.84475300 -1.53232900	H -2.54074100 1.90525000 -1.57719600
H -2.54226500 -1.76464700 -1.59554200	H 2.49930500 1.95031800 -1.54574800
H 3.34745500 -0.51576700 -2.27776300	H -3.35501400 0.57325300 -2.37098200
H -3.34893500 -0.37426400 -2.29378700	H 3.34968000 0.65190200 -2.36235900
C 1.17840500 -0.43488500 -2.52971700	C -1.18462200 0.54810900 -2.57491500
C -1.17688500 -0.38022500 -2.53659100	C 1.18115100 0.57932300 -2.57145700
H 1.16788500 -1.05109400 -3.45012700	H -1.17007800 1.19737500 -3.47023700
H -1.17886700 -0.98128400 -3.46681500	H 1.15815400 1.23727000 -3.46030500
H 1.25157700 0.61206800 -2.89171400	H -1.22882900 -0.48650400 -2.97003700
H -1.21051900 0.67465800 -2.88123500	H 1.24640500 -0.45006900 -2.97710100
C -3.32731500 -1.06077100 0.99629000	C 3.37530400 1.13465200 0.96839500
C 3.32363000 -1.06974700 1.02322100	C -3.37144000 1.12612700 0.95736500
H -2.68609600 -1.94515900 1.06802500	H 2.69750100 1.99021000 1.05694900
H 2.67196500 -1.94399400 1.11606700	H -2.69672600 1.98633900 1.02643800
C -3.38810200 1.64645400 -0.13507700	C 3.51758400 -1.51605800 -0.33926000
C 3.41862600 1.59858800 -0.19298000	C -3.50470400 -1.54710200 -0.30850800
H -4.40021000 1.28387200 0.07324100	H 4.53300100 -1.12870600 -0.20325100
H 4.42757100 1.22419000 0.01003500	H -4.52190100 -1.16322500 -0.17590100
C 0.01398900 0.95307600 1.75676400	C 0.00990500 -1.06865700 1.89147200
O 0.02174000 1.50708200 2.79224100	O 0.01364200 -1.63451200 2.92940300
C 3.06578800 2.61971900 0.88844300	C -3.22250000 -2.56269400 0.79814200
C -3.00341500 2.63347100 0.96654200	C 3.24622700 -2.55182100 0.75175600
H 3.02927800 2.18210000 1.88693800	H -3.24328900 -2.12178500 1.79547800
H -2.96156200 2.16945400 1.95282400	H 3.26758300 -2.12740300 1.75624400
H 2.09839100 3.08761100 0.69447800	H -2.24716600 -3.03446100 0.66032400
H -2.03047700 3.08960100 0.77181100	H 2.27404400 -3.02880600 0.61037600
H 3.81914500 3.41483000 0.90388500	H -3.98018300 -3.35297700 0.76976100
H -3.74255700 3.44075000 1.01263900	H 4.00970900 -3.33577900 0.70769600
C 3.44634700 2.26540700 -1.56601200	C -3.43271500 -2.22243200 -1.67568500
C -3.42364100 2.34847500 -1.49056700	C 3.44653900 -2.16872100 -1.71750700
H 2.46646200 2.64729200 -1.85766000	H -2.43165100 -2.60160500 -1.89029100
H -2.44093200 2.71928100 -1.78707200	H 2.44605300 -2.54501100 -1.93984100
H 3.79875300 1.59375200 -2.35043200	H -3.73079600 -1.55937500 -2.48922100
H -3.80015300 1.70437200 -2.28699300	H 3.74448100 -1.49135400 -2.51929700
H 4.13334400 3.11835500 -1.53685900	H -4.11542500 -3.07889700 -1.68827200
H -4.09368600 3.21306700 -1.42933100	H 4.13009100 -3.02421600 -1.74420000
C -3.54378800 -0.51176200 2.40458200	C 3.59243300 0.55312200 2.36302700
C 3.54731500 -0.49041300 2.41815900	C -3.57648800 0.56710900 2.36302500
H -4.26876300 0.30666000 2.40515900	H 4.35069500 -0.23424000 2.35291700
H 4.27953300 0.32131400 2.39973300	H -4.33294500 -0.22209400 2.37098600
H -2.62070800 -0.14689200 2.85910500	H 2.67686700 0.13919800 2.79066600
H 2.62827900 -0.10793300 2.86650800	H -2.65691100 0.16201400 2.79040700
H -3.94505500 -1.29901300 3.05123300	H 3.95031600 1.33755300 3.03771900

H 3.94285600 -1.26652600 3.08165700	H -3.93135800 1.36150100 3.02756300
C -4.65929000 -1.48453100 0.38120600	C 4.69636100 1.62257400 0.37894500
C 4.64954000 -1.52610600 0.41835800	C -4.69929000 1.59686200 0.36922300
H -4.54145000 -1.96701400 -0.59080700	H 4.57224100 2.10778400 -0.59105600
H 4.52397200 -2.02531300 -0.54423900	H -4.58564800 2.06624300 -0.60980900
H -5.34071000 -0.63785200 0.25901500	H 5.41435100 0.80624600 0.26124000
H 5.34502200 -0.69335400 0.28030700	H -5.41323000 0.77445200 0.27104900
H -5.15506000 -2.20275900 1.04356900	H 5.14981400 2.35524400 1.05524900
H 5.13303200 -2.23925600 1.09513500	H -5.15196500 2.33841300 1.03631000
H -0.86976100 -1.66096200 2.80532500	H 0.90330400 1.72848900 2.83430800
C 0.01231400 1.79267600 -0.57245000	C 0.00770500 -1.98459600 -0.54841700
O 0.01857400 2.85403000 -1.07532300	O 0.01136200 -3.09252900 -0.96917300
Mn 0.00555100 0.23184900 0.16713400	Re 0.00386500 -0.26307500 0.17641200
K -0.08330600 -3.37255300 -1.07683000	K -0.06486300 3.47474400 -1.01803700
O 0.00533400 -1.75522000 0.90000400	O 0.00461100 1.82117100 0.94233800
H 0.00201600 -3.14535300 2.42690000	H 0.00187700 3.20194900 2.47350500
H 0.88975700 -1.66977600 2.80134100	H -0.85851500 1.70742200 2.84946700
1Mn-HCH₂O⁻...K⁺-SMD(CH₃OH)	1Re-HCH₂O⁻...K⁺-SMD(CH₃OH)
O -0.18679000 -3.42177100 -0.15297000	O 0.09848700 -3.36466500 0.08478700
P -2.32245600 -0.18265000 -0.10164400	P -2.39043000 -0.24112700 -0.17157500
P 2.24583900 -0.40922200 -0.11089300	P 2.43115900 -0.10825600 -0.16757300
C -2.47727600 0.41161500 -1.85494200	C -2.46974200 0.57964700 -1.83708100
C 2.43898200 0.17362600 -1.86448600	C 2.47204200 0.72042300 -1.83025800
H -2.57033500 1.50123800 -1.81642100	H -2.61090100 1.64723600 -1.64029800
H 2.62599400 1.25089100 -1.82314500	H 2.55674600 1.79323300 -1.63027200
H -3.38229800 0.04424500 -2.34141700	H -3.34071300 0.25211300 -2.40813800
H 3.30489400 -0.27033700 -2.35824100	H 3.35948500 0.43833600 -2.40046900
C -1.22388900 -0.00155800 -2.60783000	C -1.18055200 0.32846000 -2.60295900
C 1.14970900 -0.12391200 -2.61029700	C 1.19943200 0.40518200 -2.60075800
H -1.11541000 0.63133700 -3.50434000	H -1.12446200 1.04141000 -3.44395700
H 1.10003400 0.50882400 -3.51223400	H 1.10403300 1.12255700 -3.43428300
H -1.34211100 -1.02706000 -2.99304500	H -1.21937300 -0.66507000 -3.07685800
H 1.16678300 -1.15975300 -2.98526200	H 1.29489900 -0.58011400 -3.08352000
N -0.02797800 0.09298200 -1.76487700	N 0.00587000 0.45071100 -1.75353700
C 3.12519900 0.97449900 0.82101700	C 3.40960500 1.11370800 0.87326400
C -3.05673800 1.28116100 0.83411000	C -3.40549900 0.94853300 0.87346200
H 2.56352400 1.85362800 0.48248800	H 2.87374400 2.04501200 0.65513900
H -2.44002200 2.10755900 0.46097300	H -2.84624700 1.88082800 0.73092000
C 3.34719900 -1.91602600 0.06877800	C 3.52193900 -1.61835700 -0.37023800
C -3.56291200 -1.57798100 0.08837300	C -3.41936200 -1.79418800 -0.35750000
C 3.21586800 -2.88400400 -1.10525500	C 3.15587000 -2.42249400 -1.61609500
C -3.51124000 -2.56478400 -1.07577200	C -3.03341600 -2.58447400 -1.60616800
O -0.08168100 -0.91608000 2.96221600	O 0.02513000 -0.65165800 3.25499800
H -4.54439000 -1.09433800 0.07761200	H -4.44406300 -1.43274800 -0.49164400
H 4.36970500 -1.52648100 0.07144100	H 4.52863300 -1.21462700 -0.51757900
C -3.38978900 -2.30253800 1.42194800	C -3.36927700 -2.66989200 0.89144200
C 3.09461500 -2.63355400 1.39377500	C 3.52678700 -2.49740900 0.87739100
H -3.42214200 -1.62592800 2.27715600	H -3.75596300 -2.15905800 1.77412900
H 3.20625100 -1.97651300 2.25728700	H 3.89900600 -1.97039400 1.75702600
H -2.44449400 -2.84885800 1.46060700	H -2.35165900 -2.99773200 1.11251500
H 2.09166700 -3.06423300 1.42864500	H 2.52879000 -2.87525100 1.10917400
H -4.19658600 -3.03188300 1.54792700	H -3.98128400 -3.56373700 0.73386000
H 3.81106600 -3.45348500 1.50766500	H 4.17909600 -3.36081200 0.71133700
C 3.00272100 0.90958200 2.33918900	C 3.31733400 0.86862100 2.37443900
C -2.88007300 1.23756400 2.34768700	C -3.40109700 0.63055400 2.36501000
H 3.57436600 0.07840700 2.75833000	H 3.86810500 -0.02420300 2.67802500
H -3.46744400 0.43863700 2.80557300	H -4.03021300 -0.23148800 2.59734100
H 1.96859800 0.81491900 2.67097600	H 2.28505200 0.75980600 2.70772300
H -1.83802200 1.10745500 2.64084200	H -2.39803300 0.43166300 2.74401600

H	3.40594500	1.83011500	2.77307400	H	3.75393600	1.71755300	2.91010000
H	-3.22759900	2.18269800	2.77730500	H	-3.80389900	1.48407800	2.91940100
C	4.58160000	1.15528900	0.39892500	C	4.85792300	1.28113300	0.42315100
C	-4.50779600	1.57537500	0.45990500	C	-4.82666200	1.16115400	0.36006500
H	4.70685100	1.18913100	-0.68553300	H	4.94733100	1.46290000	-0.65046400
H	-4.67003200	1.60322700	-0.62019700	H	-4.85819100	1.41559600	-0.70162500
H	5.21617200	0.35600400	0.79015100	H	5.46103400	0.40427000	0.67189500
H	-5.19109500	0.83734100	0.88743300	H	-5.44814900	0.27606800	0.51811400
H	4.96284600	2.09875300	0.80279600	H	5.30336800	2.13754300	0.93969900
H	-4.79495100	2.55303100	0.86015500	H	-5.29211300	1.98627900	0.90902100
H	0.12240800	2.72108100	1.34278600	H	0.02904100	2.19655900	1.10366400
C	0.32573000	3.80670500	1.51251900	C	-0.08073000	3.18205400	1.64244400
H	3.87547500	-3.74144400	-0.93623500	H	3.81219500	-3.29612400	-1.68377700
H	2.19989300	-3.26941200	-1.20816800	H	2.12737400	-2.78596100	-1.58436900
H	3.50882900	-2.43280900	-2.05483300	H	3.28628900	-1.84678500	-2.53428800
H	-4.25218800	-3.35366700	-0.90950500	H	-3.65932000	-3.48025700	-1.67093400
H	-3.74701100	-2.09630000	-2.03282300	H	-3.18788700	-2.01312400	-2.52337500
H	-2.53546600	-3.04629900	-1.16090000	H	-1.99233600	-2.91147700	-1.57874700
O	0.84477000	4.46464000	0.41507500	O	-0.53840100	4.21131300	0.85306600
C	-0.13549700	-2.25823300	-0.04519500	C	0.07115000	-2.18529600	0.13925700
Mn	-0.05601600	-0.54526100	0.05762900	Re	0.02476300	-0.34175000	0.18994400
C	-0.06597800	-0.70586700	1.81297900	C	0.02419800	-0.51985500	2.08717000
H	-0.64407200	4.21977700	1.87012000	H	-0.73954200	2.93738500	2.50377400
K	0.12474400	3.09314200	-1.66954300	K	-0.12875100	3.32671500	-1.56653000
H	0.98673100	3.82345900	2.40659400	H	0.92181600	3.36306000	2.08894400
Mn-TS(HCH₂O⁻...K⁺)-SMD(CH₃OH)				Re-TS(HCH₂O⁻...K⁺)-SMD(CH₃OH)			
O	-0.03882000	-3.30850500	-0.17011900	O	-0.00014700	-3.38863900	0.22198700
P	-2.26473300	-0.19934600	-0.10448000	P	2.37902500	-0.12979300	0.17117400
P	2.24865400	-0.23727800	-0.10903600	P	-2.37930700	-0.12935700	0.17123900
C	-2.44471900	0.08170100	-1.93529500	C	2.45698100	0.31240100	1.97880000
C	2.42643600	0.04675300	-1.93930800	C	-2.45710500	0.31296900	1.97882900
H	-2.51773200	1.16334400	-2.09242500	H	2.53797000	1.40319300	2.03582700
H	2.51092900	1.12797100	-2.09355900	H	-2.53759200	1.40380600	2.03578800
H	-3.35970400	-0.35242700	-2.34261100	H	3.35094500	-0.08841700	2.46058100
H	3.33526800	-0.39634000	-2.35081300	H	-3.35125600	-0.08740600	2.46064600
C	-1.19237000	-0.46477700	-2.60420100	C	1.18222000	-0.16397300	2.66184800
C	1.16547500	-0.48245500	-2.60572200	C	-1.18246800	-0.16381400	2.66182800
H	-1.19975700	-0.16400300	-3.67016900	H	1.17273700	0.23017100	3.69493500
H	1.17544500	-0.18285500	-3.67199000	H	-1.17287100	0.23017200	3.69497200
H	-1.24879800	-1.57454400	-2.61625400	H	1.22689300	-1.26714700	2.76861900
H	1.20580600	-1.59287900	-2.61617900	H	-1.22737600	-1.26699300	2.76841900
N	-0.00929900	0.02351700	-1.93361400	N	-0.00008100	0.26515700	1.93877000
C	3.16956900	1.24597800	0.60478500	C	-3.31508900	1.30007300	-0.61807200
C	-3.14884700	1.30949300	0.60326100	C	3.31502100	1.29953200	-0.61798900
H	2.52628500	2.07781600	0.29606300	H	-2.68409900	2.15274500	-0.34141200
H	-2.50355200	2.12521700	0.25709700	H	2.68446900	2.15236500	-0.34081300
C	3.40732000	-1.67176600	0.30459000	C	-3.52461200	-1.60537600	-0.05513000
C	-3.45317400	-1.60650100	0.31606200	C	3.52431300	-1.60581300	-0.05535100
C	3.46042400	-2.75267900	-0.77252400	C	-3.44517400	-2.60812700	1.09291500
C	-3.52104800	-2.69678800	-0.75094300	C	3.44539100	-2.60828900	1.09296600
O	-0.00699100	-0.69814600	3.05674800	O	0.00020600	-0.91414200	-3.22395800
H	-4.44214500	-1.14191900	0.37944800	H	4.53562000	-1.18783200	-0.06948000
H	4.40486000	-1.22733200	0.37871000	H	-4.53600900	-1.18761400	-0.06869300
C	-3.12651800	-2.22190800	1.67633700	C	3.26759700	-2.30254500	-1.39076600
C	3.05934000	-2.29189500	1.65718000	C	-3.26840300	-2.30171100	-1.39085700
H	-3.07054000	-1.48002400	2.47422800	H	3.30453000	-1.61811600	-2.23978500
H	3.02170600	-1.55688200	2.46242200	H	-3.30541100	-1.61696000	-2.23961400
H	-2.17440500	-2.75727000	1.65164400	H	2.29005200	-2.79027100	-1.39863300
H	2.09228200	-2.79853300	1.62386300	H	-2.29096300	-2.78965400	-1.39914500

H	-3.90418800	-2.94322100	1.95016100	H	4.02671200	-3.07475900	-1.55437100
H	3.81547500	-3.03759300	1.92599900	H	-4.02773100	-3.07369800	-1.55454400
C	3.21850500	1.24292800	2.13000800	C	-3.35118400	1.22390300	-2.14101100
C	-3.15315600	1.34377800	2.12839300	C	3.35045500	1.22390300	-2.14095900
H	3.90682300	0.48139200	2.50580600	H	-4.04409000	0.45258200	-2.48634700
H	-3.83191200	0.59431000	2.54350500	H	4.04025500	0.45007700	-2.48686400
H	2.23837200	1.06492500	2.57677400	H	-2.36726700	1.01221600	-2.56563400
H	-2.16008900	1.17293600	2.54861300	H	2.36560700	1.01617200	-2.56538000
H	3.58119100	2.21049000	2.49242300	H	-3.69754400	2.17739000	-2.55280400
H	-3.50154200	2.32132600	2.47789300	H	3.70041800	2.17623300	-2.55240600
C	4.56033300	1.48115900	0.02133400	C	-4.70893300	1.53730400	-0.04399500
C	-4.55157000	1.54887200	0.05138500	C	4.70928100	1.53591200	-0.04447800
H	4.55831000	1.52283000	-1.06980400	H	-4.70596100	1.61439000	1.04550600
H	-4.58071100	1.54754100	-1.04030100	H	4.70786700	1.60699700	1.04544400
H	5.26772400	0.70638800	0.32909600	H	-5.40527800	0.74350100	-0.32652000
H	-5.26292700	0.80003000	0.40980500	H	5.40636300	0.74467100	-0.33237400
H	4.95410600	2.43677500	0.38447300	H	-5.11385500	2.47557500	-0.43797000
H	-4.91784500	2.52497700	0.38777400	H	5.11216100	2.47696600	-0.43385600
H	-0.00489200	1.22397400	0.43652900	H	-0.00043700	1.43105100	-0.58298500
C	0.08231700	3.56134400	1.53527300	C	-0.00042900	3.45404700	-1.66673900
H	4.14708700	-3.54467800	-0.45412100	H	-4.11123400	-3.45139900	0.88087800
H	2.48505100	-3.21501600	-0.93589800	H	-2.43749200	-3.01053700	1.21416000
H	3.82418400	-2.37600700	-1.73012900	H	-3.75918600	-2.18003100	2.04639300
H	-4.22391100	-3.47259300	-0.42806500	H	4.11101900	-3.45182900	0.88064600
H	-3.87317000	-2.32325400	-1.71410800	H	3.76020800	-2.18009200	2.04613000
H	-2.55362200	-3.17869600	-0.90434800	H	2.43765300	-3.01034900	1.21499600
O	0.17231900	4.27779000	0.55543800	O	0.00327000	4.29580600	-0.78277000
C	-0.02638800	-2.13616500	-0.08387000	C	-0.00015200	-2.21343100	0.11923200
Mn	-0.01059300	-0.40842300	0.15999300	Re	-0.00014300	-0.34182300	-0.20438100
C	-0.00849700	-0.57460500	1.88648700	C	-0.00000300	-0.68135100	-2.06482600
H	-0.89450200	3.29775600	1.96767300	H	0.93301300	3.09233700	-2.12163900
K	0.01155800	2.75633500	-1.73336400	K	0.00059800	3.01301500	1.64386600
H	0.97388500	3.19709000	2.06697600	H	-0.93757400	3.09323800	-2.11466600
1Mn-OCH₂OH...K⁺-SMD(CH₃OH)				1Re-OCH₂OH...K⁺-SMD(CH₃OH)			
N	0.00080800	0.11614500	1.87788800	N	-0.02992300	0.30844600	1.91220900
P	2.31636900	-0.22543500	0.10009600	P	2.35851800	-0.26925600	0.19318700
P	-2.30600600	-0.25077500	0.09752800	P	-2.44113200	-0.07170000	0.17540800
C	-0.01002500	2.45788600	-1.55149000	C	0.28207100	2.56056000	-1.61678400
C	2.43989200	0.19806300	1.90385400	C	2.43001800	0.24660600	1.97920700
C	-2.43853300	0.15644600	1.90476800	C	-2.48857100	0.46303600	1.95549700
H	2.48468000	1.28986500	1.95891500	H	2.55653500	1.33359400	1.97674200
H	-2.50383500	1.24665700	1.96932600	H	-2.51800700	1.55715900	1.94503300
H	3.35359100	-0.17982600	2.36729800	H	3.30005400	-0.16472100	2.49510800
H	-3.34595700	-0.24077600	2.36407300	H	-3.39532700	0.12698600	2.46294800
C	1.18367000	-0.30983800	2.59490300	C	1.12800800	-0.13150300	2.67136700
C	-1.17404500	-0.33405700	2.59336100	C	-1.23020800	-0.02364300	2.66094100
H	1.17429800	0.07393700	3.63369500	H	1.12810300	0.32517200	3.67846200
H	-1.17099000	0.04471800	3.63400400	H	-1.19883600	0.43466200	3.66670200
H	1.25218900	-1.41268700	2.70058300	H	1.12100100	-1.22553600	2.85019300
H	-1.22384100	-1.43844700	2.69355800	H	-1.32013300	-1.11363900	2.84168800
C	-3.30373500	1.13116700	-0.70244800	C	-3.34606000	1.33895800	-0.67805600
C	3.30716300	1.15709600	-0.70845900	C	3.40273200	1.04825700	-0.64783900
H	-2.65130300	1.99863800	-0.56226900	H	-2.68658600	2.18491200	-0.45843800
H	2.65223600	2.02324500	-0.57361200	H	2.76656800	1.93510400	-0.56088900
C	-3.40631500	-1.76030500	-0.18107000	C	-3.60254900	-1.54045700	0.01845800
C	3.42935200	-1.72821900	-0.16288400	C	3.39874800	-1.82809600	0.02817500
H	-4.41462300	-1.35090000	-0.30140400	H	-4.60646100	-1.10568900	-0.01628100
H	4.43508700	-1.31237300	-0.28204700	H	4.43108700	-1.47025800	-0.04294800
C	0.00747400	-0.64052500	-1.90015800	C	-0.06159200	-0.77318900	-2.03785100

O	0.00871600	-0.91039600	-3.04227000	O	-0.07512700	-1.10774400	-3.17082000
C	3.06989200	-2.47232900	-1.44934700	C	3.06431700	-2.58688000	-1.25572000
C	-3.03571700	-2.49219600	-1.47121500	C	-3.35953000	-2.30154100	-1.28428300
H	3.03023600	-1.81663800	-2.32051400	H	3.13331800	-1.96227100	-2.14741800
H	-2.99937300	-1.83012000	-2.33766000	H	-3.38286900	-1.65511000	-2.16279300
H	2.10238400	-2.97126300	-1.36262100	H	2.05539400	-3.00210300	-1.21818400
H	-2.06394700	-2.98289900	-1.38461900	H	-2.39331800	-2.81059900	-1.27033100
H	3.82211200	-3.24276200	-1.65034100	H	3.76446000	-3.41980400	-1.37979100
H	-3.78024200	-3.26800200	-1.67998800	H	-4.13523400	-3.06378000	-1.41347000
C	3.46910000	-2.69660000	1.01702600	C	3.30670400	-2.75593800	1.23714100
C	-3.44354300	-2.73728800	0.99185100	C	-3.54539800	-2.49056600	1.21228400
H	2.49014600	-3.13294700	1.22336800	H	2.28626000	-3.10364600	1.40797200
H	-2.46181000	-3.16623000	1.20049300	H	-2.55267100	-2.92657000	1.33974900
H	3.83396400	-2.22802800	1.93247400	H	3.66682000	-2.28683800	2.15422500
H	-3.81769000	-2.27871200	1.90862500	H	-3.82955400	-2.00571500	2.14780000
H	4.15069100	-3.52150500	0.78196500	H	3.92851700	-3.63966000	1.05890400
H	-4.11637500	-3.56658400	0.74724900	H	-4.24668400	-3.31555200	1.04746100
C	-3.50702500	0.91859400	-2.20035600	C	-3.41692900	1.17546600	-2.19351500
C	3.51087200	0.93712000	-2.20520400	C	3.62493300	0.76267700	-2.13067600
H	-4.22058600	0.11302600	-2.39447500	H	-4.14475500	0.41205500	-2.48048200
H	4.22814600	0.13397300	-2.39556800	H	4.34462500	-0.04751700	-2.27567600
H	-2.57706100	0.68088900	-2.72047200	H	-2.45152000	0.90355300	-2.62603000
H	2.58159700	0.69199700	-2.72319400	H	2.70134800	0.49337800	-2.64773600
H	-3.91609400	1.82873800	-2.65121200	H	-3.73724900	2.11617200	-2.65314100
H	3.91523300	1.84670100	-2.66140900	H	4.03459100	1.65170700	-2.62087600
C	-4.63870300	1.42198700	-0.02050000	C	-4.72159700	1.64201600	-0.09122000
C	4.64029300	1.45773800	-0.02722900	C	4.73076600	1.33868900	0.04694400
H	-4.52861500	1.65842000	1.03949000	H	-4.69164000	1.79487400	0.98974700
H	4.52789500	1.69814100	1.03163100	H	4.60706800	1.61826900	1.09481700
H	-5.33642600	0.58434300	-0.10952800	H	-5.43939800	0.84451600	-0.30127300
H	5.34263300	0.62356900	-0.11196900	H	5.41041900	0.48318000	0.00258400
H	-5.11225800	2.28617300	-0.49934400	H	-5.11859100	2.55876800	-0.54048700
H	5.10963800	2.32231800	-0.50950300	H	5.23075700	2.17322300	-0.45643300
H	0.89321800	2.31909200	-2.18199200	H	1.05022600	2.08239300	-2.24995600
O	-0.05662000	3.88485900	-1.20291300	O	0.82614300	3.83838600	-1.15057100
H	-0.05733900	4.38972000	-2.02653700	H	0.83737000	4.44952800	-1.89807300
C	0.01276300	-2.02715000	0.17037900	C	-0.10774500	-2.16125500	0.18009900
O	0.01722000	-3.17513300	0.41430700	O	-0.14749000	-3.32839400	0.37864500
Mn	0.00582300	-0.33700600	-0.17947000	Re	-0.04682900	-0.33564600	-0.19399800
K	-0.05009500	2.95927300	1.85023700	K	0.19109300	3.17159000	1.66242400
O	0.00303800	1.76660200	-0.40699700	O	-0.04369000	1.84784800	-0.52602400
H	-0.89226800	2.26261900	-2.19550400	H	-0.58297700	2.80827200	-2.26490900
1Mn-HCH(OH)O⁻...K⁺-SMD(CH₃OH)				1Re-HCH(OH)O⁻...K⁺-SMD(CH₃OH)			
O	-0.20380500	-3.25818200	-0.36712400	N	0.04741200	0.19216900	-1.84440800
P	-2.37763300	-0.20650000	-0.08824100	P	-2.36932300	-0.35658100	-0.21126600
P	2.26639900	-0.41188500	-0.10959900	P	2.44130800	-0.17063600	-0.15363600
C	-2.50050700	0.20309300	-1.89216200	H	-0.01295500	2.18045600	0.86178400
C	2.39986800	0.05546400	-1.89858800	C	-0.03551200	3.27125600	1.14723600
H	-2.56610000	1.29445700	-1.95422600	C	-2.43035200	0.28123400	-1.95489300
H	2.50423800	1.14474000	-1.91630700	C	2.51872500	0.38384600	-1.92701100
H	-3.40063100	-0.19689100	-2.36136000	H	-2.56530600	1.36447600	-1.87103800
H	3.28725000	-0.35078400	-2.38759400	H	2.61349100	1.47409000	-1.90287600
C	-1.24039600	-0.29761100	-2.57334400	H	-3.29575400	-0.10099300	-2.50050400
C	1.11563500	-0.36402200	-2.58873200	H	3.40812800	0.00595000	-2.43484600
H	-1.19408300	0.12474600	-3.59400700	C	-1.13242000	-0.05530700	-2.67427300
H	1.09341600	0.07726800	-3.60311500	C	1.24796200	-0.03576500	-2.65070200
H	-1.31703600	-1.38907500	-2.71831500	H	-1.08218100	0.53705200	-3.60548600
H	1.12314600	-1.45548000	-2.75178900	H	1.18499000	0.52061400	-3.60244000
N	-0.04601600	0.06177000	-1.81432100	H	-1.16225800	-1.10481900	-3.00955200

C	3.31072500	0.90047900	0.74029500	H	1.32637500	-1.09574400	-2.94344000
C	-3.27515300	1.24300500	0.70387600	C	3.31731000	1.25172600	0.71248000
H	2.68527700	1.79668400	0.66051700	C	-3.39938200	0.92601600	0.69729800
H	-2.63644500	2.08830300	0.43274900	H	2.71773000	2.10280400	0.36806700
C	3.27958000	-1.98493600	0.12975800	H	-2.84220300	1.84164900	0.46250200
C	-3.52725400	-1.66333200	0.25066800	C	3.59001900	-1.64471900	-0.01943400
C	3.28671100	-2.92777700	-1.07089400	C	-3.37874300	-1.93748000	-0.22306000
C	-3.65554300	-2.64149600	-0.91413600	H	4.59576400	-1.22043100	-0.09721000
O	-0.02906900	-0.87467300	3.02671800	H	-4.41230300	-1.60598100	-0.36600400
H	-4.50535300	-1.19935900	0.39510600	C	0.03299200	-0.55519500	2.07874300
H	4.29989300	-1.61625000	0.26247100	O	0.03282200	-0.69026900	3.24639700
C	-3.16214700	-2.39248600	1.54154700	C	-3.28371000	-2.68680700	1.10346200
C	2.88227600	-2.73467200	1.40036100	C	3.45807800	-2.34172300	1.33288300
H	-3.08478400	-1.71930700	2.39655000	H	-3.63699100	-2.09232300	1.94651700
H	2.87790000	-2.09551300	2.28400200	H	3.62626400	-1.66602400	2.17252900
H	-2.21638800	-2.92874800	1.44688700	H	-2.25895900	-2.99759500	1.31755700
H	1.89301500	-3.18870900	1.30769600	H	2.47091800	-2.79201600	1.45673400
H	-3.93845200	-3.13003900	1.77181800	H	-3.90138800	-3.58957700	1.05603200
H	3.59907000	-3.54268200	1.58094500	H	4.19950300	-3.14442100	1.40177800
C	3.53134800	0.60535100	2.22130700	C	-3.00917500	-2.84560300	-1.39351700
C	-3.32132600	1.15041200	2.22612700	C	3.40757500	-2.63593000	-1.16661600
H	4.24311200	-0.21164400	2.36318400	H	-1.97586800	-3.19253100	-1.33200300
H	-4.01964900	0.37790300	2.55741900	H	2.40346900	-3.06317800	-1.18248700
H	2.60589900	0.34644200	2.74052700	H	-3.15201200	-2.35834000	-2.35937300
H	-2.34100700	0.93319600	2.65835600	H	3.60547600	-2.18738100	-2.14176700
H	3.94980800	1.48994000	2.71197900	H	-3.65370300	-3.73061600	-1.37645700
H	-3.66568500	2.10175200	2.64456300	H	4.11399700	-3.46260500	-1.03922700
C	4.63868000	1.17697200	0.03881900	C	3.22667000	1.20393900	2.23338900
C	-4.66294800	1.50366400	0.12355300	C	-3.40604200	0.75843200	2.21367300
H	4.50903700	1.49555000	-0.99663200	H	3.85433800	0.41405400	2.65233100
H	-4.64742300	1.61081600	-0.96300700	H	-4.02080300	-0.08931300	2.52417200
H	5.29701800	0.30362600	0.04778500	H	2.20436900	1.04625800	2.58087700
H	-5.37061600	0.71072000	0.37918000	H	-2.40338200	0.61924400	2.62184400
H	5.16408100	1.98137900	0.56296000	H	3.57807200	2.15295300	2.65085000
H	-5.06197500	2.43498100	0.53824800	H	-3.83458500	1.65248700	2.67761500
H	0.23238000	2.00540300	0.72252400	C	4.75526400	1.46422000	0.24760600
C	0.06038200	3.07657800	1.06524300	C	-4.81657300	1.07774200	0.15184100
H	3.92648600	-3.78695800	-0.84190200	H	4.84536200	1.49746900	-0.84059400
H	2.29211400	-3.31373200	-1.29881000	H	-4.83758300	1.21188600	-0.93196100
H	3.68842100	-2.45792800	-1.96980700	H	5.42002600	0.68085400	0.62055700
H	-4.36832000	-3.42702700	-0.64054700	H	-5.43842800	0.21416600	0.40123000
H	-4.03483300	-2.16406800	-1.81908800	H	5.12815100	2.41718800	0.63708800
H	-2.70938400	-3.12947600	-1.15304200	H	-5.28866500	1.95768700	0.60082500
O	0.57075600	3.96123700	0.21123400	H	0.97968000	3.52626700	1.51319400
C	-0.14394300	-2.11091000	-0.14955500	O	-0.49784800	4.06007500	0.17929700
Mn	-0.05739500	-0.41680100	0.12945300	O	-0.81707500	3.33356500	2.39024600
C	-0.04456700	-0.64511800	1.88004500	H	-1.73452300	3.17176600	2.13577700
H	-1.02559800	3.21991400	1.29327600	C	0.11285000	-2.25250400	0.15847900
O	0.73585800	3.17156200	2.36629900	O	0.16081400	-3.43253900	0.13100800
H	0.26690800	2.60543700	2.99039700	Re	0.04129700	-0.41294400	0.17552900
K	0.18801800	2.92149100	-2.13948500	K	-0.05042600	3.07933900	-2.20442100
Mn-TS(HCH(OH)O⁻...K⁺)-SMD(CH₃OH)				Re-TS(HCH(OH)O⁻...K⁺)-SMD(CH₃OH)			
O	0.13540600	-3.26215400	0.20183100	O	0.01276600	-3.39018900	0.05144900
P	2.32553800	-0.19684600	0.10463200	P	2.40572900	-0.19871600	0.16798400
P	-2.24123400	-0.31504400	0.14365400	P	-2.39058200	-0.20800200	0.21936900
C	2.50371200	0.04411600	1.93780600	C	2.48827300	0.22412700	1.97658000
C	-2.37825000	0.03715700	1.96127600	C	-2.43156800	0.22937400	2.02572100
H	2.59031000	1.12302600	2.10393000	H	2.57128100	1.31431600	2.03307100
H	-2.45528700	1.12410700	2.06468500	H	-2.50706400	1.32045200	2.07450500

H	3.41169400	-0.40823100	2.34045600	H	3.38241200	-0.18094800	2.45431500
H	-3.28158600	-0.38231900	2.40822100	H	-3.31751400	-0.16599200	2.52654000
C	1.24396800	-0.49122400	2.59846900	C	1.21561900	-0.25072400	2.66091300
C	-1.10988000	-0.47224300	2.62524600	C	-1.14671200	-0.24675000	2.68553300
H	1.24840200	-0.19200100	3.66429200	H	1.20805500	0.14207500	3.69428700
H	-1.10413900	-0.14180600	3.68226100	H	-1.11745600	0.14818700	3.71773300
H	1.28688500	-1.60037800	2.61038600	H	1.25602000	-1.35265100	2.76806900
H	-1.15042200	-1.57990500	2.67161400	H	-1.18746900	-1.34832500	2.79575900
N	0.06339200	0.00947700	1.92571300	N	0.02745100	0.18012000	1.94247500
C	-3.28953200	1.05088000	-0.61779300	C	-3.40009200	1.17948900	-0.54667100
C	3.25884500	1.29812700	-0.56185000	C	3.39684300	1.20094300	-0.60199500
H	-2.65455800	1.93461700	-0.50182100	H	-2.74697800	2.04435800	-0.38953600
H	2.63854600	2.13105000	-0.21245100	H	2.76691800	2.06925400	-0.37965000
C	-3.31088900	-1.84317000	-0.16472500	C	-3.48717300	-1.72322100	0.01593500
C	3.47493500	-1.62040900	-0.36754600	C	3.50221800	-1.70874800	-0.07246200
C	-3.29887700	-2.85530100	0.97815800	C	-3.36426700	-2.71983900	1.16569400
C	3.57717400	-2.72146800	0.68551100	C	3.39857600	-2.71814500	1.06799200
O	0.02515900	-0.65576400	-3.05051200	O	-0.03956200	-0.70337200	-3.25159200
H	4.46404000	-1.16177300	-0.46102700	H	4.52348300	-1.31510200	-0.07896900
H	-4.33097800	-1.45487500	-0.25162500	H	-4.50944500	-1.33153000	0.02037800
C	3.09905800	-2.21173700	-1.72536700	C	3.23910600	-2.38510700	-1.41755700
C	-2.94887000	-2.52459000	-1.48412000	C	-3.24316500	-2.41530500	-1.32442200
H	3.03779600	-1.45742700	-2.51120300	H	3.29691700	-1.69223300	-2.25800900
H	-2.96241900	-1.83870200	-2.33196800	H	-3.32270500	-1.73391800	-2.17228000
H	2.13825700	-2.72883300	-1.68415500	H	2.25386000	-2.85492700	-1.43995700
H	-1.95688700	-2.97790500	-1.43887300	H	-2.25402200	-2.87565700	-1.35964300
H	3.85598400	-2.94308000	-2.02887700	H	3.98499900	-3.16952500	-1.58353600
H	-3.66874300	-3.32299100	-1.69428500	H	-3.98471600	-3.20856800	-1.46612500
C	-3.54181000	0.83909700	-2.10872500	C	-3.60089400	1.00530700	-2.04921900
C	3.30373400	1.34068900	-2.08668100	C	3.52603200	1.07765900	-2.11753800
H	-4.26463800	0.03637200	-2.27784000	H	-4.35253700	0.24093600	-2.26206300
H	3.99320000	0.59102800	-2.48354900	H	4.25195800	0.30805900	-2.39169900
H	-2.63189600	0.59844800	-2.66015300	H	-2.67905400	0.72596900	-2.56316400
H	2.32500300	1.16933700	-2.54010000	H	2.57697300	0.83317500	-2.59917900
H	-3.96216500	1.75128300	-2.54409500	H	-3.95795400	1.94296100	-2.48640400
H	3.66245800	2.31922700	-2.42236000	H	3.88230100	2.02364700	-2.53767500
C	-4.60787000	1.31235200	0.10806600	C	-4.73238800	1.45460600	0.14641200
C	4.65597200	1.49528800	0.02296600	C	4.76261600	1.43775400	0.03849200
H	-4.46698800	1.57797700	1.15742300	H	-4.62157100	1.64599700	1.21557100
H	4.65812700	1.51252400	1.11473400	H	4.70499100	1.56863400	1.12087900
H	-5.27942600	0.45006100	0.06395900	H	-5.43782600	0.62893700	0.02017000
H	5.35051300	0.71763500	-0.30537300	H	5.45803000	0.62032300	-0.16915000
H	-5.12671400	2.14900500	-0.37237600	H	-5.19485700	2.34284000	-0.29718100
H	5.06168400	2.45325300	-0.31991800	H	5.20495200	2.34928800	-0.37731200
H	-0.04897600	1.34709000	-0.46296900	H	0.03212400	1.53269300	-0.55578700
C	-0.03728800	2.89095500	-1.15970500	C	0.24777200	2.92271900	-1.30313300
H	-3.95103700	-3.69686100	0.71978200	H	-4.01482100	-3.57821700	0.96705000
H	-2.30152800	-3.26050900	1.15780000	H	-2.34635000	-3.09925100	1.27173200
H	-3.67025000	-2.43543800	1.91455900	H	-3.67218800	-2.29503100	2.12264800
H	4.27437800	-3.48951700	0.33346000	H	4.04755600	-3.57322600	0.85063500
H	3.95659200	-2.35472700	1.64092000	H	3.72052700	-2.30277500	2.02449900
H	2.61803700	-3.21053300	0.86359500	H	2.38313700	-3.10057400	1.18585500
O	-0.48236600	3.68171300	-0.30985200	O	0.42705200	3.79949500	-0.43368000
C	0.09947300	-2.09604400	0.08373900	C	0.00743500	-2.21207000	0.00129000
Mn	0.04371600	-0.37491000	-0.15025300	Re	0.00492300	-0.34061500	-0.19831000
C	0.03308300	-0.53167600	-1.88240600	C	-0.02136400	-0.55610600	-2.08081400
H	1.03501200	2.77924300	-1.33888500	H	1.08134800	2.50662200	-1.87719300
O	-0.78677200	2.69914300	-2.28762100	O	-0.90415200	3.02335000	-2.05053100
H	-0.30655700	2.12446900	-2.90039900	H	-0.90053400	2.33777400	-2.73374100
K	-0.01707900	2.75708000	2.12103000	K	0.03360800	2.96357800	2.02265900

1Mn-OOCH ⁻ ...K ⁺ -SMD(CH ₃ OH)				1Re-OOCH ⁻ ...K ⁺ -SMD(CH ₃ OH)			
O	-0.00028200	-3.15991500	-0.53472000	O	-0.00012700	-3.32601300	0.40226100
P	-2.30194400	-0.21267800	-0.10264500	P	2.39938700	-0.14394000	0.18617000
P	2.30174000	-0.21319900	-0.10285300	P	-2.39949400	-0.14366400	0.18622600
C	-2.44503300	0.23832900	-1.89893100	C	2.46590600	0.36880900	1.97344000
C	2.44467500	0.23782400	-1.89914400	C	-2.46595200	0.36924600	1.97344400
H	-2.52402700	1.32936000	-1.93722300	H	2.56047900	1.45934000	1.97926100
H	2.52378800	1.32885100	-1.93738200	H	-2.56046500	1.45978500	1.97913500
H	-3.34974300	-0.15699500	-2.36464200	H	3.35117400	-0.02083200	2.47987500
H	3.34927400	-0.15758800	-2.36499900	H	-3.35124900	-0.02028900	2.47991700
C	-1.18058100	-0.23042900	-2.60292800	C	1.18212500	-0.06079500	2.67027700
C	1.18007200	-0.23069800	-2.60302300	C	-1.18222700	-0.06041200	2.67034300
H	-1.17144700	0.18735100	-3.62760100	H	1.16393500	0.39776500	3.67561900
H	1.17094900	0.18707100	-3.62770100	H	-1.16395200	0.39835100	3.67559200
H	-1.23422800	-1.32901400	-2.74310500	H	1.22033600	-1.15298300	2.84887200
H	1.23346500	-1.32929600	-2.74318600	H	-1.22062600	-1.15255800	2.84916500
N	-0.00017600	0.18339900	-1.86837900	N	-0.00000800	0.32520800	1.91312100
C	3.23033200	1.19583100	0.73094200	C	-3.31588200	1.26372200	-0.65843000
C	-3.23029600	1.19646800	0.73124000	C	3.31582400	1.26345200	-0.65839500
H	2.59736100	2.05637300	0.49132500	H	-2.67303200	2.11863100	-0.42163700
H	-2.59716500	2.05692800	0.49174100	H	2.67287600	2.11834300	-0.42181200
C	3.42771600	-1.70164300	0.16291600	C	-3.52630600	-1.63426400	0.00271300
C	-3.42815300	-1.70095100	0.16325000	C	3.52618300	-1.63454900	0.00248100
C	3.47420500	-2.66585600	-1.02033900	C	-3.44987500	-2.59697000	1.18530200
C	-3.47494100	-2.66515200	-1.02000600	C	3.44990100	-2.59730700	1.18504000
O	-0.00001600	-1.07585200	2.98816200	O	-0.00028800	-1.15247900	-3.14553800
H	-4.42942000	-1.27605900	0.28368000	H	4.53934000	-1.22193200	-0.03172100
H	4.42906700	-1.27691200	0.28322600	H	-4.53947400	-1.22166000	-0.03141600
C	-3.07127300	-2.44984900	1.44696700	C	3.25740000	-2.37192700	-1.30841300
C	3.07084800	-2.45046200	1.44668500	C	-3.25758500	-2.37170700	-1.30815500
H	-3.02840900	-1.79648700	2.31982300	H	3.30315200	-1.71686700	-2.17965700
H	3.02814300	-1.79706900	2.31952600	H	-3.30341400	-1.71669100	-2.17942600
H	-2.10624400	-2.95342800	1.35736600	H	2.27390300	-2.84699500	-1.29952200
H	2.10574500	-2.95392200	1.35718200	H	-2.27407300	-2.84675200	-1.29931000
H	-3.82733400	-3.21686200	1.64563300	H	4.00653600	-3.15867700	-1.44550300
H	3.82682300	-3.21756900	1.64531200	H	-4.00670800	-3.15848600	-1.44515400
C	3.28312200	1.05766700	2.24939300	C	-3.36733700	1.12192100	-2.17654500
C	-3.28316300	1.05814800	2.24967700	C	3.36755300	1.12150400	-2.17649100
H	3.96358400	0.25841500	2.55468200	H	-4.08004500	0.35185400	-2.48218500
H	-3.96382800	0.25902500	2.55485000	H	4.08030800	0.35139800	-2.48192500
H	2.30265900	0.85131900	2.68312000	H	-2.39392000	0.87076500	-2.60346100
H	-2.30276200	0.85152200	2.68341100	H	2.39421100	0.87030700	-2.60355100
H	3.65449300	1.98707600	2.69326500	H	-3.69646500	2.06495800	-2.62455900
H	-3.65433100	1.98759400	2.69364300	H	3.69676100	2.06449500	-2.62454000
C	4.62086000	1.45740700	0.15851100	C	-4.70214900	1.53711500	-0.08223500
C	-4.62075000	1.45835600	0.15878400	C	4.70196000	1.53702200	-0.08197400
H	4.61079100	1.59211300	-0.92504700	H	-4.68670200	1.67296900	1.00127200
H	-4.61060900	1.59321300	-0.92475400	H	4.68629600	1.67296200	1.00152000
H	5.31861800	0.64925200	0.39360400	H	-5.40421200	0.73174100	-0.31354200
H	-5.31865600	0.65028900	0.39373400	H	5.40414200	0.73169600	-0.31308500
H	5.03057700	2.37331200	0.59801200	H	-5.10741400	2.45468200	-0.52180000
H	-5.03033300	2.37426800	0.59839600	H	5.10721400	2.45459300	-0.52154100
H	4.16133900	-3.48616800	-0.78624500	H	-4.12260400	-3.44145900	1.00233700
H	2.49863300	-3.10880700	-1.22861200	H	-2.44511400	-3.00271200	1.31778000
H	3.83713300	-2.19253700	-1.93400700	H	-3.75943200	-2.13431500	2.12386000
H	-4.16216000	-3.48536800	-0.78582200	H	4.12255500	-3.44182400	1.00192300
H	-3.83792600	-2.19178100	-1.93362400	H	3.75965300	-2.13471300	2.12356400
H	-2.49946200	-3.10824300	-1.22841500	H	2.44514700	-3.00300300	1.31767500
O	0.00293300	3.70900000	1.56865200	O	0.00066400	3.77516000	-1.69075500

C -0.0007800 -0.73200500 1.86808600	C -0.00020600 -0.79704300 -2.02089100
C 0.00107800 2.46166400 1.53298200	C 0.00026900 2.53548000 -1.62324300
C -0.00029800 -2.02433500 -0.25027500	C -0.00013600 -2.16298300 0.19858600
Mn -0.00014300 -0.34647100 0.15743600	Re -0.00007900 -0.34046300 -0.17875000
K 0.00004600 3.01643900 -1.83356400	K 0.00052600 3.17951400 1.74461100
O 0.00017300 1.76908900 0.47669800	O -0.00005500 1.87533600 -0.53730400
H 0.00013100 1.91411000 2.49470400	H 0.00011200 1.95179700 -2.56159700
1Mn-HCOO⁻...K⁺-SMD(CH₃OH)	1Re-HCOO⁻...K⁺-SMD(CH₃OH)
O -0.00713500 -3.40879400 0.04134200	O -0.04281500 -3.40308700 -0.20575700
P 2.29655600 -0.33238000 0.11124400	P 2.40071400 -0.28081900 0.18414100
P -2.29942700 -0.32693300 0.10799600	P -2.41442800 -0.22684000 0.17596900
C 2.45304300 0.17007200 1.89164300	C 2.47340600 0.37246100 1.92195700
C -2.45865000 0.17318600 1.88872100	C -2.47146900 0.47282300 1.89659400
H 2.56793800 1.25858000 1.89271000	H 2.60750700 1.45513100 1.83039400
H -2.57374600 1.26166400 1.89173200	H -2.55697800 1.55746500 1.77366900
H 3.34664800 -0.23686800 2.36753000	H 3.34304800 -0.00582200 2.46342500
H -3.35299800 -0.23419900 2.36277400	H -3.36010300 0.14677800 2.44119100
C 1.18423300 -0.24513200 2.61559500	C 1.18152800 0.04123200 2.65369000
C -1.19125800 -0.24349200 2.61429600	C -1.19962000 0.10773600 2.64729900
H 1.11611000 0.30525600 3.57087300	H 1.12528300 0.65843500 3.56799500
H -1.12339100 0.30714500 3.56926100	H -1.12636200 0.74287400 3.54845800
H 1.25268100 -1.30647300 2.90575200	H 1.22153900 -0.99743400 3.01873500
H -1.26101500 -1.30475800 2.90435800	H -1.28389400 -0.91901400 3.03760300
N -0.00269400 -0.00462500 1.79424900	N -0.00190600 0.25223700 1.81919500
C -3.15681500 1.12069900 -0.74361800	C -3.39704200 1.06079700 -0.78122900
C 3.16158400 1.10986900 -0.74134000	C 3.39814500 1.01857300 -0.73988000
H -2.53895200 1.96114900 -0.40729200	H -2.88297000 1.98062000 -0.47675300
H 2.54042800 1.95249800 -0.41639700	H 2.87592900 1.93302000 -0.43245500
C -3.44998800 -1.79050400 -0.13104400	C -3.48359200 -1.76497500 0.25210200
C 3.44244900 -1.80021800 -0.12276500	C 3.44180900 -1.83966800 0.21089100
C -3.36939100 -2.80169400 1.01027100	C -3.11451500 -2.65778300 1.43445800
C 3.35733700 -2.80903200 1.02041100	C 3.06783500 -2.75575000 1.37392000
O -0.00171200 -0.77696300 -3.00738000	O 0.00598300 -0.66522500 -3.25718400
H 4.45027700 -1.37375700 -0.11926600	H 4.46395300 -1.48519900 0.37855700
H -4.45634100 -1.36049600 -0.12791300	H -4.49704100 -1.38779800 0.42230600
C 3.20874900 -2.48447900 -1.46914100	C 3.39532400 -2.58409200 -1.12030600
C -3.21666800 -2.47259300 -1.47844500	C -3.46716900 -2.54163800 -1.06092500
H 3.26321600 -1.79241900 -2.31067000	H 3.76674600 -1.97895800 -1.94841100
H -3.26769600 -1.77858400 -2.31856400	H -3.83823700 -1.94889600 -1.89815900
H 2.23423800 -2.97600900 -1.50336500	H 2.38157700 -2.90670300 -1.36734200
H -2.24381600 -2.96747100 -1.51255700	H -2.46243300 -2.88783100 -1.31222500
H 3.97189200 -3.25394600 -1.62461500	H 4.02308800 -3.47899300 -1.05891200
H -3.98221600 -3.23910400 -1.63677400	H -4.11013800 -3.42315500 -0.97074400
C -3.10488600 1.08759500 -2.26687600	C -3.26607900 0.94259300 -2.29548700
C 3.12378200 1.06508900 -2.26481600	C 3.29686200 0.91919100 -2.25760900
H -3.76016300 0.31523100 -2.67597900	H -3.76791700 0.05326600 -2.68292600
H 3.78737800 0.29318300 -2.66143900	H 3.82154400 0.04335900 -2.64561700
H -2.09753700 0.92007200 -2.64858100	H -2.22321500 0.91152400 -2.61362200
H 2.12106800 0.88873500 -2.65448000	H 2.26114100 0.87474500 -2.59722400
H -3.45118400 2.04796300 -2.66187700	H -3.73185700 1.81215100 -2.77011600
H 3.46831100 2.02415100 -2.66425600	H 3.75747100 1.80226300 -2.71170100
C -4.58364300 1.35669300 -0.25347600	C -4.85709200 1.16549900 -0.35102800
C 4.58379000 1.34942400 -0.24022000	C 4.84989000 1.12032200 -0.28110700
H -4.65641200 1.39395800 0.83554100	H -4.97078500 1.25061200 0.73230300
H 4.64586900 1.40073000 0.84885200	H 4.94290300 1.19456200 0.80490700
H -5.26750300 0.58392600 -0.61398700	H -5.43874800 0.30381300 -0.68820400
H 5.26971400 0.57085500 -0.58392500	H 5.43863600 0.26228100 -0.61538400
H -4.94664500 2.31499600 -0.63912900	H -5.30753600 2.05645900 -0.80040200
H 4.95250300 2.30203000 -0.63454300	H 5.30801500 2.01613800 -0.71269000

H -0.00867500	2.03854900	-0.94493500	H -0.00182500	2.18690200	-0.94852600
H -4.06677100	-3.62208100	0.81109100	H -3.77755800	-3.52905900	1.44548900
H -2.37298500	-3.23702800	1.10372900	H -2.08944000	-3.02655700	1.36885200
H -3.64650500	-2.36892100	1.97303000	H -3.23445300	-2.14672700	2.39119000
H 4.05251400	-3.63190500	0.82332200	H 3.73262900	-3.62577200	1.37156200
H 3.63469600	-2.37540400	1.98269200	H 3.18089500	-2.26419500	2.34167200
H 2.35945000	-3.24108500	1.11359400	H 2.04405600	-3.12573300	1.29375200
O -0.00932400	3.92794400	-0.22978800	O 0.04256100	4.10440500	-0.31555900
C -0.00130600	-0.61745400	-1.85056300	C -0.00046400	-0.52334600	-2.09067200
C 0.00945400	3.12746000	-1.20118800	C 0.05240200	3.26441200	-1.25199000
O 0.04731400	3.41556600	-2.41589200	O 0.11726900	3.49217000	-2.47719000
C -0.00452400	-2.24192700	-0.03532400	C -0.02973200	-2.22252600	-0.20793300
Mn -0.00190700	-0.52597400	-0.08846000	Re -0.00863700	-0.38099300	-0.18839200
K -0.00040400	2.92883500	2.22146700	K 0.05398900	3.18515200	2.17588400
Mn-TS(HCO₂⁻...K⁺)-SMD(CH₃OH)			Re-TS(HCO₂⁻...K⁺)-SMD(CH₃OH)		
O 0.00002500	-3.29700800	0.04334900	O -0.00028600	-3.41728600	0.01456800
P 2.27022000	-0.24065100	0.13554500	P 2.38251200	-0.17057800	0.20126800
P -2.27017700	-0.24063600	0.13566000	P -2.38257000	-0.17043200	0.20117700
C 2.43816600	-0.09397300	1.98083000	C 2.45739200	0.13606800	2.03623700
C -2.43799900	-0.09373200	1.98092800	C -2.45734800	0.13709700	2.03599400
H 2.51765600	0.97396400	2.20865100	H 2.53704000	1.22031600	2.16789800
H -2.51734400	0.97424200	2.20862800	H -2.53651300	1.22145000	2.16709200
H 3.34856200	-0.55949600	2.36283800	H 3.35154600	-0.29581300	2.48970300
H -3.34842700	-0.55910300	2.36304700	H -3.35169300	-0.29418800	2.48965400
C 1.17878100	-0.67666600	2.60254700	C 1.18360100	-0.38818900	2.68481500
C -1.17864200	-0.67650700	2.60262500	C -1.18380700	-0.38749100	2.68481400
H 1.18412400	-0.45884700	3.68809200	H 1.17170900	-0.06251800	3.74143200
H -1.18391800	-0.45862200	3.68815800	H -1.17185600	-0.06161000	3.74136500
H 1.22295700	-1.78363300	2.52794200	H 1.23006700	-1.49516600	2.72086100
H -1.22293100	-1.78347300	2.52808500	H -1.23074600	-1.49444100	2.72106700
N 0.00008600	-0.12714700	1.96775900	N 0.00004100	0.08503300	1.98954200
C -3.19961000	1.28408400	-0.46812900	C -3.31001800	1.31708100	-0.48161400
C 3.19961000	1.28419400	-0.46802700	C 3.30981000	1.31728700	-0.48095000
H -2.53588400	2.09837600	-0.15747800	H -2.65370900	2.14117900	-0.17905500
H 2.53603700	2.09843300	-0.15690300	H 2.65292000	2.14115800	-0.17896300
C -3.42569600	-1.64210500	-0.38606600	C -3.53029200	-1.62200000	-0.14213000
C 3.42571700	-1.64204800	-0.38642200	C 3.53030000	-1.62188700	-0.14292700
C -3.50498800	-2.78945400	0.61844800	C -3.46731100	-2.70375500	0.93225000
C 3.50505900	-2.78952400	0.61794400	C 3.46758800	-2.70410200	0.93100300
O -0.00011200	-0.56584400	-3.05121100	O 0.00015800	-0.72044100	-3.23523000
H 4.41843100	-1.18415900	-0.44726400	H 4.53917400	-1.19754600	-0.13777300
H -4.41841700	-1.18422500	-0.44691000	H -4.53920600	-1.19775900	-0.13690600
C 3.06147800	-2.17634800	-1.77073100	C 3.26342600	-2.22307500	-1.52223200
C -3.06153000	-2.17657200	-1.77033000	C -3.26365200	-2.22365400	-1.52127300
H 3.01018900	-1.39195400	-2.52697900	H 3.26855800	-1.47725000	-2.31849900
H -3.01030200	-1.39226700	-2.52667300	H -3.26901100	-1.47807200	-2.31777600
H 2.09795500	-2.69050000	-1.75728500	H 2.29826100	-2.73407000	-1.54919400
H -2.09799800	-2.69070200	-1.75688600	H -2.29844900	-2.73457600	-1.54827400
H 3.81775700	-2.89916000	-2.09578900	H 4.03728800	-2.96199900	-1.75555000
H -3.81781700	-2.89943400	-2.09525500	H -4.03750600	-2.96270400	-1.75421800
C -3.32402500	1.33511800	-1.98866200	C -3.39525600	1.32436700	-2.00519600
C 3.32357100	1.33576800	-1.98857300	C 3.39614500	1.32430300	-2.00446600
H -4.05950300	0.61151900	-2.34991700	H -4.12652100	0.59711000	-2.36712700
H 4.05873600	0.61211100	-2.35034600	H 4.12782100	0.59709300	-2.36565300
H -2.37665600	1.13757900	-2.49251300	H -2.43514000	1.10543100	-2.47570500
H 2.37598000	1.13869100	-2.49218900	H 2.43643200	1.10508300	-2.47562900
H -3.66753900	2.32708900	-2.29975600	H -3.72093300	2.31029200	-2.35212100
H 3.66724700	2.32776600	-2.29940300	H 3.72191600	2.31020700	-2.35135800
C -4.56048900	1.50633400	0.18778900	C -4.68441800	1.54907900	0.14075400

C 4.56067900	1.50611500	0.18760500	C 4.68374600	1.55001700	0.14219200
H -4.50123200	1.55721600	1.27691900	H -4.65435900	1.58508200	1.23179900
H 4.50173100	1.55640100	1.27677900	H 4.65317200	1.58593700	1.23322300
H -5.27444200	0.72116600	-0.07633900	H -5.39931800	0.77630500	-0.15397000
H 5.27456900	0.72110200	-0.07715200	H 5.39924800	0.77768800	-0.15225200
H -4.98289300	2.45490100	-0.16114500	H -5.08538500	2.50703200	-0.20714900
H 4.98297300	2.45487600	-0.16093400	H 5.08432100	2.50822800	-0.20545300
H 0.00001400	1.30156000	-0.34220600	H -0.00017200	1.46678300	-0.44572500
H -4.19887500	-3.54900300	0.24220700	H -4.14171400	-3.52233900	0.65881900
H -2.53783800	-3.27533100	0.76136800	H -2.46455200	-3.12515000	1.02580800
H -3.87383900	-2.47032900	1.59475000	H -3.77949000	-2.34093200	1.91302300
H 4.19895600	-3.54900800	0.24158800	H 4.14171200	-3.52269500	0.65691600
H 3.87392500	-2.47051700	1.59427700	H 3.78022500	-2.34179100	1.91181700
H 2.53792400	-3.27544300	0.76082200	H 2.46478100	-3.12534800	1.02474800
O -0.00022100	3.72872900	-0.32633200	O -0.00485000	3.81905600	-0.45811100
C -0.00006100	-0.47718800	-1.88032500	C 0.00006100	-0.56170900	-2.06551100
C -0.00030400	3.01812700	-1.26724400	C -0.00068800	3.07070100	-1.37159300
O -0.00043400	2.69088500	-2.38920900	O 0.00337800	2.72545100	-2.49014700
C 0.00002400	-2.12396600	0.00117600	C -0.00018800	-2.23827000	-0.00901300
Mn 0.00001300	-0.39025800	-0.14360300	Re -0.00003400	-0.35492100	-0.18339900
K 0.00031800	2.59999900	2.14988400	K 0.00113000	2.84437700	2.08573700
2Mn⁺...K⁺...H₂O-SMD(CH₃OH)			2Re⁺...K⁺...H₂O-SMD(CH₃OH)		
O -0.02888400	-3.20358000	-0.54544100	O 0.01347600	-3.20279700	-0.99870200
P -2.25488600	-0.09966500	-0.07873500	P -2.37182400	-0.03591400	-0.11386800
P 2.24197800	-0.13183000	-0.08692700	P 2.37468000	-0.02508400	-0.10716200
C -2.44067000	0.37477200	-1.86982900	C -2.45256200	0.78648700	-1.78395300
C 2.42844500	0.33641300	-1.87945100	C 2.45659200	0.80028400	-1.77544500
H -2.51819600	1.46634900	-1.91117600	H -2.53787500	1.86207600	-1.59881200
H 2.52286100	1.42660300	-1.92305300	H 2.53705900	1.87913600	-1.58807800
H -3.35575000	-0.01863700	-2.31663300	H -3.34820200	0.50039300	-2.34125800
H 3.33533500	-0.07199200	-2.32940500	H 3.35654400	0.51827900	-2.32912200
C -1.19001800	-0.09620300	-2.59602400	C -1.17985600	0.47433300	-2.55777800
C 1.16766900	-0.11537500	-2.60051600	C 1.18637000	0.48019200	-2.55228800
H -1.19923500	0.31591700	-3.62419300	H -1.17266500	1.08711300	-3.48128700
H 1.17952800	0.29631200	-3.62880100	H 1.18177500	1.09349600	-3.47533200
H -1.24770200	-1.19834800	-2.72467300	H -1.22568300	-0.57783500	-2.90717300
H 1.20730500	-1.21831400	-2.72909200	H 1.24134800	-0.57151000	-2.90204000
N -0.00632100	0.31775700	-1.87879300	N 0.00198700	0.73521300	-1.75989800
C 3.12258900	1.30868800	0.75919400	C 3.24957200	1.23280800	0.98898800
C -3.11133600	1.35082500	0.77495100	C -3.25384200	1.21827300	0.97783400
H 2.51040600	2.15568400	0.42827000	H 2.60245000	2.10710400	0.86436600
H -2.48550900	2.19008300	0.45002000	H -2.61030300	2.09488300	0.84909100
C 3.43439900	-1.57311500	0.17269000	C 3.56175600	-1.48314500	-0.18609300
C -3.46489200	-1.52577100	0.18405000	C -3.55220800	-1.49918700	-0.19614900
C 3.45744600	-2.56559400	-0.98727300	C 3.51114000	-2.22670100	-1.51772200
C -3.50634700	-2.51574600	-0.97772600	C -3.48575100	-2.25196300	-1.52188500
O -0.01072000	-1.03816600	2.99047700	O 0.00232100	-1.66674800	2.96514000
H -4.45237100	-1.06047500	0.26052700	H -4.55411600	-1.07038200	-0.09935900
H 4.42768600	-1.11937700	0.24220400	H 4.56073700	-1.04760700	-0.07757700
C -3.17678700	-2.26315400	1.49115000	C -3.31913100	-2.45907800	0.97017000
C 3.14555700	-2.30424000	1.48309100	C 3.32332100	-2.44870100	0.97162600
H -3.14440900	-1.59823200	2.35586900	H -3.35932900	-1.96601300	1.94260200
H 3.12475500	-1.63694800	2.34637900	H 3.35386900	-1.95898400	1.94744900
H -2.22249000	-2.79314100	1.44176200	H -2.34442700	-2.95019300	0.88291300
H 2.18573300	-2.82494700	1.44078100	H 2.35435900	-2.94303700	0.87679900
H -3.95930600	-3.00699400	1.67638700	H -4.08609400	-3.24057500	0.96210200
H 3.92140200	-3.05562200	1.66599400	H 4.09659800	-3.22677300	0.96723600
C 3.05114700	1.26508600	2.28168700	C 3.23941300	0.86133500	2.46751700
C -3.04275300	1.29680700	2.29708000	C -3.24236700	0.85030400	2.45823300

H	3.69256700	0.48127200	2.69212000	H	3.92692400	0.04035800	2.68115200
H	-3.69181200	0.51636200	2.70193500	H	-3.92777200	0.02855400	2.67546900
H	2.03457800	1.09579600	2.64198400	H	2.24122600	0.57218200	2.81017800
H	-2.02794500	1.11762300	2.65737800	H	-2.24359400	0.56460100	2.80210800
H	3.39842300	2.21673300	2.69808000	H	3.55975600	1.71794000	3.06733800
H	-3.38141700	2.24952200	2.71785200	H	-3.56833300	1.70836500	3.05470700
C	4.55317200	1.54892900	0.28515100	C	4.65357600	1.61097500	0.52723400
C	-4.53753500	1.61625100	0.30091500	C	-4.65946700	1.58468100	0.51416100
H	4.63589700	1.57533000	-0.80371800	H	4.69100800	1.88880300	-0.52884300
H	-4.61819500	1.65264500	-0.78782600	H	-4.69807000	1.86059000	-0.54337200
H	5.23880300	0.78342500	0.65808200	H	5.36909000	0.79936200	0.68762700
H	-5.23508700	0.85807200	0.66681400	H	-5.37049500	0.76974400	0.67778600
H	4.91165500	2.51198800	0.66473000	H	5.01132700	2.46956100	1.10519500
H	-4.88169300	2.58149100	0.68789100	H	-5.02238500	2.44371600	1.08831900
H	-0.00340400	1.21102800	0.58718200	H	-0.01154000	1.27627100	0.93146100
H	4.17495100	-3.36314800	-0.76472800	H	4.21614500	-3.06390300	-1.48949000
H	2.48549700	-3.03788300	-1.14130400	H	2.51937000	-2.63851300	-1.71026600
H	3.76717200	-2.10761900	-1.92812100	H	3.78969300	-1.59602200	-2.36267800
H	-4.23352700	-3.30393900	-0.75341100	H	-4.18883700	-3.09079600	-1.49484600
H	-3.81377400	-2.05184100	-1.91637800	H	-3.75990000	-1.62821400	-2.37445100
H	-2.54144100	-3.00082000	-1.13656100	H	-2.49084800	-2.66287000	-1.70348800
H	0.07876100	2.73503400	1.38295400	H	-0.03240300	2.80974100	1.59308900
O	0.08284900	3.70976900	1.29498300	O	0.00324800	3.78422400	1.52119500
C	-0.01972400	-2.05220500	-0.30915400	C	0.00929700	-2.09304800	-0.60042100
C	-0.00981200	-0.75996600	1.84704700	C	0.00128100	-1.14655700	1.90145200
H	0.77440500	4.01070200	1.89569200	H	-0.59474500	4.10916300	2.20490900
K	0.01813700	3.03959700	-1.40322200	K	-0.00352800	3.45594500	-1.17993300
Mn	-0.00841800	-0.36746000	0.15574100	Re	0.00151300	-0.35903800	0.18633400
2Mn⁻...K⁺...H₂O-TS(H⁺ transfer, H₂ formation)-SMD(CH₃OH)				2Re⁻...K⁺...H₂O-TS(H⁺ transfer, H₂ formation)-SMD(CH₃OH)			
O	0.00100100	-2.64357900	-1.73709800	O	0.10322300	-3.13101900	-1.01949300
P	-2.27549300	-0.11364800	-0.01112600	P	-2.37552000	-0.10267200	-0.14405000
P	2.27524000	-0.12357100	-0.00276400	P	2.42186700	0.01162700	-0.10051900
C	-2.43440600	1.06993600	-1.43244800	C	-2.46231100	0.85565000	-1.73669000
C	2.45183800	1.04165100	-1.43735200	C	2.47793800	1.01115800	-1.66845300
H	-2.50431500	2.06813400	-0.98930200	H	-2.62092000	1.90166500	-1.45690900
H	2.53985800	2.04381600	-1.00657400	H	2.55186700	2.05886000	-1.35969200
H	-3.34409400	0.91608200	-2.01580800	H	-3.31844100	0.56141700	-2.34692200
H	3.35889200	0.86678300	-2.01869200	H	3.36941800	0.79364200	-2.26029800
C	-1.17559500	0.94436400	-2.27873200	C	-1.15441000	0.69089700	-2.49609300
C	1.19058200	0.92470300	-2.28132000	C	1.20547900	0.77325000	-2.46629100
H	-1.16877700	1.76063100	-3.02839800	H	-1.14094400	1.41977900	-3.32671400
H	1.19147200	1.73541300	-3.03695700	H	1.16826900	1.50983900	-3.28939700
H	-1.23384100	0.01413200	-2.87920400	H	-1.14383500	-0.30221900	-2.98409600
H	1.23762000	-0.01026800	-2.87530000	H	1.27036700	-0.21287600	-2.96402800
N	0.00898200	0.99722200	-1.44240800	N	0.01009700	0.87676900	-1.63664900
C	3.08178800	0.84543500	1.39282000	C	3.27913100	1.17018000	1.10654800
C	-3.09581200	0.83792600	1.38855000	C	-3.30699400	1.03079900	1.02909600
H	2.45427400	1.74393700	1.41796600	H	2.63919700	2.05684000	1.03307400
H	-2.46873500	1.73573700	1.43157800	H	-2.72951800	1.95696600	0.92612800
C	3.45410100	-1.55531600	-0.32993900	C	3.59790000	-1.42933800	-0.33791700
C	-3.45360800	-1.54006300	-0.36365100	C	-3.46871200	-1.61239100	-0.35336100
C	3.52235000	-1.96941000	-1.79848600	C	3.46258100	-2.08509400	-1.70950400
C	-3.51476700	-1.93558100	-1.83752700	C	-3.31470700	-2.27998000	-1.71741800
O	-0.01003500	-2.31098200	2.32087500	O	-0.02003200	-1.73955900	2.90823300
H	-4.44224300	-1.16776800	-0.07819800	H	-4.49199400	-1.23225000	-0.27644700
H	4.44167900	-1.18100400	-0.04330300	H	4.59874900	-0.99174500	-0.26931200
C	-3.12927500	-2.75703500	0.50098100	C	-3.23922000	-2.62365600	0.76900700
C	3.12231600	-2.76169100	0.54661900	C	3.43753500	-2.46231900	0.77571300

H	-3.07722900	-2.51784400	1.56411100	H	-3.32767800	-2.18170600	1.76274300
H	3.06265100	-2.51044300	1.60660400	H	3.56231700	-2.03239400	1.77063700
H	-2.17651200	-3.20609000	0.21099000	H	-2.25028200	-3.08138600	0.69215000
H	2.17118700	-3.21279400	0.25420600	H	2.45452800	-2.93720400	0.73665700
H	-3.90665900	-3.51739700	0.37111700	H	-3.98208100	-3.42457900	0.69588100
H	3.89970400	-3.52432900	0.43107700	H	4.19196500	-3.24696300	0.65818100
C	2.97117200	0.16397100	2.75283200	C	3.24575000	0.69512000	2.55507200
C	-2.99863000	0.14083100	2.74168900	C	-3.23542100	0.60660100	2.49211100
H	3.60154400	-0.72695600	2.81232200	H	3.94227700	-0.12907100	2.72560700
H	-3.62668000	-0.75266700	2.78516300	H	-3.84850500	-0.27603900	2.68975300
H	1.94533500	-0.12807900	2.98638600	H	2.24932800	0.36863300	2.86014700
H	-1.97442200	-0.15034900	2.98335700	H	-2.21331300	0.39091300	2.80950400
H	3.30661700	0.85165300	3.53607300	H	3.54502000	1.51518500	3.21563300
H	-3.34465800	0.81884000	3.52881500	H	-3.61674400	1.41467300	3.12479300
C	4.51860400	1.27588100	1.10985800	C	4.69134300	1.56794000	0.68599100
C	-4.52950000	1.27240400	1.09594300	C	-4.74572700	1.31500200	0.60607800
H	4.62724700	1.77284300	0.14297500	H	4.73986900	1.91553100	-0.34842300
H	-4.62774100	1.78115100	0.13408100	H	-4.82662400	1.61568400	-0.44118000
H	5.21085900	0.43021000	1.13628200	H	5.39692800	0.74130100	0.80136000
H	-5.22290800	0.42725900	1.10517700	H	-5.39258100	0.44789200	0.76259200
H	4.84589100	1.98310000	1.87938400	H	5.04447100	2.38552600	1.32301300
H	-4.86410800	1.97075700	1.87044400	H	-5.14929100	2.13210500	1.21302000
H	0.02687200	0.72193800	1.44633100	H	0.32005700	1.27982700	1.47008300
H	4.24584500	-2.78455600	-1.90599600	H	4.18770600	-2.90197400	-1.78743000
H	2.56238100	-2.33688700	-2.16608700	H	2.47045400	-2.51395100	-1.86061400
H	3.85030000	-1.15794400	-2.45000000	H	3.66566400	-1.39146600	-2.52721300
H	-4.24077700	-2.74645800	-1.95966900	H	-3.98373000	-3.14553500	-1.76803300
H	-3.83595100	-1.11441100	-2.48020800	H	-3.58055700	-1.61653500	-2.54196100
H	-2.55422100	-2.30201100	-2.20463300	H	-2.29875200	-2.64350900	-1.88182900
H	-0.02926800	1.50809000	1.20608500	H	-0.08195900	1.98460400	1.35466400
O	-0.09524200	3.16244900	1.56166300	O	-0.59372900	3.60864200	1.50308000
C	-0.00023000	-1.73283300	-1.00610500	C	0.06436500	-2.03482000	-0.58610900
C	-0.00649300	-1.52229700	1.45700100	C	-0.00083500	-1.18906400	1.86979200
Mn	-0.00048200	-0.40519400	0.10923500	H	-0.87290200	3.55910200	2.42272300
H	-0.12677800	3.03238700	2.51484600	K	-0.10688900	3.64554100	-0.98707600
K	0.05948700	3.76066200	-0.90161200	Re	0.02199200	-0.34252900	0.16642200

Table S17. Computed energetic data for all structures optimized in methanol

H₂-SMD(CH₃OH) HF= -1.178394 ZPE= 0.01003 NImag= 0 Htot = -1.165058 Gtot = -1.165058 SP(M06-SCRF)= -1.170229	CH₃OH-SMD(CH₃OH) HF= -115.733956 ZPE= 0.051139 NImag= 0 Htot = -115.678536 Gtot = -115.705577 SP(M06-SCRF)= -115.7030033
CH₂O-SMD(CH₃OH) HF= -114.503457 ZPE= 0.026838 NImag= 0 Htot = -114.472808 Gtot = -114.497627 SP(M06-SCRF)= -114.4822947	H₂O-SMD(CH₃OH) HF= -76.444748 ZPE= 0.021154 NImag= 0 Htot = -76.419815 Gtot = -76.441245 SP(M06-SCRF)= -76.433431
HOCH₂OH-SMD(CH₃OH) HF= -190.969546 ZPE= 0.057314 NImag= 0 Htot = -190.907408 Gtot = -190.936555 SP(M06-SCRF)= -190.9358401	HCOOH-SMD(CH₃OH) HF= -189.7477813 ZPE= 0.033838 NImag= 0 Htot = -189.73325 Gtot = -189.761413 SP(M06-SCRF)= -189.771184
CO₂-SMD(CH₃OH) HF= -188.575297 ZPE= 0.011666 NImag= 0 Htot = -188.560068 Gtot = -188.584975 SP(M06-SCRF)= -188.5675991	OH⁻-SMD(CH₃OH) HF= -75.934977 ZPE= 0.008695 NImag= 0 Htot = -75.922977 Gtot = -75.94253 SP(M06-SCRF)= -75.9239424
CH₃O⁻-SMD(CH₃OH) HF= -115.224172 ZPE= 0.036948 NImag= 0 Htot = -115.183364 Gtot = -115.208463 SP(M06-SCRF)= -115.1957265	HOCH₂O⁻-SMD(CH₃OH) HF= -190.470740 ZPE= 0.042706 NImag= 0 Htot = -190.423464 Gtot = -190.452779 SP(M06-SCRF)= -190.4399412
HCOO⁻-SMD(CH₃OH) HF= -189.309466 ZPE= 0.020596 NImag= 0 Htot = -189.284954 Gtot = -189.312027 SP(M06-SCRF)= -189.2876886	K⁺-SMD(CH₃OH) HF= -28.084513 ZPE= 0 NImag= 0 Htot = -28.082152 Gtot = -28.099689 SP(M06-SCRF)= -28.034514
1Mn(C1)-SMD(CH₃OH) HF= -1699.470826 ZPE= 0.516918 NImag= 0 Htot = -1698.921173 Gtot = -1699.014802 SP(M06-SCRF)= -1699.150302	1Re(C1)-SMD(CH₃OH) HF= -1674.748575 ZPE= 0.516415 NImag= 0 Htot = -1674.199222 Gtot = -1674.293852 SP(M06-SCRF)= -1674.351315
2Mn(Cs)-SMD(CH₃OH)	2Re(Cs)-SMD(CH₃OH)

HF= -1700.652679 ZPE= 0.538867 NImag= 0 Htot = -1700.107246 Gtot = -1700.199972 SP(M06-SCRF)= -1700.355528	HF= -1675.956453 ZPE= 0.538262 NImag= 0 Htot = -1675.385299 Gtot = -1675.478950 SP(M06-SCRF)= -1675.553430
1Mn+H₂(ads)-SMD(CH₃OH) HF= -1700.630638 ZPE= 0.533547 NImag= 0 Htot = -1700.068787 Gtot = -1700.162656 SP(M06-SCRF)= -1700.3148	1Re+H₂(ads)-SMD(CH₃OH) HF= -1675.907964 ZPE= 0.532222 NImag= 0 Htot = -1675.342998 Gtot = -1675.438487 SP(M06-SCRF)= -1675.51014
1Mn + H₂-TS(1M/2M)-SMD(CH₃OH) HF= -1700.613055 ZPE= 0.532023 NImag= -886.1906 Htot = -1700.064177 Gtot = -1700.157222 SP(M06-SCRF)= -1700.305677	1Re+ H₂-TS(1M/2M)-SMD(CH₃OH) HF= -1675.897639 ZPE=0.530885 NImag= -906.3676 Htot = -1675.333794 Gtot = -1675.42736 SP(M06-SCRF)= -1675.497755
1Mn + H₂-TS(H₂O-H⁺)-SMD(CH₃OH) HF= -1777.09523 ZPE= 0.554714 NImag= -389.8106 Htot = -1776.504923 Gtot = -1776.603628 SP(M06-SCRF)= -1776.766104	1Re + H₂-TS(H₂O-H⁺)-SMD(CH₃OH) HF= -1752.365656 ZPE= 0.553227 NImag= -923.7158 Htot = -1751.776303 Gtot = -1751.877278 SP(M06-SCRF)= -1751.958742
1Mn + H₂-TS(CH₃OH-H⁺)-SMD(CH₃OH) HF= -1816.383886 ZPE= 0.583659 NImag= -655.43 Htot = -1815.763293 Gtot = -1815.866186 SP(M06-SCRF)= -1816.038966	1Re + H₂-TS(CH₃OH-H⁺)-SMD(CH₃OH) HF= -1791.654293 ZPE= 0.582421 NImag= -962.1873 Htot = -1791.034548 Gtot = -1791.138456 SP(M06-SCRF)= -1791.231783
1Mn + H₂-interm(H₂O-H₂)-SMD(CH₃OH) HF= -1777.100971 ZPE= 0.559499 NImag= 0 Htot = -1776.505165 Gtot = -1776.605947 SP(M06-SCRF)= -1776.769831	1Re + H₂-interm(H₂O-H₂)-SMD(CH₃OH) HF= ZPE= 0.558181 NImag= 0 Htot = -1751.77407 Gtot = -1751.876124 SP(M06-SCRF)= -1751.958742
1Mn + H₂-interm(CH₃OH-H₂)-SMD(CH₃OH) HF= -1816.389332 ZPE= 0.588303 NImag= 0 Htot = -1815.763486 Gtot = -1815.86866 SP(M06-SCRF)= -1816.042133	1Re + H₂-interm(CH₃OH-H₂)-SMD(CH₃OH) HF= -1791.657288 ZPE= 0.586613 NImag= 0 Htot = -1791.032807 Gtot = -1791.138458 SP(M06-SCRF)= -1791.233647
1Mn + H₂-TS(H₂O-H-H)-SMD(CH₃OH) HF= -1777.096636 ZPE= 0.55776 NImag= -446.1294	1Re + H₂-TS(H₂O-H-H)-SMD(CH₃OH) HF= -1752.366149 ZPE= 0.558052 NImag= -263.2779

Htot = -1776.503144 Gtot = -1776.601964 SP(M06-SCRF)= -1776.765826	Htot = -1751.772481 Gtot = -1751.871662 SP(M06-SCRF)= -1751.959488
1Mn + H₂-TS(CH₃OH-H-H)-SMD(CH₃OH) HF= -1816.385815 ZPE= 0.586952 NImag= -400.1286 Htot = -1815.761917 Gtot = -1815.864024 SP(M06-SCRF)= -1816.040044	1Re + H₂-TS(CH₃OH-H-H)-SMD(CH₃OH) HF= -1791.654493 ZPE= 0.586887 NImag= -63.0455 Htot = -1791.030501 Gtot = -1791.134135 SP(M06-SCRF)= -1791.233027
Mn-TS1-H⁺-SMD(CH₃OH) HF= -1815.195763 ZPE= 0.566496 NImag= -936.9764 Htot = -1814.593247 Gtot = -1814.694548 SP(M06-SCRF)= -1814.853504	Re-TS1-H⁺-SMD(CH₃OH) HF= -1790.474069 ZPE= 0.565798 NImag= -925.6305 Htot = -1789.871791 Gtot = -1789.975852 SP(M06-SCRF)= -1790.056465
3Mn⁺-OCH₃⁻-SMD(CH₃OH) HF= -1815.199796 ZPE= 0.571273 NImag= 0 Htot = -1814.592997 Gtot = -1814.691226 SP(M06-SCRF)= -1814.861047	3Re⁺-OCH₃⁻-SMD(CH₃OH) HF= -1790.477309 ZPE= 0.571692 NImag= 0 Htot = -1789.869705 Gtot = -1789.96986 SP(M06-SCRF)= -1790.061717
Mn-TS1-H⁻-SMD(CH₃OH) HF= -1815.181916 ZPE= 0.567236 NImag= -76.0497 Htot = -1814.578907 Gtot = -1814.678828 SP(M06-SCRF)= -1814.846701	Re-TS1-H⁻-SMD(CH₃OH) HF= -1790.459679 ZPE= 0.567762 NImag= -110.8579 Htot = -1789.856277 Gtot = -1789.956015 SP(M06-SCRF)= -1790.044255
Mn-TS(CH₃OH)-SMD(CH₃OH) HF= -1815.193734 ZPE= 0.56679 NImag= -693.7236 Htot = -1814.59111 Gtot = -1814.690444 SP(M06-SCRF)= -1814.851361	Re-TS(CH₃OH)-SMD(CH₃OH) HF= -1790.051532 ZPE= 0.566868 NImag= -658.8587 Htot = -1789.866613 Gtot = -1789.96692 SP(M06-SCRF)= -1790.469459
2Mn-OCH₃-SMD(CH₃OH) HF= -1815.221193 ZPE= 0.573378 NImag= 0 Htot = -1814.612158 Gtot = -1814.709922 SP(M06-SCRF)= -1814.885549	2Re-OCH₃-SMD(CH₃OH) HF= -1790.499387 ZPE= 0.572867 NImag= 0 Htot = -1789.890499 Gtot = -1789.99012 SP(M06-SCRF)= -1790.088411
Mn-TS(H₂O)-SMD(CH₃OH) HF= -1775.910432 ZPE= 0.538483 NImag= -1177.3117 Htot = -1775.337909 Gtot = -1775.43373 SP(M06-SCRF)= -1775.584635	Re-TS(H₂O)-SMD(CH₃OH) HF= -1751.186459 ZPE= 0.539791 NImag= -469.7149 Htot = -1750.612812 Gtot = -1750.708253 SP(M06-SCRF)= -1750.785599
2Mn-OH-SMD(CH₃OH)	2Re-OH-SMD(CH₃OH)

HF= -1775.934719 ZPE= 0.544586 NImag= 0 Htot = -1775.355518 Gtot = -1775.451768 SP(M06-SCRF)= -1775.610526	HF= -1751.212809 ZPE= 0.545157 NImag= 0 Htot = -1750.633149 Gtot = -1750.729423 SP(M06-SCRF)= -1750.813242
Mn-TS2-OH-SMD(CH₃OH) HF= -1890.438877 ZPE= 0.574259 NImag= -61.0422 Htot = -1889.827246 Gtot = -1889.930005 SP(M06-SCRF)= -1890.100797	Re-TS2-OH-SMD(CH₃OH) HF= -1865.715673 ZPE= 0.574371 NImag= -80.4681 Htot = -1865.103775 Gtot = -1865.207947 SP(M06-SCRF)= -1865.303019
3Mn⁺-O(H)CH₂O-SMD(CH₃OH) HF= -1890.447963 ZPE= 0.578293 NImag= 0 Htot = -1889.832959 Gtot = -1889.933213 SP(M06-SCRF)= -1890.109275	3Re⁺-O(H)CH₂O-SMD(CH₃OH) HF= -1865.723453 ZPE= 0.577949 NImag= 0 Htot = -1865.108746 Gtot = -1865.209947 SP(M06-SCRF)= -1865.311301
Mn-TS2-H⁺-SMD(CH₃OH) HF= -1890.432593 ZPE= 0.573994 NImag= -499.2595 Htot = -1889.822749 Gtot = -1889.920656 SP(M06-SCRF)= -1890.09342	Re-TS2-H⁺-SMD(CH₃OH) HF= -1865.714478 ZPE= 0.572319 NImag= -783.0439 Htot = -1865.105557 Gtot = -1865.20681 SP(M06-SCRF)= -1865.300398
2Mn-OCH₂OH-SMD(CH₃OH) HF= -1890.458646 ZPE= 0.577563 NImag= 0 Htot = -1889.843954 Gtot = -1889.946032 SP(M06-SCRF)= -1890.121162	2Re-OCH₂OH-SMD(CH₃OH) HF= -1865.738594 ZPE= 0.577721 NImag= 0 Htot = -1865.123592 Gtot = -1865.226814 SP(M06-SCRF)= -1865.325445
Mn-TS(HOCH₂OH)-SMD(CH₃OH) HF= -1890.430099 ZPE= 0.572427 NImag= -734.754 Htot = -1889.820962 Gtot = -1889.923206 SP(M06-SCRF)= -1890.085587	Re-TS(HOCH₂OH)-SMD(CH₃OH) HF= -1865.706792 ZPE= 0.573663 NImag= -149.1026 Htot = -1865.096435 Gtot = -1865.19892 SP(M06-SCRF)= -1865.287686
Mn-TS3-H⁺-SMD(CH₃OH) HF= -1890.434016 ZPE= 0.571896 NImag= -867.6534 Htot = -1889.825185 Gtot = -1889.927495 SP(M06-SCRF)= -1890.090708	Re-TS3-H⁺-SMD(CH₃OH) HF= -1865.711418 ZPE= 0.571744 NImag= -660.2084 Htot = -1865.102573 Gtot = -1865.206304 SP(M06-SCRF)= -1865.293917
3Mn⁺-HCH(OH)O-SMD(CH₃OH) HF= -1890.439277 ZPE= 0.576288 NImag= 0	3Re⁺-HCH(OH)O-SMD(CH₃OH) HF= -1865.717733 ZPE= 0.577155 NImag= 0

Htot = -1889.826433 Gtot = -1889.926709 SP(M06-SCRF)= -1890.099874	Htot = -1865.103295 Gtot = -1865.207127 SP(M06-SCRF)= -1865.301272
Mn-TS3-H-SMD(CH₃OH) HF= -1890.432985 ZPE= 0.5734912 NImag= -545.8865 Htot = -1889.823304 Gtot = -1889.923454 SP(M06-SCRF)= -1890.095559	Re-TS3-H-SMD(CH₃OH) HF= -1865.70906 ZPE= 0.572599 NImag= -489.8278 Htot = -1865.099725 Gtot = -1865.20169 SP(M06-SCRF)= -1865.29298
Mn-TS4-H-SMD(CH₃OH) HF= -1889.251276 ZPE= 0.548533 NImag= -1269.4451 Htot = -1888.666205 Gtot = -1888.770277 SP(M06-SCRF)= -1888.914515	Re-TS4-H-SMD(CH₃OH) HF= -1864.527287 ZPE= 0.551153 NImag= -1029.1351 Htot = -1863.940432 Gtot = -1864.040756 SP(M06-SCRF)= -1864.114732
3Mn⁺-OOCH-SMD(CH₃OH) HF= -1889.272853 ZPE= 0.554358 NImag= 0 Htot = -1888.68208 Gtot = -1888.783117 SP(M06-SCRF)= -1888.941478	3Re⁺-OOCH-SMD(CH₃OH) HF= -1864.55323 ZPE= 0.555947 NImag= 0 Htot = -1863.960686 Gtot = -1864.063578 SP(M06-SCRF)= -1864.143837
Mn-TS4-H-SMD(CH₃OH) HF= -1889.248848 ZPE= 0.550492 NImag= -396.1174 Htot = -1888.662373 Gtot = -1888.762388 SP(M06-SCRF)= -1888.924353	Re-TS4-H-SMD(CH₃OH) HF= -1864.524563 ZPE= 0.54942 NImag= -415.5505 Htot = -1863.93854 Gtot = -1864.041312 SP(M06-SCRF)= -1864.11977
Mn-TS(HCOOH)-SMD(CH₃OH) HF= -1889.270508 ZPE= 0.549901 NImag= -286.3223 Htot = -1888.684821 Gtot = -1888.784183 SP(M06-SCRF)= -1888.936349	Re-TS(HCOOH)-SMD(CH₃OH) HF= -1864.52935 ZPE= 0.548835 NImag= -700.1692 Htot = -1863.944311 Gtot = -1864.045533 SP(M06-SCRF)= -1864.121856
2Mn-OOCH-SMD(CH₃OH) HF= -1889.291002 ZPE= 0.555264 NImag= 0 Htot = -1888.699406 Gtot = -1888.800066 SP(M06-SCRF)= -1888.959454	2Re-OOCH-SMD(CH₃OH) HF= -1864.565846 ZPE= 0.555866 NImag= 0 Htot = -1863.973819 Gtot = -1864.074003 SP(M06-SCRF)= -1864.160156
1Mn-TS(HOCH₂OH-H-H)-SMD(CH₃OH) HF= -1891.626034 ZPE= 0.592312 NImag= -467.9015 Htot = -1890.995838 Gtot = -1891.100831 SP(M06-SCRF)= -1891.277215	1Re-TS(HOCH₂OH-H-H)-SMD(CH₃OH) HF= -1866.898109 ZPE= 0.592466 NImag= -504.0507 Htot = -1866.267666 Gtot = -1866.373131 SP(M06-SCRF)= -1866.473586
1Mn-TS(HCOOH-H-H)-SMD(CH₃OH)	1Re-TS(HCOOH-H-H)-SMD(CH₃OH)

HF= -1890.449925 ZPE= 0.568735 NImag= -864.283 Htot = -1889.843961 Gtot = -1889.948466 SP(M06-SCRF)= -1890.108817	HF= -1865.723448 ZPE= 0.568559 NImag= -1038.6082 Htot = -1865.117355 Gtot = -1865.222676 SP(M06-SCRF)= -1865.30613
1Mn-OCH₃⁻-SMD(CH₃OH) HF= -1814.685351 ZPE= 0.555765 NImag= 0 Htot = -1814.093609q Gtot = -1814.193064 SP(M06-SCRF)= -1814.356463	1Re-OCH₃⁻-SMD(CH₃OH) HF= -1789.972792 ZPE= 0.555777 NImag= 0 Htot = -1789.380767 Gtot = -1789.481637 SP(M06-SCRF)= -1789.566194
1Mn-HCH₂O⁻-SMD(CH₃OH) HF= -1814.675403 ZPE= 0.554494 NImag= 0 Htot = -1814.084539 Gtot = -1814.185207 SP(M06-SCRF)= -1814.342234	1Re-HCH₂O⁻-SMD(CH₃OH) HF= -1789.965347 ZPE= 0.555733 NImag= 0 Htot = -1789.372696 Gtot = -1789.477159 SP(M06-SCRF)= -1789.550136
1Mn-TS(HCH₂O)-SMD(CH₃OH) HF= -1814.649551 ZPE= 0.549285 NImag= -86.3017 Htot = -1814.064132 Gtot = -1814.165437 SP(M06-SCRF)= -1814.321298	1Re-TS(HCH₂O)-SMD(CH₃OH) HF= -1789.936682 ZPE=0.550481 NImag= -114.5156 Htot = -1789.350235 Gtot = -1789.451377 SP(M06-SCRF)= -1789.526112
1Mn-OCH₂OH⁻-SMD(CH₃OH) HF= -1889.940179 ZPE= 0.560743 NImag= 0 Htot = -1889.343134 Gtot = -1889.442616 SP(M06-SCRF)= -1889.606947	1Re-OCH₂OH⁻-SMD(CH₃OH) HF= -1865.225272 ZPE= 0.561017 NImag= 0 Htot = -1864.627613 Gtot = -1864.729107 SP(M06-SCRF)= -1864.816445
1Mn-HCH(OH)O⁻-SMD(CH₃OH) HF= -1889.931698 ZPE= 0.561491 NImag= 0 Htot = -1889.332163 Gtot = -1889.440004 SP(M06-SCRF)= -1889.586114	1Re-HCH(OH)O⁻-SMD(CH₃OH) HF= -1865.212192 ZPE= 0.560639 NImag= 0 Htot = -1864.613032 Gtot = -1864.724419 SP(M06-SCRF)= -1864.790975
Mn-TS(HCH(OH)O)-SMD(CH₃OH) HF= -1889.902065 ZPE= 0.55617 NImag= -708.4999 Htot = -1889.309458 Gtot = -1889.410064 SP(M06-SCRF)= -1889.570052	Re-TS(HCH(OH)O)-SMD(CH₃OH) HF= -1865.188471 ZPE= 0.556082 NImag= -526.3419 Htot = -1864.595508 Gtot = -1864.698329 SP(M06-SCRF)= -1864.777173
1Mn-OOCH⁻-SMD(CH₃OH) HF= -1888.764462 ZPE= 0.538844 NImag= 0	1Re-OOCH⁻-SMD(CH₃OH) HF= -1864.046077 ZPE= 0.537987 NImag= 0

Htot = -1888.189101 Gtot = -1888.290823 SP(M06-SCRF)= -1888.439303	Htot = -1863.470804 Gtot = -1863.576723 SP(M06-SCRF)= -1863.643585
1Mn-HCOO⁻-SMD(CH₃OH) HF= -1888.769926 ZPE= 0.538939 NImag= 0 Htot = -1888.193382 Gtot = -1888.30182 SP(M06-SCRF)= -1888.431742	1Re-HCOO⁻-SMD(CH₃OH) HF= -1864.050274 ZPE= 0.538758 NImag= 0 Htot = -1863.473921 Gtot = -1863.581432 SP(M06-SCRF)= -1863.637773
Mn-TS(HCO₂)-SMD(CH₃OH) HF= -1888.71723 ZPE= 0.531212 NImag= -347.2109 Htot = -1888.149003 Gtot = -1888.253271 SP(M06-SCRF)= -1888.401335	Re-TS(HCO₂)-SMD(CH₃OH) HF= -1864.003663 ZPE= 0.532703 NImag= -351.8376 Htot = -1863.434071 Gtot = -1863.53849 SP(M06-SCRF)= -1863.605181
2Mn⁻-SMD(CH₃OH) HF= -1700.146478 ZPE= 0.522385 NImag= 0 Htot = -1699.591749 Gtot = -1699.683401 SP(M06-SCRF)= -1699.831778	2Re⁻-SMD(CH₃OH) HF= -1675.433205 ZPE= 0.521765 NImag= 0 Htot = -1674.87857 Gtot = -1674.972477 SP(M06-SCRF)= -1675.036714
2Mn⁻...H₂O-SMD(CH₃OH) HF= -1776.608019 ZPE= 0.545706 NImag= 0 Htot = -1776.026898 Gtot = -1776.125357 SP(M06-SCRF)= -1776.285598	2Re⁻...H₂O-SMD(CH₃OH) HF= -1751.893269 ZPE= 0.543642 NImag= 0 Htot = -1751.313525 Gtot = -1751.41489 SP(M06-SCRF)= -1751.488828
Mn-TS(H⁺ transfer, H₂ formation)-SMD(CH₃OH) HF= -1776.570798 ZPE= 0.543837 NImag= -578.9689 Htot = -1775.992074 Gtot = -1776.088995 SP(M06-SCRF)= -1776.247467	Re-TS(H⁺ transfer, H₂ formation)-SMD(CH₃OH) HF= -1751.845731 ZPE= 0.541324 NImag= -542.3147 Htot = -1751.268417 Gtot = -1751.369162 SP(M06-SCRF)= -1751.442249
1Mn-OCH₃⁻...K⁺-SMD(CH₃OH) HF= -1842.800629 ZPE= 0.558106 NImag= 0 Htot = -1842.205078 Gtot = -1842.307072 SP(M06-SCRF)= -1842.429333	1Re-OCH₃⁻...K⁺-SMD(CH₃OH) HF= -1818.088109 ZPE= 0.55767 NImag= 0 Htot = -1817.492425 Gtot = -1817.59676 SP(M06-SCRF)= -1817.639713
1Mn-HCH₂O⁻...K⁺-SMD(CH₃OH) HF= -1842.796857 ZPE= 0.557431 NImag= 0 Htot = -1842.20053 Gtot = -1842.309569 SP(M06-SCRF)= -1842.41244	1Re-HCH₂O⁻...K⁺-SMD(CH₃OH) HF= -1818.075979 ZPE= 0.558488 NImag= 0 Htot = -1817.479219 Gtot = -1817.584604 SP(M06-SCRF)= -1817.619786
Mn-TS(HCH₂O⁻...K⁺)-SMD(CH₃OH)	Re-TS(HCH₂O⁻...K⁺)-SMD(CH₃OH)

HF= -1842.763034 ZPE= 0.550749 NImag= -57.7858 Htot = -1842.173894 Gtot = -1842.28123 SP(M06-SCRF)= -1842.392289	HF= -1818.04958 ZPE= 0.551936 NImag= -27.1608 Htot = -1817.459614 Gtot = -1817.565264 SP(M06-SCRF)= -1817.597329
1Mn-OCH₂OH...K⁺-SMD(CH₃OH) HF= -1918.041192 ZPE= 0.561506 NImag= 0 Htot = -1917.440224 Gtot = -1917.548432 SP(M06-SCRF)= -1917.66838	1Re-OCH₂OH...K⁺-SMD(CH₃OH) HF= -1893.327789 ZPE= 0.562459 NImag= 0 Htot = -1892.726006 Gtot = -1892.834195 SP(M06-SCRF)= -1892.877857
1Mn-HCH(OH)O⁻...K⁺-SMD(CH₃OH) HF= -1918.033368 ZPE= 0.561332 NImag= 0 Htot = -1917.432088 Gtot = -1917.542457 SP(M06-SCRF)= -1917.652698	1Re-HCH(OH)O⁻...K⁺-SMD(CH₃OH) HF= -1893.321642 ZPE= 0.563134 NImag= 0 Htot = -1892.719134 Gtot = -1892.827352 SP(M06-SCRF)= -1892.865243
Mn-TS(HCH(OH)O⁻...K⁺)-SMD(CH₃OH) HF= -1918.015081 ZPE= 0.557128 NImag= -670.3226 Htot = -1917.419403 Gtot = -1917.524793 SP(M06-SCRF)= -1917.641975	Re-TS(HCH(OH)O⁻...K⁺)-SMD(CH₃OH) HF= -1893.300302 ZPE= 0.557353 NImag= -715.1374 Htot = -1892.704014 Gtot = -1892.811729 SP(M06-SCRF)= -1892.847077
1Mn-OOCH⁻...K⁺-SMD(CH₃OH) HF= -1916.87882 ZPE= 0.540036 NImag= 0 Htot = -1916.300189 Gtot = -1916.406691 SP(M06-SCRF)= -1916.511419	1Re-OOCH⁻...K⁺-SMD(CH₃OH) HF= -1892.16044 ZPE= 0.540125 NImag= 0 Htot = -1891.581632 Gtot = -1891.689151 SP(M06-SCRF)= -1891.716571
1Mn-HCOO⁻...K⁺-SMD(CH₃OH) HF= -1916.877033 ZPE= 0.540384 NImag= 0 Htot = -1916.29751 Gtot = -1916.406416 SP(M06-SCRF)= -1916.502406	1Re-HCOO⁻...K⁺-SMD(CH₃OH) HF= -1892.157049 ZPE= 0.540292 NImag= 0 Htot = -1891.577547 Gtot = -1891.687971 SP(M06-SCRF)= -1891.706622
Mn-TS(HCO₂⁻...K⁺)-SMD(CH₃OH) HF= -1916.827699 ZPE= 0.534975 NImag= -489.3937 Htot = -1916.254806 Gtot = -1916.359133 SP(M06-SCRF)= -1916.468113	Re-TS(HCO₂⁻...K⁺)-SMD(CH₃OH) HF= ZPE= NImag= 0 Htot = Gtot = SP(M06-SCRF)=
2Mn⁻...K⁺-SMD(CH₃OH)-SMD(CH₃OH) HF= -1728.254187 ZPE= 0.52297 NImag= 0	2Re⁻...K⁺-SMD(CH₃OH)-SMD(CH₃OH) HF= -1892.1129 ZPE= 0.533895 NImag= -460.9803

Htot = -1727.696431 Gtot = -1727.794353 SP(M06-SCRF)= -1727.895721	Htot = -1891.540304 Gtot = -1891.648036 SP(M06-SCRF)= -1891.672179
2Mn⁻...K⁺...H₂O-SMD(CH₃OH) HF= -1804.706292 ZPE= 0.545972 NImag= 0 Htot = -1804.121845 Gtot = -1804.228646 SP(M06-SCRF)= -1804.342254	2Re⁻...K⁺...H₂O-SMD(CH₃OH) HF= -1779.991444 ZPE= 0.545598 NImag= 0 Htot = -1779.40704 Gtot = -1779.517775 SP(M06-SCRF)= -1779.545154
2Mn⁻...K⁺...H₂O-TS(H⁺ transfer, H₂ formation)-SMD(CH₃OH) HF= -1804.680557 ZPE= 0.543173 NImag= -523.9842 Htot = -1804.09949 Gtot = -1804.203859 SP(M06-SCRF)= -1804.313576	2Re⁻...K⁺...H₂O-TS(H⁺ transfer, H₂ formation)-SMD(CH₃OH) HF= -1779.958018 ZPE= 0.543134 NImag= -308.202 Htot = -1779.376763 Gtot = -1779.483864 SP(M06-SCRF)= -1779.513226

References

1. A. Schäfer, C. Huber and R. Ahlrichs, *J. Chem. Phys.*, 1994, **100**, 5829-5835.
2. P. J. Hay and W. R. Wadt, *J. Chem. Phys.*, 1985, **82**, 299-310.
3. A. V. Marenich, C. J. Cramer and D. G. Truhlar, *J. Phys. Chem. B*, 2009, **113**, 6378-6396.
4. E. Alberico, A. J. J. Lennox, L. K. Vogt, H. Jiao, W. Baumann, H.-J. Drexler, M. Nielsen, A. Spannenberg, M. P. Checinski, H. Junge and M. Beller, *J. Am. Chem. Soc.*, 2016, **138**, 14890-14904.
5. D. R. Lide, *Standard thermodynamic properties of chemical substances*, CRC Press, Boca Raton, FL, 2007.
6. D. H. Nguyen, X. Trivelli, F. Capet, J.-F. Paul, F. Dumeignil and R. M. Gauvin, *ACS Catal.*, 2017, **7**, 2022-2032.
7. A. M. Tondreau, R. Michalczyk and J. M. Boncella, *Organometallics*, 2017, **36**, 4179-4183.