Supplementary Information

Unveiling a unique outer-sphere pathway in manganese-catalyzed acceptorless dehydrogenation reaction

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1. The calculation details of standard state correction.

For the experimental condition (383.15 K), the molar volume of an ideal gas in the gas phase state (383.15 K, 1 atm) (eq. S1):

$$V_m = \frac{RT}{P} = \frac{8.314 \times 383.15}{101325} = 0.03144 \text{ m}^3/\text{mol} = 31.44 \text{ L/mol}$$

(S1)

The free energy change of the process of compressing 1M ideal gas into 1M solution concentration in the standard state (eq. S2):

$$\Delta G_{1\text{atm}\rightarrow 1\text{M}}^{383.15\text{K}} = RTln(\frac{V_a}{V_b}) = \frac{8.314 \times 383.15 \times \ln(31.44)}{1000} = 10.98 \text{ KJ/mol} = 2.62 \text{ kcal/mol}$$

(S2)

Therefore, a correction factor of 2.62 kcal/mol was applied for the standard state change from 1 atm to 1 M.

2. The comparison of free energy barriers using different hybrid functionals.

Table S1. The comparison of free energy barriers using different hybrid functionals (kcal/mol).

	Functional				
	M06L	M06	PBE0-D3BJ	B3LYP-D3BJ	WB97XD
IM6	0	0	0	0	0
TS2	29.0	31.8	33.9	32.2	36.2
TS3	30.6	33.3	33.8	31.6	35.7
TS6	28.7	31.3	33.7	32.7	36.4
TS7	26.3	27.0	30.0	27.4	31.9

To select a suitable functional for our calculations, we compared a series of functionals commonly used in computational studies of dehydrogenation reactions and applied different hybrid functionals to calculate the rate-determining transition state and intermediate. The results show that, starting from intermediate IM6, the energy barrier for the TS7 pathway is lowest under the M06-L functional among the five tested functionals, with this functional also providing the most stable structure. Considering both computational cost and accuracy, we ultimately selected M06-L as our functional for the calculations.

3. Conformational Search Performed with Crest.

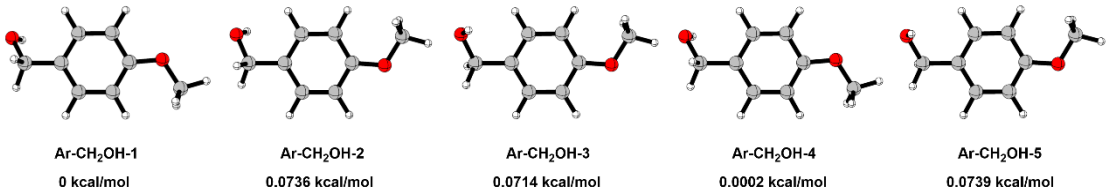

Figure S1. Crest conformational search for Ar-CH_2OH (Top five most stable structures selected).

To ensure the identification of the lowest-energy conformers of the benzylic substrate, we utilized the Conformer-Rotamer Ensemble Sampling Tool (CREST, version 2.11) in combination with DFT optimizations using the xTB package (version 6.1). The conformers generated by CREST were initially optimized using GFN2-xTB, and the solvation effect in toluene was calculated with the GBSA implicit solvation model. The five most stable conformers of the benzylic substrate are shown in Figure S1, where it can be observed that the relative energy differences among the various conformers are all less than 0.1 kcal/mol. Such small differences are not expected to significantly affect the selectivity of the reaction mechanism.

4. The kinetic isotope effect (KIE) calculation results.

Table S2. The Calculated Result of KIEs in Mn System.

Labeling species	KIE_{Cal} Free Energy	KIE_{Cal} Enthalpy	KIE_{expt}
IM1/TS2	5.24	21.38	2.23
IM6/TS7	4.12	2.08	2.23

The KIEs calculation[1, 2] is based on the transition state theory, the rate constants can be calculated using eq. S3

$$k^{TST}(T) = \frac{k_S T}{h} K^{\circ \neq} e^{-\Delta G^{\circ \neq}/RT} \quad (S3)$$

Since the TS1 including the hydrogen transfer process, the tunneling effects must be taken into consideration, here we use Winger tunneling approximation[3, 4] (eq. S4):

$$k^{tunneling} = \kappa(T) k^{TST}(T) \quad (S4)$$

where κ(T) refer to (eq. S5):

$$\kappa(T) = 1 + \frac{1}{24}\left(\frac{\hbar\omega^{\neq}}{kT}\right) \quad (S5)$$

In the Eyring KIE calculation, the activation free energy ($\Delta G^{\neq}$) for the hydrogen and deuterium substitution reactions in the gas phase at room temperature (T = 383.15 K) was considered, where R is the gas constant, ħ is Planck's constant, and k_B is the Boltzmann constant. To further validate our computational results, we performed kinetic isotope effect (KIE) calculations for the rate-determining steps, incorporating Wigner tunneling corrections (i.e., for the deuterated analogues of IM1/TS2 and IM6/TS7). However, the results are not consistent with the experimentally observed KIE values. The experimentally measured KIE value is 2.23, while our calculated KIE value is 4.12. We believe that the discrepancy between our calculated results and the experimental values may arise from uncertainties in the computed entropy contributions and some approximations in the theoretical model. Additionally, we found that when the KIE was calculated using enthalpy values, the result was 2.08, which is very close to the experimental value of 2.23.[5] Therefore, while there is some discrepancy, our computational results still represent a reasonable approximation.

References

1. J. Bigeleisen and M. Wolfsberg, Theoretical and experimental aspects of isotope effects in chemical kinetics, *Adv. Chem. Phys.*, 1957, 15-76.
2. P. Barman, P. Upadhyay, A.S. Faponle, J. Kumar, S.S. Nag, D. Kumar, C.V. Sastri and S.P. de Visser, Deformylation Reaction by a Nonheme Manganese (III) ‑ Peroxo Complex via Initial Hydrogen ‑ Atom Abstraction, *Angew. Chem.*, 2016, **128**, 11257-11261.
3. M. Szaleniec, T. Borowski, K. Schühle, M. Witko and J. Heider, Ab Inito Modeling of Ethylbenzene Dehydrogenase Reaction Mechanism, *J. Am. Chem. Soc.*, 2010, **132**, 6014-6024.

4. S. Ghafoor, A. Mansha and S.P. de Visser, Selective Hydrogen Atom Abstraction from Dihydroflavonol by a Nonheme Iron Center Is the Key Step in the Enzymatic Flavonol Synthesis and Avoids Byproducts, *J. Am. Chem. Soc.*, 2019, **141**, 20278-20292.
5. A. Mondal, H.J. Phukan, D. Pal, S. Kumar, M. Roy and D. Srimani, Well-Defined Mn(II)-complex Catalyzed Switchable De(hydrogenative) Csp(3) -H Functionalization of Methyl Heteroarenes: A Sustainable Approach for Diversification of Heterocyclic Motifs, *Chem.-Eur. J.*, 2024, **30**, e202303315.

5. Driving Forces for Precatalyst Activation with KOH and KBr Models.

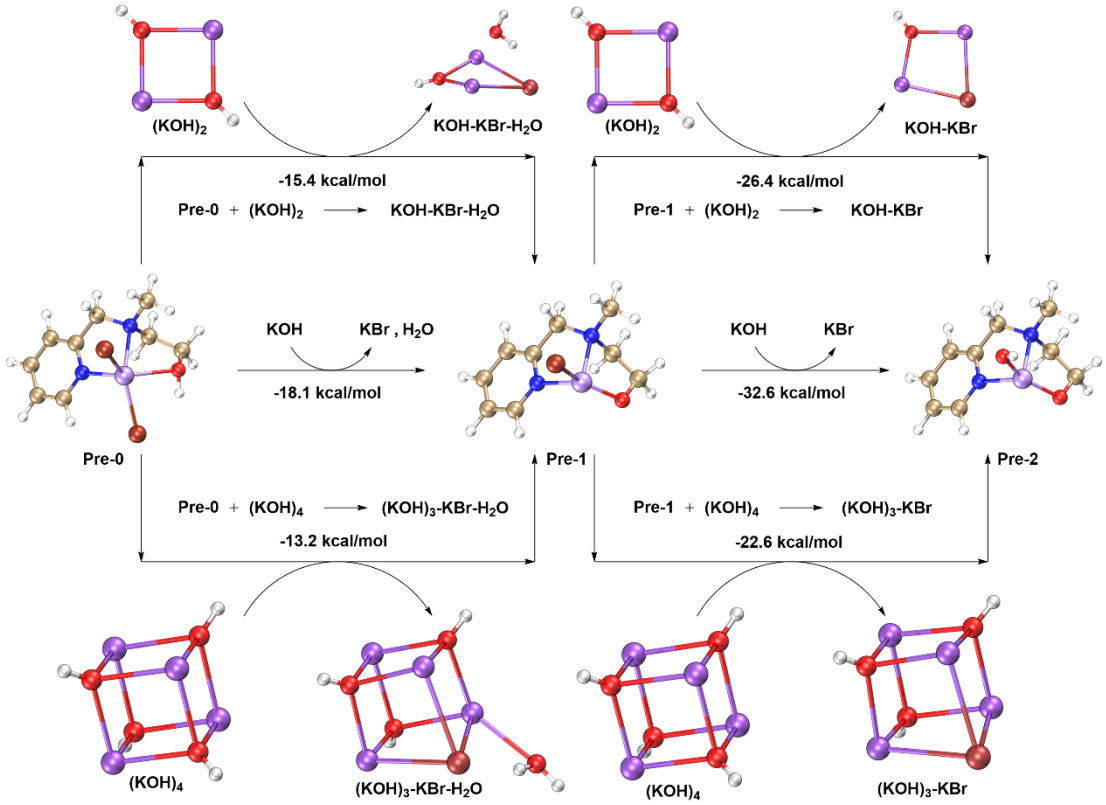

Figure S2. Evaluation of Driving Forces for Potential Precatalyst Activation Steps Using KOH and KBr Models, Including Single Molecules and Aggregates ($(KOH)_2$ and $(KOH)_4$).

To further confirm the reliability of our results, we followed the suggestion to perform calculations using the $(KOH)_2$ and $(KOH)_4$ clusters, examining the influence of these aggregates on the driving forces. The results indicate that, even with these aggregation models, the trends and qualitative conclusions remain similar to those obtained with the single-molecule model.

6. The comparison of free energy barriers using different hybrid functionals.

Table S3. Spin contamination values of intermediates and transition states in the sextet state.

Structural	S^2	Structural	S^2	Structural	S^2	Structural	S^2
Expect	8.75	Pre-0	8.76	Pre-1	8.76	Pre-2	8.77
IM1	8.77	TS1	8.76	IM5	8.76	TS5	8.76
IM2	8.76	TS2	8.77	IM6	8.76	TS6	8.76
IM3	8.76	TS3	8.77	IM7	8.76	TS7	8.77
IM4	8.77	TS4	8.76	IM8	8.77	TS8	8.76

We used the unrestricted Kohn-Sham (UKS) formalism to handle open-shell systems in our study. We monitored spin contamination throughout the calculations and found that the $\langle S^2 \rangle$ values were close to the expected value of 8.75, as detailed in Table S3. This indicated an extremely low level of spin contamination, with deviations kept at around 0.1 or less. All deviations were within an acceptable range, thereby ensuring the high reliability of our computational results.

7. The reaction pathway of active species Pre-1 dehydrogenation.

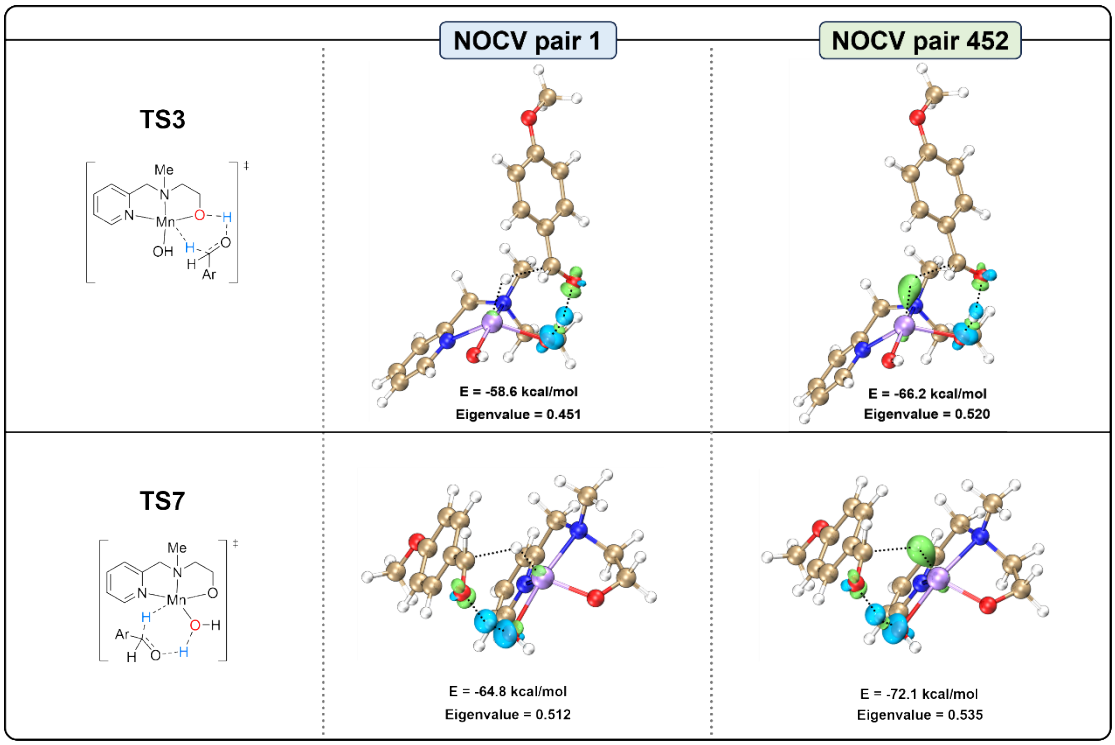

Figure S3. The ETS-NOCV analysis of the TS3 and TS7.

8. Geometric structure diagrams.

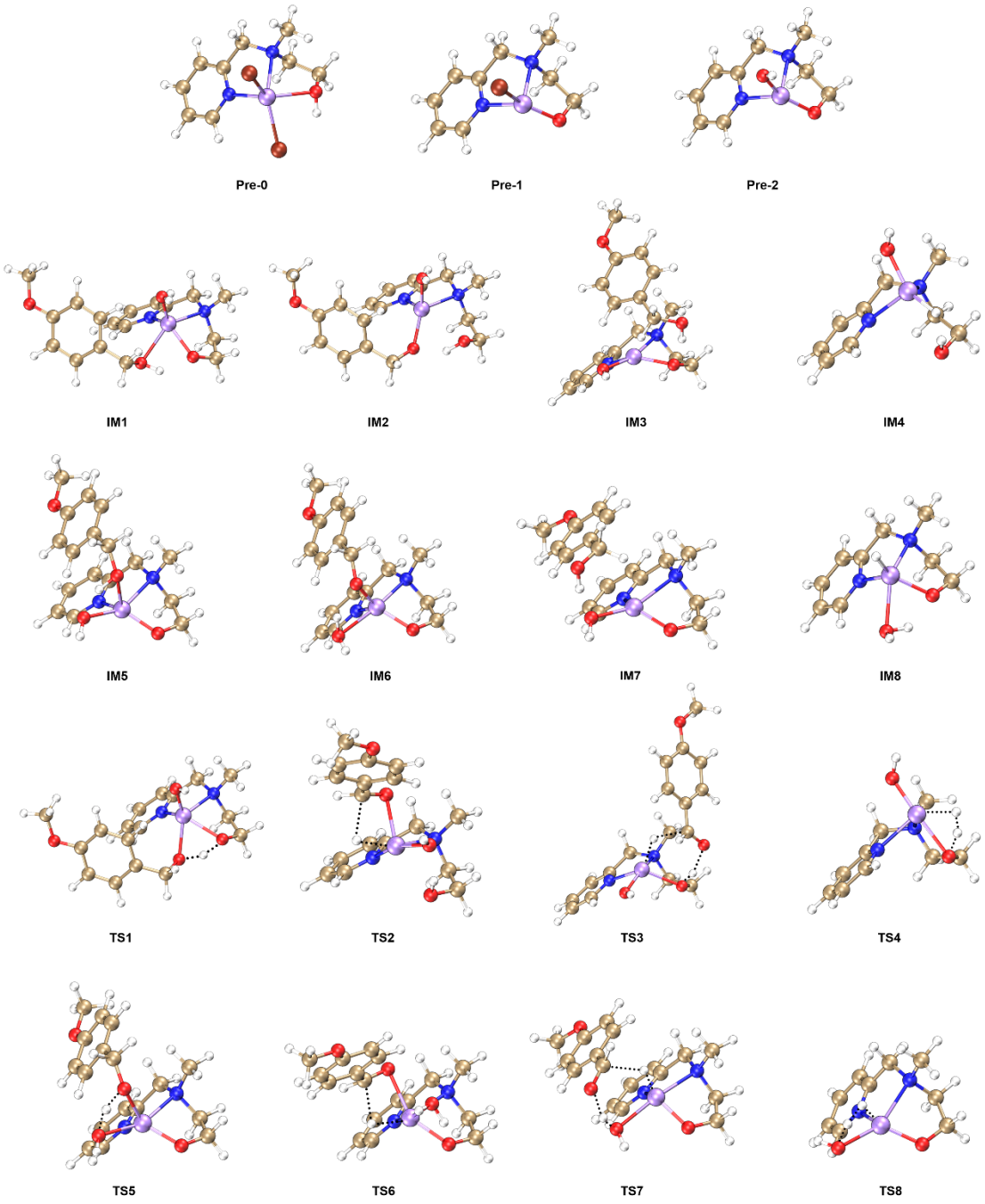

Figure S4. Geometric structure diagrams of all intermediates and transition states in the Mn(II) catalysts

9. The DFT calculated energies of all optimized structures

Species	Gc (2.62) hartree	G(gas) hartree	Esp + G_{SOL} hartree	Final G (2.62) hartree	*i* (cm^{-1})
Ar-CH_2OH	0.123391	-460.766638	-461.4111395	-461.2877485	
Ar-CHO	0.100094	-459.597928	-460.2183579	-460.1182639	
H_2	-0.001647	-1.168683	-1.171163	-1.172809816	
pre-catalyst activation					
KOH	-0.013634	-675.604056	-675.7861273	-675.7997613	
KBr	-0.028131	-3173.691139	-3174.07524	-3174.103371	
H_2O	0.001948	-76.346006	-76.44737071	-76.44542271	
$(KOH)_2$	-0.01467	-1351.29055	-1351.635018	-1351.649688	
KOH-KBr	-0.028656	-3849.36753	-3849.918888	-3849.947544	
KOH-KBr-H_2O	-0.009724	-3925.72572	-3926.384799	-3926.394523	
$(KOH)_4$	-0.00517	-2702.6551	-2703.340811	-2703.345981	
$(KOH)_3$-KBr-H_2O	-0.001259	-5277.08337	-5278.085991	-5278.087250	
$(KOH)_3$-KBr	-0.01843	-5200.72811	-5201.622973	-5201.641403	
pre-0	0.161797	-6833.99797	-6835.548091	-6835.386294	
pre-1	0.154556	-4259.589273	-4260.820582	-4260.666026	
pre-2	0.166337	-1761.530155	-1762.55198	-1762.385643	
Catalytic Cycle					
IM1	0.312212	-2222.319259	-2223.988251	-2223.676039	
IM2	0.311889	-2222.317594	-2223.987297	-2223.675408	
IM3	0.316063	-2222.313125	-2223.985567	-2223.669504	
IM4	0.185822	-1762.675232	-1763.719246	-1763.533424	
IM5	0.31688	-2222.321325	-2223.99174	-2223.67486	
IM6	0.315607	-2222.327468	-2223.994367	-2223.67876	
IM7	0.316131	-2222.313289	-2223.98905	-2223.672919	
IM8	0.186066	-1762.690542	-1763.728293	-1763.542227	
TS1	0.309648	-2222.31395	-2223.979403	-2223.669755	-541.52
TS2	0.307889	-2222.275465	-2223.940427	-2223.632538	-373.38
TS3	0.307428	-2222.266269	-2223.937531	-2223.630103	-409.00
TS4	0.18151	-1762.66426	-1763.699016	-1763.517506	-1127.45
TS5	0.313793	-2222.320282	-2223.984872	-2223.671079	-668.02
TS6	0.308018	-2222.278353	-2223.941062	-2223.633044	-447.28
TS7	0.310349	-2222.280618	-2223.94718	-2223.636831	-460.79
TS8	0.179731	-1762.668309	-1763.700923	-1763.521192	-1204.88

Table S4. The DFT calculated energies of all optimized structures

- The $\mathbf{G_C}$ **(2.62)** designate the thermal correction of Enthalpy and Gibbs Free Energy at M06L/def2-SVP level.
- The **G(gas)** designate Enthalpy and Gibbs Free Energy in the gas phase at the M06L/def2-SVP level.
- The $\mathbf{E_{SP}}$ **+** $\mathbf{G_{SOL}}$ designates the sum of single point energy at M06L/def2-TZVP level and the solvation free energy calculated by SMD continuum solvent mode.
- The **Final G (2.62)** designates the sum of $\mathbf{E_{SP}}$ **+** $\mathbf{G_{SOL}}$ and $\mathbf{G_C}$ **(2.62)**.

- The ***i*** designates the imaginary frequency of transition states.

10. The cartesian coordinates for all structures

Ar-CH_2OH

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-1.36074	0.29661	0.00065
C	-0.91342	-1.02948	0.00096
C	0.44384	-1.32529	0.00065
C	1.39324	-0.29625	0.00016
C	0.9606	1.03561	-0.0003
C	-0.4055	1.31488	-0.00007
H	-1.64988	-1.8342	0.00131
H	0.79919	-2.35759	0.00081
H	1.6765	1.85868	-0.00096
H	-0.7301	2.36054	-0.00054
C	-2.82428	0.63107	0.00153
H	-3.05022	1.26775	-0.87975
H	-3.05064	1.26125	0.88738
O	-3.5878	-0.54526	-0.00283
H	-4.51669	-0.29852	-0.0008
O	2.69587	-0.67549	0.00001
C	3.67241	0.32897	-0.00066
H	4.64631	-0.17242	-0.00059
H	3.6069	0.97152	-0.89544
H	3.60713	0.97234	0.89357

Ar-CHO

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-1.48002	0.19024	0
C	-0.73159	-0.99429	-0.00006
C	0.65586	-0.96358	-0.00006
C	1.32068	0.27532	0.0001
C	0.58026	1.46971	0
C	-0.80257	1.42047	-0.00001
H	-1.27184	-1.94441	-0.00017
H	1.21875	-1.89782	-0.0002
H	1.12416	2.41561	0.00003
H	-1.38162	2.34931	0.00001
C	-2.94758	0.1424	0.00002
H	-3.4371	1.15573	-0.00001
O	-3.61105	-0.87028	0.00005
O	2.66028	0.4112	-0.00016
C	3.45481	-0.7495	0.00012
H	4.49765	-0.4169	0.00036
H	3.27827	-1.36663	0.8958
H	3.27883	-1.36679	-0.8956

H_2

Atomic Type	Coordinates (Angstroms) X	Y	Z
H	1.07562	0.06088	0.024
H	2.07562	0.06088	0.024

KOH

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-1.48002	0.19024	0
C	-0.73159	-0.99429	-0.00006

KBr

Atomic Type	Coordinates (Angstroms) X	Y	Z
Br	1.03883	0.07189	0.05766
K	4.26883	0.07189	0.05766

H_2O

Atomic Type	Coordinates (Angstroms) X	Y	Z
O	1.02369	-0.09104	0.03391
H	0.69036	-0.97456	0.36299
H	2.02369	-0.09104	0.03391

$(KOH)_2$

Atomic Type	Coordinates (Angstroms) X	Y	Z
O	0.00076	-1.72606	-0.00023
H	-0.00017	-2.68571	-0.00034
K	-1.72227	-0.0001	0.00012
O	0.00025	1.72606	-0.00024
H	-0.00003	2.68565	-0.00031
K	1.72186	0.0001	0.00012

KOH-KBr

Atomic Type	Coordinates (Angstroms) X	Y	Z
O	2.41575	0.00259	0.00002
H	3.37598	0.00461	0.00002
K	0.85914	-1.86232	0.00001
K	0.85403	1.86394	0
Br	-1.57864	-0.00161	-0.00001

KOH-KBr-H_2O

Atomic Type	Coordinates (Angstroms) X	Y	Z
O	-2.44177	-0.00123	-0.79439
H	-3.29082	-0.00109	-1.24101

K	-0.93345	-1.75641	-0.0916
O	-0.36213	0.00346	2.05422
H	0.53003	0.00227	1.62288
K	-0.93368	1.75582	-0.09422
H	-0.18146	0.00439	2.99957
Br	1.73853	-0.00034	-0.2837

$(KOH)_4$

Atomic Type	Coordinates (Angstroms) X	Y	Z
O	-0.25056	-2.01691	-0.9725
H	-0.3597	-2.87651	-1.3876
K	0.14509	0.21682	-2.18987
O	2.02027	0.84774	-0.53682
H	2.87869	1.21181	-0.76881
K	0.2461	1.97396	0.95216
O	-1.61842	1.39089	-0.7258
H	-2.30684	1.98512	-1.03593
K	-1.97649	-0.82968	0.52706
O	-0.15082	-0.22165	2.23514
H	-0.21329	-0.31697	3.18922
K	1.58516	-1.3613	0.71081

$(KOH)_3$-KBr-H_2O

Atomic Type	Coordinates (Angstroms) X	Y	Z
O	2.17286	-1.64024	-0.00211
H	2.76049	-2.40106	-0.00393
K	0.5539	-1.18789	1.93313
O	-3.26036	2.00722	-0.02805
H	-3.19205	1.02943	-0.03609
K	-0.61026	1.97893	0.00317
O	1.11587	1.29492	1.83287
H	1.18598	1.85286	2.61255
K	2.84918	0.85224	-0.00128
O	1.11431	1.29538	-1.82942
H	1.17503	1.85424	-2.60923
K	0.54971	-1.18671	-1.93537
H	-4.18278	2.17659	0.18087
Br	-2.01132	-1.05272	0.00218

$(KOH)_3$-KBr

Atomic Type	Coordinates (Angstroms) X	Y	Z
O	1.29957	1.68765	-1.24107
H	1.57905	2.42814	-1.78672
K	2.7871	0.00059	0.0014
K	-0.09373	-1.78871	1.31789
O	1.2952	0.23353	2.08107
H	1.57482	0.33715	2.99498
K	-0.0942	2.03611	0.88953
O	1.29877	-1.92138	-0.83673
H	1.57936	-2.7646	-1.20333
K	-0.08872	-0.24774	-2.20639
Br	-2.388	-0.00011	-0.0022

Pre-1

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-3.193707	0.164565	-1.022702
C	-1.855168	-0.063563	-0.699173
C	-2.01705	1.330815	1.140838
C	-3.350888	1.619687	0.87821
C	-3.949945	1.019365	-0.227086
H	-3.631452	-0.327156	-1.89411
H	-1.504741	1.774843	2.000086
H	-3.905187	2.296023	1.530055
H	-4.998194	1.212281	-0.465008
C	-0.965792	-0.912546	-1.567405
H	-1.57873	-1.637453	-2.141196
N	0.103547	-1.550349	-0.818721
C	1.185818	-2.006876	-1.678869
C	-0.370039	-2.597302	0.109176
H	1.606163	-1.157984	-2.235401
H	0.856508	-2.781528	-2.397315
H	1.989951	-2.432836	-1.064889
H	-0.567564	-3.543967	-0.434492
H	-1.332862	-2.252544	0.521431
C	0.617014	-2.768926	1.266338
H	0.145292	-3.473164	1.987677
H	1.511965	-3.32428	0.890648
O	0.938378	-1.568563	1.835776
N	-1.287789	0.511395	0.3759
Br	2.11624	1.755898	-0.357818
Mn	0.880828	-0.018055	0.71041
H	-0.499039	-0.247405	-2.31654

Pre-2

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-2.675612	1.242948	0.440847
C	-1.395125	0.687519	0.454892
C	-2.172067	-1.241414	-0.554827
C	-3.478059	-0.765655	-0.595705
C	-3.732229	0.505484	-0.085401
H	-2.834223	2.247518	0.839289
H	-1.923747	-2.230592	-0.952921
H	-4.273366	-1.377317	-1.024007
H	-4.741778	0.92179	-0.104555
C	-0.221523	1.407607	1.062439
H	-0.437362	2.494713	1.125609
N	1.021782	1.111862	0.378078
C	2.189949	1.427532	1.181476
C	1.098344	1.597117	-1.008976
H	2.183369	0.806788	2.08911
H	2.244093	2.497574	1.461682
H	3.099096	1.18116	0.616842
H	1.397047	2.665602	-1.046329
H	0.08241	1.530788	-1.432282
C	2.024407	0.693379	-1.83245

H	1.943761	1.036611	-2.889697
H	3.083036	0.934095	-1.553837
O	1.717252	-0.627158	-1.681337
N	-1.15747	-0.539705	-0.041633
Mn	1.035847	-1.170693	0.040774
H	-0.114036	1.051485	2.103146
O	1.226809	-1.807523	1.79777
H	1.964358	-2.347654	2.088243

IM1

Atomic	Coordinates (Angstroms)		
Type	X	Y	Z
C	-1.653685	3.433096	0.385949
C	-1.788435	2.116365	-0.053499
C	0.259583	1.546478	0.871997
C	0.473558	2.843062	1.32474
C	-0.503755	3.805169	1.077457
H	-2.448752	4.154839	0.184872
H	0.982688	0.747341	1.063546
H	1.387358	3.084829	1.869362
H	-0.376941	4.832169	1.427046
C	-2.973233	1.666165	-0.867255
H	-3.83934	2.332736	-0.672818
N	-3.283317	0.263019	-0.66576
C	-4.040256	-0.310305	-1.765409
C	-3.873662	-0.017129	0.652682
H	-4.170996	-1.387366	-1.600516
H	-3.481052	-0.189397	-2.702997
H	-5.043123	0.145682	-1.881285
H	-4.928451	0.329622	0.697518
H	-3.306187	0.577864	1.389254
C	-3.735277	-1.50021	1.009551
H	-4.075185	-1.602838	2.065513
H	-4.497657	-2.073668	0.425658
O	-2.464295	-1.95398	0.80387
N	-0.840848	1.192148	0.19179
Mn	-1.261505	-0.896419	-0.436768
H	-2.72352	1.804916	-1.934418
C	2.254588	-1.180902	-0.691502
C	3.312046	-0.350949	-1.067718
C	4.31236	-0.030381	-0.14209
C	4.242661	-0.549074	1.159245
C	3.185369	-1.372675	1.520423
C	2.178025	-1.705181	0.603425
H	1.451443	-1.400277	-1.411976
H	3.344216	0.040571	-2.085725
H	5.034363	-0.290679	1.865129
H	3.135739	-1.765563	2.54061
C	0.971849	-2.482597	1.032518
H	1.22025	-3.168802	1.861669
H	0.590796	-3.09555	0.19232
O	-0.017772	-1.54537	1.444488
H	-0.891028	-1.979583	1.619489
O	5.37614	0.766025	-0.411204
C	5.490994	1.293874	-1.705243
H	5.569836	0.502757	-2.469765
H	6.407376	1.893683	-1.724248
H	4.637789	1.943012	-1.965711
O	-0.58593	-1.516683	-2.116965
H	-0.714388	-2.440764	-2.348677

IM2

Atomic	Coordinates (Angstroms)		
Type	X	Y	Z
C	-1.325292	3.486268	0.409295
C	-1.447604	2.187356	-0.083204
C	0.628535	1.610087	0.759928
C	0.834895	2.889513	1.267375
C	-0.162025	3.844788	1.087055
H	-2.136457	4.202802	0.261862
H	1.371226	0.818057	0.897023
H	1.75845	3.12103	1.800125
H	-0.04144	4.85715	1.479303
C	-2.640961	1.725592	-0.870552
H	-3.489214	2.426666	-0.728118
N	-3.00288	0.347307	-0.572204
C	-3.861355	-0.211382	-1.609305
C	-3.514033	0.1829	0.790943
H	-4.023178	-1.279067	-1.422084
H	-3.334479	-0.1386	-2.569207
H	-4.84203	0.2993	-1.671736
H	-4.399639	0.828069	0.978016
H	-2.721586	0.524976	1.480294
C	-3.870574	-1.268696	1.093243
H	-4.017598	-1.367459	2.185245
H	-4.847202	-1.508876	0.639819
O	-2.94408	-2.181607	0.588736
N	-0.47919	1.273118	0.090833
Mn	-0.983661	-0.83583	-0.567076
H	-2.378881	1.765642	-1.942544
C	2.009795	-1.484635	-0.462786
C	3.07278	-0.737685	-0.972374
C	4.04135	-0.226019	-0.099281
C	3.927133	-0.476923	1.274544
C	2.854241	-1.217095	1.760948
C	1.869163	-1.73281	0.908298
H	1.263121	-1.862302	-1.173421
H	3.134165	-0.564146	-2.047757
H	4.693258	-0.075221	1.941139
H	2.769459	-1.39128	2.838244
C	0.630412	-2.420121	1.433677
H	0.765269	-2.592163	2.52323
H	0.575168	-3.441097	0.985815
O	-0.507791	-1.67708	1.179243
H	-2.093377	-2.162139	1.112344
O	5.110036	0.512996	-0.491197
C	5.257628	0.77629	-1.860207
H	5.367983	-0.148723	-2.451096
H	6.167919	1.375111	-1.973257
H	4.405782	1.347244	-2.267514
O	-0.892131	-1.045967	-2.455548
H	-0.933491	-1.913516	-2.864686

IM3

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	3.153186	-2.430119	-0.812306
C	2.236317	-1.387396	-0.665731
C	3.172699	-0.781463	1.37275
C	4.105519	-1.81045	1.305607
C	4.098626	-2.642264	0.186922
H	3.116583	-3.067023	-1.699234
H	3.090781	-0.08357	2.215092
H	4.825068	-1.952601	2.113265
H	4.824216	-3.453693	0.093639
C	1.115258	-1.164579	-1.646971
H	1.437758	-1.469421	-2.664824
N	0.585364	0.183101	-1.602065
C	-0.782884	0.276382	-2.086699
C	1.468121	1.155873	-2.259405
H	-1.392121	-0.508705	-1.620599
H	-0.853769	0.169381	-3.187276
H	-1.218104	1.242536	-1.794221
H	1.52667	0.965059	-3.352572
H	2.485386	1.002769	-1.853987
C	1.007638	2.580354	-1.95706
H	1.806744	3.268884	-2.308109
H	0.130763	2.816916	-2.603188
O	0.71661	2.737849	-0.622512
N	2.271162	-0.577355	0.401742
Mn	0.914002	1.195089	0.595272
H	0.300345	-1.859177	-1.37485
C	-1.514902	-0.028232	1.512792
C	-1.79947	-1.368712	1.25655
C	-2.872232	-1.714392	0.426342
C	-3.654175	-0.699642	-0.145529
C	-3.33688	0.635312	0.097119
C	-2.269692	0.999399	0.9237
H	-0.698451	0.226223	2.204892
H	-1.210738	-2.16969	1.709994
H	-4.500965	-0.942631	-0.789615
H	-3.925898	1.42455	-0.378528
C	-1.95828	2.462531	1.149395
H	-1.028576	2.53907	1.754369
O	-1.888869	3.203022	-0.033819
H	-0.948718	3.164586	-0.338087
O	-3.081104	-3.040915	0.22896
C	-4.170241	-3.424663	-0.566174
H	-5.130314	-3.074046	-0.151483
H	-4.177684	-4.519731	-0.589591
H	-4.082512	-3.05027	-1.600702
H	-2.751173	2.904838	1.780736
O	1.298469	1.262109	2.479145
H	1.176489	2.064134	2.993316

IM4

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-2.459244	0.421585	1.380226
C	-1.232415	-0.011548	0.876786
C	-2.173468	-0.416952	-1.199109
C	-3.431864	-0.004363	-0.772619
C	-3.574743	0.417598	0.546622
H	-2.53035	0.763851	2.414896
H	-2.006834	-0.749973	-2.228618
H	-4.276052	-0.010166	-1.463357
H	-4.54434	0.753936	0.920543
C	0.02412	-0.051705	1.698077
H	-0.1069	0.519686	2.638428
N	1.167951	0.416645	0.912526
C	2.43147	0.060151	1.549219
C	1.097718	1.852932	0.596436
H	3.268764	0.411173	0.929556
H	2.485631	-1.035226	1.622607
H	2.537718	0.516239	2.552512
H	1.594637	2.442052	1.392979
H	0.0407	2.162092	0.590218
C	1.669855	2.183571	-0.770127
H	1.821116	3.276152	-0.828565
H	2.676411	1.731552	-0.875039
O	0.810319	1.784029	-1.795659
N	-1.10836	-0.429442	-0.395733
Mn	0.987014	-1.09803	-0.857261
H	0.23175	-1.106955	1.952422
H	1.674121	-0.62309	-2.372348
H	1.148499	0.940436	-2.178265
O	1.090326	-2.512901	0.423135
H	1.578905	-3.328062	0.293126

IM5

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	1.317151	2.525074	-0.729255
C	0.279968	1.596862	-0.616714
C	-0.191361	2.308628	1.536433
C	0.832936	3.247962	1.509269
C	1.597116	3.359648	0.347411
H	1.907909	2.571199	-1.647506
H	-0.812622	2.143579	2.423428
H	1.028107	3.875495	2.380214
H	2.410609	4.085969	0.28533
C	0.017205	0.570659	-1.685706
H	0.241326	0.998152	-2.686041
N	-1.313754	0.001008	-1.604631
C	-1.408487	-1.305494	-2.232479
C	-2.345255	0.933247	-2.096558
H	-0.624779	-1.965158	-1.835276
H	-1.300661	-1.259065	-3.334453
H	-2.380314	-1.761207	-2.000259
H	-2.302843	1.006606	-3.204934
H	-2.093686	1.930004	-1.695101
C	-3.730308	0.541351	-1.583726
H	-4.425567	1.350773	-1.909112
H	-4.076704	-0.354979	-2.159635
O	-3.729561	0.345378	-0.236977
N	-0.46563	1.515822	0.494357
Mn	-2.063035	-0.066657	0.663461
H	0.752759	-0.241481	-1.535488
C	1.783241	-2.56519	-0.434277

C	2.914338	-1.779281	-0.672349
C	3.134133	-0.637579	0.107558
C	2.22589	-0.314097	1.125385
C	1.105757	-1.102364	1.347919
C	0.86256	-2.243431	0.564859
H	1.612953	-3.448716	-1.058486
H	3.605075	-2.059107	-1.469116
H	2.412802	0.582726	1.721649
H	0.389761	-0.815956	2.129326
C	-0.36096	-3.086448	0.811102
H	-0.18959	-3.752812	1.678582
H	-0.527807	-3.75716	-0.048069
O	-1.536831	-2.339654	1.007545
H	-1.551121	-1.899121	1.910937
O	4.177824	0.213198	-0.058442
C	5.105126	-0.074609	-1.069594
H	5.600703	-1.047685	-0.91403
H	5.865031	0.713661	-1.040405
H	4.6386	-0.079312	-2.070179
O	-1.732255	-0.387339	2.614071
H	-2.41608	-0.270097	3.278764

IM6

Atomic	Coordinates (Angstroms)		
Type	X	Y	Z
C	0.987707	2.730158	-0.759591
C	0.134764	1.629664	-0.65783
C	-0.644213	2.365129	1.395745
C	0.184865	3.480263	1.372921
C	1.01731	3.665235	0.269505
H	1.627204	2.838613	-1.638658
H	-1.311568	2.16048	2.238893
H	0.174845	4.188188	2.202974
H	1.682254	4.529799	0.211728
C	0.134269	0.538882	-1.693897
H	0.417565	0.958688	-2.682077
N	-1.116393	-0.195198	-1.731857
C	-0.98287	-1.505826	-2.344568
C	-2.226608	0.586036	-2.308023
H	-0.172502	-2.064812	-1.855519
H	-0.764329	-1.449886	-3.429278
H	-1.913515	-2.074639	-2.213262
H	-2.138198	0.629983	-3.414718
H	-2.12266	1.618038	-1.932244
C	-3.578268	0.036905	-1.844432
H	-4.350935	0.740756	-2.234258
H	-3.778893	-0.913729	-2.403201
O	-3.625762	-0.113702	-0.492705
N	-0.669804	1.462483	0.40613
Mn	-1.948755	-0.387946	0.457501
H	0.940397	-0.169726	-1.424043
C	1.918824	-2.465716	-0.108492
C	3.054776	-1.715876	-0.430441
C	3.277411	-0.490995	0.210448
C	2.365904	-0.04794	1.179465
C	1.24492	-0.808865	1.480405
C	0.989835	-2.03079	0.839296
H	1.748851	-3.416673	-0.625351
H	3.749931	-2.088164	-1.184825
H	2.557695	0.907207	1.67483
H	0.525967	-0.449547	2.223504
C	-0.267258	-2.809	1.175475
H	-0.032583	-3.476632	2.03738
H	-0.45806	-3.51782	0.333608
O	-1.345382	-2.010966	1.453673
H	-1.950537	-0.958297	2.710656
O	4.329372	0.329288	-0.046477
C	5.276477	-0.096719	-0.987042
H	5.754494	-1.04686	-0.693876
H	6.046391	0.680693	-1.040846
H	4.836258	-0.227187	-1.991027
O	-2.345886	-0.048233	2.743515
H	-3.271631	-0.185181	2.974463

IM7

Atomic	Coordinates (Angstroms)		
Type	X	Y	Z
C	-1.401587	-2.540793	-0.217488
C	-0.257297	-1.740164	-0.220213
C	-0.674528	-1.055362	1.955114
C	-1.825203	-1.82891	2.035588
C	-2.191793	-2.588796	0.924537
H	-1.669694	-3.107881	-1.11198
H	-0.344309	-0.404752	2.772574
H	-2.422652	-1.830852	2.949076
H	-3.093572	-3.2055	0.944045
C	0.592034	-1.595849	-1.455143
H	0.682223	-2.577389	-1.964932
N	1.885556	-0.992889	-1.190248
C	2.428096	-0.287021	-2.340161
C	2.837804	-1.983295	-0.651511
H	1.695778	0.444273	-2.708999
H	2.693166	-0.964609	-3.175263
H	3.33166	0.262594	-2.044495
H	3.11797	-2.715879	-1.438481
H	2.302468	-2.543177	0.135558
C	4.050396	-1.295179	-0.030458
H	4.638672	-2.089048	0.484887
H	4.724618	-0.952529	-0.854181
O	3.673051	-0.280849	0.798376
N	0.095601	-1.026174	0.859114
Mn	1.848395	0.349396	0.802938
H	0.037773	-0.948725	-2.154701
C	-1.047372	1.418756	-1.884191
C	-2.186027	0.623106	-1.905565
C	-2.968662	0.490192	-0.749783
C	-2.602442	1.183154	0.40819
C	-1.451523	1.972405	0.412236
C	-0.646669	2.092476	-0.720756
H	-0.460441	1.5318	-2.803367
H	-2.502628	0.09991	-2.811134
H	-3.202947	1.110301	1.316701
H	-1.151779	2.495695	1.321973
C	0.606212	2.943783	-0.692115
H	1.489717	2.263489	-0.860605

O	0.755572	3.716147	0.437027
H	0.919498	3.075803	1.181356
O	-4.054608	-0.32171	-0.846504
C	-4.947981	-0.346612	0.233759
H	-4.48168	-0.739948	1.15417
H	-5.774684	-1.007384	-0.050025
H	-5.353348	0.654894	0.45591
H	0.614773	3.603272	-1.579467
O	1.182066	1.668181	2.074459
H	1.802044	1.918705	2.766765

IM8

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	2.699653	-1.415115	-0.17367
C	1.417441	-0.980314	0.16295
C	2.081395	1.234811	0.037785
C	3.385699	0.880344	-0.288872
C	3.700328	-0.472947	-0.394009
H	2.902823	-2.484667	-0.263682
H	1.766026	2.279918	0.106329
H	4.134914	1.653334	-0.466038
H	4.711658	-0.791738	-0.655936
C	0.303923	-1.94569	0.467346
H	0.501508	-2.918291	-0.030814
N	-0.99935	-1.396478	0.146335
C	-2.081464	-2.107544	0.804508
C	-1.22322	-1.231021	-1.298194
H	-1.927176	-2.10147	1.892233
H	-2.172402	-3.157802	0.463652
H	-3.034289	-1.600368	0.605086
H	-1.464733	-2.204318	-1.776053
H	-0.273025	-0.883201	-1.736473
C	-2.293232	-0.169431	-1.558324
H	-2.320143	-0.004452	-2.659178
H	-3.294356	-0.609482	-1.326711
O	-2.043933	0.969956	-0.849298
N	1.122701	0.327884	0.266969
Mn	-0.98641	0.864687	0.871811
H	0.321357	-2.156113	1.552578
H	-1.385137	1.051215	2.519962
H	-1.077525	3.598404	0.119918

TS1

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-1.616644	3.459707	0.353532
C	-1.700235	2.145921	-0.106441
C	0.385176	1.646871	0.772363
C	0.550796	2.94341	1.24804
C	-0.46956	3.866771	1.030754
H	-2.44695	4.149158	0.184732
H	1.138913	0.871237	0.942869
H	1.459696	3.2139	1.787318
H	-0.380235	4.891702	1.397828
C	-2.885023	1.629608	-0.878098
H	-3.771804	2.268935	-0.687707
N	-3.134078	0.222686	-0.612111
C	-3.921022	-0.415862	-1.655297
C	-3.630296	-0.027977	0.74552
H	-3.972916	-1.495628	-1.467869
H	-3.412522	-0.28544	-2.619429
H	-4.952091	-0.017391	-1.722492
H	-4.648922	0.391216	0.891013
H	-2.961712	0.513725	1.437781
C	-3.601219	-1.520986	1.077501
H	-3.768671	-1.622361	2.169314
H	-4.477803	-2.012916	0.608068
O	-2.434925	-2.131586	0.652743
N	-0.70612	1.265581	0.097855
Mn	-1.060247	-0.848279	-0.543212
H	-2.664251	1.727968	-1.955817
C	2.113662	-1.356924	-0.483273
C	3.166126	-0.594112	-0.991255
C	4.149743	-0.101809	-0.124382
C	4.061856	-0.382507	1.245897
C	3.002242	-1.138312	1.734227
C	2.008138	-1.640461	0.88377
H	1.346529	-1.709336	-1.18669
H	3.207034	-0.393604	-2.062939
H	4.839499	0.005791	1.906798
H	2.938929	-1.340543	2.807931
C	0.787728	-2.337859	1.420872
H	0.985939	-2.6799	2.456196
H	0.592753	-3.258276	0.827108
O	-0.305533	-1.463233	1.380827
H	-1.421587	-1.942744	1.284647
O	5.210774	0.646507	-0.518261
C	5.336323	0.938938	-1.883647
H	5.434909	0.026656	-2.495903
H	6.245792	1.538659	-1.998611
H	4.479202	1.519966	-2.264623
O	-0.715363	-1.307082	-2.360764
H	-0.868535	-2.215026	-2.63628

TS1（Quartet）

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	2.087261	3.166327	0.341203
C	1.881357	1.802534	0.250442
C	-0.319736	2.16024	-0.50188
C	-0.162467	3.528069	-0.414405
C	1.054686	4.066065	0.034151
H	3.073998	3.527538	0.643221
H	-1.241965	1.704862	-0.871055
H	-0.991512	4.175083	-0.707866
H	1.205394	5.143575	0.111153
C	2.943867	0.779352	0.543433
H	2.794371	0.360781	1.552377
N	2.827862	-0.340349	-0.396184
C	3.194935	0.020527	-1.755146
C	3.36529	-1.62862	0.036392

H	2.925448	-0.785969	-2.448763
H	2.630206	0.907648	-2.071232
H	4.277713	0.230911	-1.851947
H	4.419082	-1.771096	-0.276383
H	3.350257	-1.645665	1.137042
C	2.491697	-2.764398	-0.486933
H	2.887805	-3.729721	-0.121692
H	2.541275	-2.811141	-1.590726
O	1.146973	-2.603814	-0.102349
N	0.664371	1.285655	-0.140211
Mn	0.549467	-0.640538	-0.303291
H	3.94511	1.253766	0.523357
C	-1.846757	-1.55284	0.714946
C	-2.916824	-1.256064	-0.132766
C	-3.630174	-0.066056	0.045166
C	-3.270891	0.805959	1.08463
C	-2.19595	0.503269	1.908715
C	-1.460701	-0.677344	1.742292
H	-1.309454	-2.497449	0.57552
H	-3.174198	-1.950556	-0.93327
H	-3.83648	1.732056	1.203336
H	-1.901498	1.211896	2.688464
C	-0.21834	-0.975062	2.539161
H	-0.019678	-0.140777	3.236372
H	-0.361423	-1.875448	3.168079
O	0.891885	-1.157263	1.693303
H	1.043787	-2.182533	1.012178
O	-4.665139	0.326627	-0.733829
C	-5.006736	-0.481753	-1.828884
H	-5.345416	-1.483361	-1.514229
H	-5.830606	0.018787	-2.348531
H	-4.163319	-0.600391	-2.529598
O	0.012071	-0.621007	-2.060615
H	-0.130632	-1.534066	-2.343952

TS1（Doublet）

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-2.152205	3.17864	-0.211296
C	-1.884199	1.822407	-0.179502
C	0.375529	2.221951	0.254794
C	0.171643	3.590264	0.21423
C	-1.108435	4.098645	-0.035926
H	-3.179378	3.515369	-0.372853
H	1.350577	1.790069	0.489536
H	1.016091	4.257972	0.397012
H	-1.295298	5.172917	-0.068383
C	-2.903121	0.742716	-0.370438
H	-2.851264	0.351317	-1.399806
N	-2.559946	-0.388056	0.522851
C	-2.813762	-0.042414	1.925044
C	-3.188809	-1.67385	0.152703
H	-2.475381	-0.854206	2.576467
H	-2.235708	0.847384	2.199023
H	-3.890491	0.143875	2.08632
H	-4.203085	-1.75624	0.585484
H	-3.29376	-1.683727	-0.942625
C	-2.281923	-2.818715	0.582582
H	-2.734459	-3.773425	0.24793
H	-2.25098	-2.877327	1.689844
O	-0.993771	-2.646453	0.08115
N	-0.621212	1.326824	0.026883
Mn	-0.544993	-0.585681	0.158356
H	-3.93128	1.108289	-0.193358
C	1.664443	-1.557458	-0.646435
C	2.716811	-1.231982	0.221923
C	3.480002	-0.087556	-0.003606
C	3.212009	0.716029	-1.127052
C	2.14688	0.411541	-1.958332
C	1.345093	-0.718902	-1.731918
H	1.145227	-2.508685	-0.507797
H	2.917531	-1.879668	1.075737
H	3.82935	1.601374	-1.29084
H	1.914538	1.071201	-2.799608
C	0.148505	-1.041696	-2.588367
H	-0.031611	-0.218625	-3.301645
H	0.327027	-1.949187	-3.197413
O	-0.997214	-1.217813	-1.783815
H	-1.015305	-2.171897	-1.096716
O	4.48762	0.329212	0.798098
C	4.707851	-0.380114	1.989755
H	5.034453	-1.416506	1.79999
H	5.503908	0.144055	2.529107
H	3.803116	-0.405993	2.62006
O	0.056916	-0.512966	1.899846
H	0.192816	-1.430566	2.176295

TS2

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-4.063285	1.949844	-0.964439
C	-3.117956	0.970131	-0.65076
C	-2.598949	2.04321	1.33363
C	-3.521203	3.05471	1.095648
C	-4.266364	3.005539	-0.082602
H	-4.631425	1.875364	-1.894571
H	-1.973162	2.038691	2.231913
H	-3.651875	3.860867	1.818948
H	-5.000992	3.781581	-0.309185
C	-2.811303	-0.165309	-1.586943
H	-3.712997	-0.417406	-2.183376
N	-2.265052	-1.316102	-0.889165
C	-1.524201	-2.204699	-1.774154
C	-3.298372	-2.008584	-0.114622
H	-0.756237	-1.623461	-2.30054
H	-2.178627	-2.701097	-2.517741
H	-0.994959	-2.960246	-1.180537
H	-3.959843	-2.600893	-0.782409
H	-3.932988	-1.241139	0.358078
C	-2.732599	-2.889001	0.980194
H	-3.578656	-3.380211	1.493561

H	-2.125952	-3.70174	0.541708
O	-1.976798	-2.145129	1.898252
N	-2.406687	1.025255	0.486973
Mn	-0.662879	-0.389568	0.635758
H	-2.049018	0.192845	-2.298003
C	2.700879	-0.468155	-0.745605
C	4.019001	-0.858924	-0.592137
C	4.979658	0.056797	-0.129757
C	4.596785	1.369404	0.181974
C	3.265777	1.746236	0.030128
C	2.302125	0.844378	-0.431256
H	1.941398	-1.179363	-1.081575
H	4.345824	-1.874403	-0.824799
H	5.326611	2.095726	0.54179
H	2.962867	2.76714	0.282314
C	0.905146	1.257044	-0.613558
H	0.702369	2.334312	-0.418532
H	0.335831	0.971265	1.290415
O	0.076105	0.559555	-1.25066
H	-1.017712	-2.388327	1.735375
O	6.243127	-0.412688	-0.016552
C	7.236904	0.462139	0.447153
H	8.1741	-0.10406	0.468216
H	7.021832	0.829145	1.464715
H	7.364159	1.332517	-0.218277
O	0.28687	-2.123942	0.783288
H	1.196919	-2.142914	1.091911

TS3

Atomic	Coordinates (Angstroms)		
Type	X	Y	Z
C	-4.240807	-2.358495	0.56796
C	-3.118692	-1.553404	0.375368
C	-4.088797	-0.531337	-1.471668
C	-5.236435	-1.310395	-1.351771
C	-5.312481	-2.237834	-0.314619
H	-4.268654	-3.068659	1.397823
H	-3.935726	0.248046	-2.231486
H	-6.05906	-1.18383	-2.057522
H	-6.202673	-2.858339	-0.186904
C	-1.884164	-1.656643	1.228427
H	-2.127989	-2.126714	2.204274
N	-1.210901	-0.376789	1.372769
C	0.183734	-0.524654	1.76406
C	-1.956941	0.533582	2.238285
H	0.695132	-1.188559	1.054675
H	0.29613	-0.942281	2.784796
H	0.698715	0.444228	1.714263
H	-1.990268	0.171429	3.288575
H	-3.001467	0.550837	1.881061
C	-1.392022	1.938787	2.202242
H	-2.077173	2.611307	2.746826
H	-0.423685	1.984853	2.727635
O	-1.234298	2.369038	0.868365
N	-3.057422	-0.661662	-0.624504
Mn	-1.38176	0.841383	-0.780732
H	-1.180619	-2.346601	0.730637
C	3.219585	0.361993	-1.684181
C	4.290233	-0.512166	-1.728396
C	4.978326	-0.841406	-0.54742
C	4.576697	-0.276303	0.669084
C	3.495066	0.603454	0.694941
C	2.796384	0.929949	-0.470772
H	2.676105	0.605806	-2.602178
H	4.624389	-0.963301	-2.664564
H	5.107792	-0.50581	1.594198
H	3.182591	1.069924	1.632959
C	1.676715	1.892334	-0.422906
H	0.387955	0.661654	-0.954044
O	1.325565	2.4355	0.647917
H	-0.276138	2.641168	0.755572
O	6.013132	-1.704835	-0.683282
C	6.735993	-2.054223	0.46592
H	7.213398	-1.178284	0.936818
H	7.518252	-2.752829	0.150191
H	6.101194	-2.550814	1.21934
H	1.436597	2.363128	-1.401756
O	-2.387098	1.624659	-2.204941
H	-2.045312	2.333893	-2.752539

TS4

Atomic	Coordinates (Angstroms)		
Type	X	Y	Z
C	-2.574895	1.300615	0.424269
C	-1.324613	0.682205	0.482051
C	-2.190745	-1.253033	-0.44254
C	-3.470254	-0.712597	-0.524174
C	-3.663022	0.59196	-0.077565
H	-2.684796	2.331608	0.767425
H	-1.988915	-2.269994	-0.793597
H	-4.291236	-1.301524	-0.935433
H	-4.649405	1.058205	-0.130131
C	-0.11318	1.372124	1.043332
H	-0.308733	2.458232	1.151473
N	1.088116	1.090418	0.265317
C	2.291129	1.473154	0.990367
C	1.06866	1.576494	-1.121557
H	3.17757	1.243755	0.382943
H	2.34294	0.879112	1.913578
H	2.314346	2.554289	1.228793
H	1.493187	2.597679	-1.193887
H	0.019725	1.639601	-1.452405
C	1.786517	0.58103	-2.024915
H	1.819592	0.99526	-3.054071
H	2.855491	0.515471	-1.706146
O	1.14954	-0.64403	-1.972208
N	-1.150511	-0.580983	0.053711
Mn	1.02031	-1.219498	0.22236
H	0.070961	0.956093	2.050611
H	2.236492	-2.258136	-0.880739
H	1.870578	-1.586926	-1.531067
O	1.116686	-1.202844	2.12721
H	1.663819	-1.78804	2.654843

TS5

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-1.270194	-2.576705	-0.638017
C	-0.263712	-1.611244	-0.57013
C	0.260484	-2.239669	1.596757
C	-0.731261	-3.213343	1.612969
C	-1.508407	-3.385824	0.467404
H	-1.868437	-2.673278	-1.547299
H	0.890036	-2.035803	2.469301
H	-0.890409	-3.821288	2.504795
H	-2.297027	-4.141036	0.439168
C	-0.048365	-0.619825	-1.681576
H	-0.294069	-1.087264	-2.658482
N	1.274764	-0.027262	-1.658273
C	1.333723	1.260144	-2.329327
C	2.316803	-0.95776	-2.130827
H	0.547586	1.919755	-1.936531
H	1.205175	1.177075	-3.42668
H	2.302174	1.739491	-2.132155
H	2.273067	-1.059611	-3.236612
H	2.080337	-1.947284	-1.703392
C	3.698218	-0.534511	-1.630857
H	4.404834	-1.338851	-1.942776
H	4.028373	0.356122	-2.224683
O	3.700275	-0.314424	-0.287043
N	0.491985	-1.466326	0.529219
Mn	2.033523	0.166315	0.576792
H	-0.791769	0.186636	-1.538861
C	-1.747138	2.527017	-0.424509
C	-2.888114	1.762234	-0.688215
C	-3.153025	0.630095	0.091299
C	-2.283131	0.298634	1.139677
C	-1.154587	1.067563	1.383744
C	-0.858094	2.194894	0.59974
H	-1.54185	3.402872	-1.049273
H	-3.551207	2.049816	-1.505663
H	-2.50691	-0.586884	1.740175
H	-0.47071	0.780098	2.190102
C	0.393667	2.993752	0.873856
H	0.20921	3.662939	1.740594
H	0.575704	3.675931	0.020406
O	1.521335	2.211241	1.100947
H	1.591033	1.588361	2.095922
O	-4.206231	-0.204511	-0.101783
C	-5.097346	0.095226	-1.141129
H	-5.579697	1.077882	-1.004935
H	-5.872104	-0.679045	-1.131839
H	-4.601215	0.087107	-2.127469
O	1.786909	0.472171	2.66293
H	2.537134	0.503612	3.264187

TS5（Quartet）

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-0.218714	2.492304	-1.596717
C	0.28965	1.320523	-1.072487
C	1.494296	2.496525	0.541057
C	0.998825	3.703114	0.083022
C	0.128115	3.727099	-1.017733
H	-0.910106	2.441007	-2.442299
H	2.186907	2.448763	1.387654
H	1.299673	4.62699	0.581876
H	-0.268128	4.665055	-1.408854
C	-0.143461	-0.04013	-1.520172
H	-0.499374	-0.03536	-2.567567
N	0.943028	-1.014285	-1.338172
C	0.449358	-2.387513	-1.29711
C	2.014814	-0.822858	-2.345216
H	-0.29219	-2.480369	-0.492179
H	-0.020646	-2.683736	-2.252443
H	1.277143	-3.076575	-1.085694
H	1.677389	-1.168814	-3.342611
H	2.183706	0.263775	-2.413054
C	3.27256	-1.511551	-1.853011
H	4.13301	-1.145059	-2.449806
H	3.215947	-2.60305	-2.071917
O	3.432256	-1.268572	-0.503299
N	1.166534	1.29622	-0.02096
Mn	2.000742	-0.561145	0.462178
H	-0.989294	-0.376389	-0.894264
C	-2.048329	-1.346238	1.40791
C	-3.181123	-1.363978	0.593813
C	-3.692726	-0.157222	0.095304
C	-3.058001	1.047532	0.425666
C	-1.93121	1.042449	1.238558
C	-1.400848	-0.152432	1.741579
H	-1.645093	-2.289369	1.788798
H	-3.660316	-2.315614	0.357875
H	-3.461668	1.977782	0.020605
H	-1.430615	1.989576	1.46484
C	-0.163618	-0.176536	2.592835
H	0.226806	0.859081	2.690443
H	-0.432476	-0.492163	3.622337
O	0.803355	-1.053509	2.085615
H	1.981345	-0.796062	2.501999
O	-4.783062	-0.064169	-0.705762
C	-5.451299	-1.247243	-1.049158
H	-5.841801	-1.775565	-0.162946
H	-6.294697	-0.96339	-1.687755
H	-4.802982	-1.942674	-1.609627
O	3.007379	-0.346256	2.171418
H	3.752805	-0.955783	2.231458

TS5（Doublet）

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	0.00865	2.215719	1.862682
C	-0.386549	1.067937	1.200998
C	-1.753726	2.31336	-0.239602
C	-1.374321	3.491593	0.375972
C	-0.47821	3.464765	1.453711
H	0.71669	2.130218	2.691246
H	-2.452655	2.283045	-1.079578

H	-1.784849	4.434886	0.009836
H	-0.172559	4.381227	1.96006
C	0.134752	-0.300892	1.486958
H	0.472771	-0.406922	2.53495
N	-0.900457	-1.291855	1.142432
C	-0.331359	-2.609096	0.883612
C	-1.973088	-1.332449	2.165412
H	0.373216	-2.542408	0.043327
H	0.2029	-3.011327	1.764176
H	-1.129149	-3.312101	0.611101
H	-1.643626	-1.906335	3.0539
H	-2.139109	-0.291607	2.487404
C	-3.240678	-1.863285	1.525551
H	-4.084082	-1.709932	2.230356
H	-3.167743	-2.968863	1.403887
O	-3.442469	-1.22165	0.320685
N	-1.279894	1.094796	0.156541
Mn	-1.946207	-0.54557	-0.526992
H	1.010731	-0.508614	0.847915
C	2.146706	-1.000633	-1.554671
C	3.281625	-1.126101	-0.752937
C	3.762047	-0.008552	-0.055777
C	3.094319	1.217651	-0.177348
C	1.966222	1.320613	-0.981368
C	1.467782	0.215001	-1.682114
H	1.769494	-1.875793	-2.092034
H	3.786408	-2.090784	-0.680156
H	3.476828	2.076072	0.378575
H	1.441102	2.278917	-1.047183
C	0.232252	0.309049	-2.526026
H	-0.204207	1.323167	-2.4287
H	0.50053	0.192705	-3.595117
O	-0.705934	-0.683826	-2.185774
H	-1.765609	-0.36253	-2.542469
O	4.851426	-0.023039	0.750107
C	5.555515	-1.227827	0.886096
H	5.955533	-1.585079	-0.077774
H	6.394148	-1.03199	1.562735
H	4.930807	-2.026754	1.320931
O	-2.901078	0.073788	-2.154609
H	-3.657145	-0.493842	-2.345551

TS6

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-4.177762	1.870891	-1.024139
C	-3.204408	0.931447	-0.673643
C	-2.626581	2.164863	1.196704
C	-3.56515	3.150132	0.911309
C	-4.357219	2.994684	-0.225227
H	-4.783702	1.714296	-1.91955
H	-1.974723	2.233865	2.074391
H	-3.673635	4.014862	1.567597
H	-5.110984	3.741806	-0.484075
C	-2.914239	-0.260559	-1.542735
H	-3.831945	-0.552773	-2.095769
N	-2.328362	-1.364546	-0.809213
C	-1.634237	-2.297263	-1.681883
C	-3.276934	-2.020258	0.101519
H	-0.86388	-1.759194	-2.249744
H	-2.31877	-2.80638	-2.388953
H	-1.124653	-3.062213	-1.083148
H	-3.997199	-2.652973	-0.460113
H	-3.863036	-1.222548	0.588582
C	-2.535883	-2.811051	1.178934
H	-3.302707	-3.15569	1.909426
H	-2.156483	-3.757875	0.71936
O	-1.538317	-2.072429	1.759597
N	-2.453618	1.085675	0.427742
Mn	-0.805843	-0.46795	0.753967
H	-2.180673	0.064432	-2.299765
C	2.75434	-0.391158	-0.955572
C	4.103377	-0.695631	-0.881194
C	4.989949	0.179679	-0.23316
C	4.50345	1.364871	0.338161
C	3.144317	1.65325	0.258578
C	2.252222	0.786538	-0.378291
H	2.054114	-1.066365	-1.452289
H	4.509773	-1.607169	-1.323914
H	5.17545	2.059773	0.843462
H	2.760211	2.570901	0.715037
C	0.815541	1.113966	-0.485257
H	0.567308	2.168801	-0.222646
H	0.37087	0.768061	1.348606
O	0.026565	0.431638	-1.182527
H	0.078741	-2.525187	1.253424
O	6.289055	-0.196685	-0.209494
C	7.21253	0.646108	0.426929
H	8.193112	0.166336	0.339592
H	6.979168	0.782136	1.496263
H	7.261416	1.639842	-0.049025
O	0.77296	-2.210656	0.615062
H	1.550185	-2.003893	1.147053

TS7

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-0.987335	2.822581	-0.131647
C	-0.009103	1.852192	0.084252
C	-0.711385	0.659521	-1.771179
C	-1.710285	1.585514	-2.054095
C	-1.856057	2.683231	-1.210014
H	-1.060231	3.677706	0.544031
H	-0.552826	-0.227407	-2.39275
H	-2.358164	1.442772	-2.920985
H	-2.632654	3.429804	-1.393143
C	0.931051	1.929125	1.257231
H	1.074765	2.990274	1.551975
N	2.180053	1.236501	1.012284
C	2.880161	0.888949	2.235566
C	3.045803	1.926501	0.039624
H	2.230009	0.283021	2.88217
H	3.216229	1.778499	2.804256
H	3.762743	0.281184	1.997345
H	3.562355	2.786932	0.516369

H	2.387355	2.336937	-0.744283
C	4.019205	0.944379	-0.617212
H	4.563384	1.521637	-1.400998
H	4.816519	0.689306	0.127354
O	3.374371	-0.147671	-1.111916
N	0.113489	0.784428	-0.724924
Mn	1.7201	-0.721089	-0.257929
H	0.435237	1.44555	2.118939
C	-1.047938	-1.151673	1.835366
C	-2.065747	-0.214599	1.822538
C	-2.998468	-0.201046	0.769047
C	-2.90405	-1.156272	-0.247284
C	-1.86208	-2.085521	-0.225302
C	-0.912506	-2.089984	0.797768
H	-0.313639	-1.153573	2.648969
H	-2.172495	0.53	2.615236
H	-3.627854	-1.177214	-1.063933
H	-1.772633	-2.834444	-1.016753
C	0.164359	-3.128436	0.795285
H	1.553227	-1.96531	0.996051
O	0.347327	-3.865654	-0.188216
H	0.706462	-2.851602	-1.463457
O	-3.943485	0.769839	0.824279
C	-4.928801	0.783369	-0.17332
H	-4.498182	0.933853	-1.178859
H	-5.599499	1.619832	0.051564
H	-5.516873	-0.149583	-0.185019
H	0.48722	-3.45283	1.809758
O	0.996475	-2.016765	-1.931419
H	1.77383	-2.259609	-2.448708

TS8

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	2.618751	-1.516317	0.181156
C	1.364564	-0.939276	0.385179
C	2.12862	1.105679	-0.390229
C	3.406716	0.607508	-0.615128
C	3.653741	-0.732588	-0.321384
H	2.774368	-2.572218	0.413787
H	1.870324	2.148303	-0.607196
H	4.187177	1.25554	-1.016318
H	4.642218	-1.165526	-0.489659
C	0.211627	-1.704797	0.977609
H	0.370185	-2.794463	0.836421
N	-1.066507	-1.248125	0.46594
C	-2.178485	-1.626899	1.321039
C	-1.284046	-1.631756	-0.941328
H	-2.024854	-1.237352	2.336509
H	-2.31689	-2.72452	1.378562
H	-3.107536	-1.186366	0.93677
H	-1.575984	-2.701118	-1.013814
H	-0.315621	-1.52413	-1.459151
C	-2.287925	-0.693773	-1.611413
H	-2.328891	-0.990409	-2.684875
H	-3.310836	-0.937918	-1.226766
O	-1.944225	0.612475	-1.436926
N	1.1354	0.353434	0.097412
Mn	-0.982874	1.126337	0.152847
H	0.21989	-1.540766	2.070328
H	-1.662113	1.681762	1.90393
H	0.470343	3.177186	1.181871
O	-0.367756	3.08089	0.714319
H	-1.107704	2.4628	1.542798