Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.
This journal is © the Owner Societies 2016

How does Ammonia Bind to the Oxygen-Evolving Complex in the S_2 state of Photosynthetic Water Oxidation? Theoretical Support and Implications for the W1 Substitution Mechanism

Yu Guo, Lan-Lan He, Dong-Xia Zhao*, Li-Dong Gong, Cui Liu, Zhong-Zhi Yang*

School of Chemistry and Chemical Engineering, Liaoning Normal University, Dalian 116029, People's Republic of China

*Corresponding author: Tel: (86) 411-82159607 Fax: (86) 411-82158977

E-mail: zzyang@lnnu.edu.cn; zhaodxchem@lnnu.edu.cn

Supplementary Information

Contents: Presentations of complementary specification, computed Gibbs free energies, Mulliken spin populations and free energy profiles for all spin states with representative structures shown in 3D image and optimized Cartesian coordinates. Movies for representative reaction paths uploaded

by movies.rar.

I. Additional remarks for computational details……....S3

II. Definition of spin topologies in the S_2 state and the relevance to PES crossing……..S5

III. O5 substitution scheme

a. Closed-cubane structure as reactant S7

b. Open-cubane structure as reactant.....S31

IV. W1 substitution scheme

a. Open-cubane structure as reactant…….....S66

b. Closed-cubane structure as reactant.. .....S79

c. Wx binding to (or disassociating from) Mn4 .....S97

V. Mn4 addition scheme

a. NH_3 binding to Mn4 of the closed-cubane structure as an additional ligand……..……...S103

b. Models for Figure 4 of ref. [19]…….……....S137

VI. Ammonia departure time analysis

a. NH_3 hydrolysis in the S_3 state…….…….. S145

b. NH_3 hydrolysis in the S_4, S’ 4 or S' 0

state……....S149

c. NH_3 hydrolysis in the S_0 state……..……S150

VII. Implications for O-O bond formation……...S182

VIII. Notes and references…….....S184

I. Additional remarks for computational details

Model construnction

We retained Mn_4CaO_5 cluster with its four terminal water ligands coordinated to Ca and Mn, keeping their original protonation conditions for the S_2 state.[1] All the first-sphere amino acid ligands including D1-Asp170, D1-Glu189, D1-His332, D1-Glu333, D1-Asp342, D1-Ala344, and CP43-Glu354 were preserved after being conventionally cut off from their alpha-carbon atoms and capped with methyl groups, with an exception that the peptide bond was saved between the adjacent His332 and Glu333 ligands. All the second-sphere ligands and vicinal water molecules were deleted for hardly any impacts on electronic or geometric properties considered here. NH_3 was manually added to suitable locations in a variety of situations. There are over 100 atoms and this size is sufficient for characterization of metal-ligand interactions and electronic effects involved in our subject.

Oxidation state scheme

The high-oxidation scheme[2] was adopted in this paper because it is better acknowledged over the low-oxidation scheme[3] for the comprehensive advisement on the geometric, energetic, electronic and spectroscopic properties and coherence with experimental observables.

Approximation treatment

It is worth mentioning that groups including Asp61, Ser169 and HOH559 which lie in the hydrogen bond interaction region with W1 were excluded in our models as a result of the severe interference against Mn4-ligand binding and dissociation courses in practice during TS searching in our preceding attempts. Superficially, this led to some omission in the vicinity of the active region. However, this is a rational approximate treatment, because barriers related to NH_3 attacking processes must be dominated by metal-ligand chemical bonding interactions rather than the comparatively much weaker intermolecular forces. Additionally, Asp61 exhibited great flexibility in molecular dynamics simulations,[4] which may bring about its nonparticipation in the NH_3 binding event and justify its elimination from our model. Fortunately, this circumstance resembles the method successfully applied in the water binding case taking place in the S_2~S_3 transition.[5]

Full degree of freedom optimization

Fixing certain atoms or backbone constraints[6] may lead to unexpected imaginary frequencies which will not only raise the energies in varying degrees even for the same molecular system in different spin states, but also make Hessian calculations in frequency analyses lose rigor to some extent owing to the non-stationary-point character on potential energy surfaces (PES). Besides, redundant imaginary vibrations confuse TS identifications in the strict sense. These factors will inevitably introduce errors making energy comparisons inaccurate and bringing influence on thermodynamic and kinetic values. Fortunately, ligands in the full optimized structures did not fall apart and basically preserved their origin positions as displayed in the XRD crystallization.[7,8] It has been clarified that rotation of His332 imidazole ring because of the omission of one hydrogen bond in small QM models would affect

the spectroscopic signature like Mn1 hyperfine coupling (HFC) constant, but was testified to bring almost no change to the energetic property considered here,[9] so we did not impose any restriction during optimizations.

SCF iteration algorithm details

We utilized normal, tight convergence in the self-consistent field (SCF) iterations with ultrafine grid for numerical integrations and full accuracy of the integrals throughout, with two-electron integral accuracy parameter set to 10^{-12}. When wavefunctions were difficult to converge in some extreme circumstances, steepest descent or quadratic algorithm[10] was mixed with the regular SCF for smooth solutions.

II. Definition of spin topologies in the S_2 State and the relevance to PES crossing

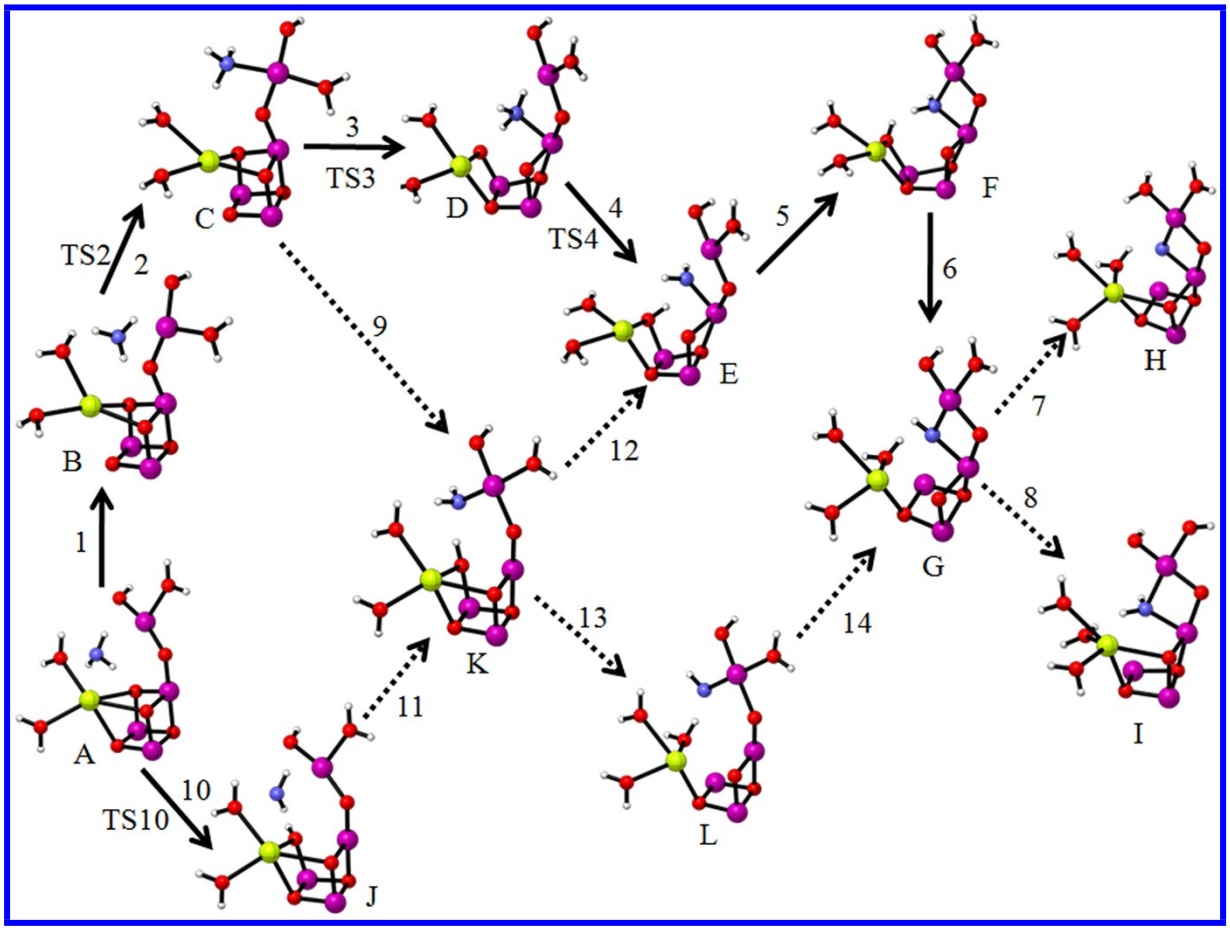
First of all, we need to illustrate the spin states and spin topologies introduced for the open and closed-cubane structures in the S_2 state, which are set up based on the oxidation state distributions of Mn1-Mn4 (III, IV, IV, IV) and (IV, IV, IV, III), respectively. What complicates spin assignments is the potential spin flip[11] of unpaired electrons in the d orbitals, causing various ferromagnetic and antiferromagnetic coupling between manganese ions. This leads to diversification of the overall spin multiplicities or different spin coupling ways in the same spin state, which may interconvert to each other by intersystem crossing (ISC)[12] among different PESs through non-adiabatic spin-forbidden reactions.[13] Attention is paid to avoid electrons pairing in the d-orbital for the proven excessively high energy inactivating in chemical reactions. For the open-cubane structure, possible spin topologies are αααβ, αβαβ, αββα on the doublet surface, βααα on the sextet surface, αααβ, ααβα,

αβαα on the octet surface and αααα on the 14-et surface. For the closed-cubane structure, they change to ββαα, βαβα, αββα on the doublet surface, αααβ on the sextet surface, βααα, ααβα, αβαα on the octet surface and αααα on the 14-et surface. In fact, ααββ and αβαβ are equivalent to ββαα and βαβα, respectively, but they are differently marked lest computation would be confused because of the net negative spin multiplicity.

It is important that all the electrons in the d-orbitals of the individual manganeses must keep spin-parallel for energetically steady states and activities in chemical reactions. As energy landscapes may be affected by the spin state designation, magnetic coupling property, and possible electron transfer participated by open-shell metals in spin-allowed reactions whose reactivity may present disparities on different PESs, it makes sense to investigate reactions under these circumstances for potential spin-related events. However, computational results reveal that except for valence state isomerizations, the reaction mechanisms are independent of the spin state selections because of the modest varieties among different spin surfaces including the pivotal rate-determining steps. Thus, searching for the minimum energy crossing points (MECPs)[14-16] is not essential and not performed here because of the adequate proximity found later in the thermodynamics and kinetics of key steps among these spin states which might make hopping between different surfaces facile but indecisive and unconvincing for substance transformation on a definitive PES. Moreover, the undistinguishable reactivity for each spin state according to the computed results suggests the subequal probability, so it is more significative to determine the reaction pathway than the reactive spin state. Hence, it is insignificant to further calculate the magnitude of SOC matrix element and probability for ISC for our subject under discussion.

III. O5 substitution scheme

IIIa. Closed-cubane structure as reactant



Scheme S1. CYLview[17] is used in this paper for graphic molecular images. Sequence numbers with TS stand for each reaction with its respective transition state, and letters (A-L) express reactants and products; solid lines show reactions we have studied while dotted lines denote conjectural reactions (similarly hereinafter). Here are specific annotations for each step: 1: NH_3 approaching the Mn4; 2: NH_3 binding to Mn4; 3: Mn3 ligand exchange between NH_3 and O5; 4: PT from NH_3 to O5; 5: NH_2^- flipping and binding to Mn4; 6: proton-coupled electron transfer (PCET) of proton transfer (PT) from NH_2^- to $O5H^-$ and electron transfer (ET) from Mn4 to Mn1;

7: PT from NH^{2-} to W2; 8: two-step PT from W1 to W2 and then to NH^{2-}; 9: PCET of PT from NH_3 to O5 and ET from Mn4 to Mn3; 10: PCET of PT from NH_3 to O5 and ET from N to Mn3 (N refers to N of NH_3 rather than His332 unless otherwise specified, the same below); 11: $NH_2\cdot$ binding to Mn4 and ET from Mn4 to N; 12: Mn3 ligand exchange between NH_2^- and $O5H^-$ accompanied with ET from Mn3 to Mn4; 13: PCET of PT from NH_2^- to $O5H^-$ and ET from N to Mn1; 14: $NH\cdot^-$ binding to Mn3 and ET from Mn3 to N. The reason why the ideal electron donor of step9 and 13 is different is that the active Mn4 in C is in formal state III and apt to transfer an electron while Mn4 in K is IV, and about -1.0 spins on N atom was found in a trial optimization of L.

Table SIIIa. Gibbs free energies and Mulliken spin populations for the O5 substitution scheme with the closed-cubane structure as reactant:

Spin states	Spin topology (Mn1-Mn4)	Gibbs Free energy (a.u.)			
		A	B	TS2	C
doublet	αββα	-3347.6447	-3347.6338	-3347.6297	-3347.6391
	βαβα	-3347.6435	-3347.6330	-3347.6290	-3347.6384
	ββαα	-3347.6407	-3347.6323	-3347.6275	-3347.6369
sextet	αααβ	-3347.6490	-3347.6355	-3347.6318	-3347.6411
octet	ααβα	-3347.6460	-3347.6354	-3347.6313	-3347.6409
	αβαα	-3347.6455	-3347.6329	-3347.6278	-3347.6372
	βααα	-3347.6458	-3347.6337	-3347.6289	-3347.6380
14-et	αααα	-3347.6482	-3347.6350	-3347.6304	-3347.6396
		TS3	D	TS4*	E
	αββα	-3347.5865	-3347.6051	-3347.6067	-3347.6079

doublet	βαβα	-3347.5873	-3347.6053	-3347.6066	-3347.6086
	ββαα	-3347.5879	-3347.6053	-3347.6077	-3347.6090
sextet	αααβ	-3347.5885	-3347.6065	-3347.6078	-3347.6095
octet	ααβα	-3347.5890	-3347.6076	-3347.6090	-3347.6103
	αβαα	-3347.5885	-3347.6056	-3347.6077	-3347.6089
	βααα	-3347.5881	-3347.6055	-3347.6079	-3347.6099
14-et	αααα	-3347.5894	-3347.6062	-3347.6083	-3347.6104

		F	G	TS10	J
doublet	αββα	-3347.6079	-3347.5912	-3347.5987	-3347.6030
	βαβα	-3347.6085	-3347.5699	-3347.6014	-3347.6050
	ββαα	-3347.6091	-3347.5736	-3347.5951	-3347.6014
sextet	αααβ	-3347.6095	-3347.5710	-3347.6020	-3347.6054
octet	ααβα	-3347.6102	-3347.5923	-3347.6019	-3347.6064
	αβαα	-3347.6089	-3347.5952	-3347.6014	-3347.6050
	βααα	-3347.6099	-3347.5805	-3347.5986	-3347.6030
14-et	αααα	-3347.6104	-3347.5970	-3347.6013	-3347.6046

Spin states	Spin topology (Mn1-Mn4)		Mulliken spin density			
			A	B	TS2	C
doublet	α	Mn1	2.94	2.93	2.93	2.93
	β	Mn2	-2.93	-2.93	-2.93	-2.93
	β	Mn3	-2.81	-2.79	-2.79	-2.78
	α	Mn4	3.82	3.81	3.82	3.85
		O4	-0.07	-0.10	-0.12	-0.13

		O5	0.02	0.00	0.00	0.01
		N	0.00	0.00	0.00	-0.01
	β	Mn1	-2.93	-2.92	-2.92	-2.92
	α	Mn2	2.94	2.95	2.95	2.95
	β	Mn3	-2.79	-2.76	-2.76	-2.77
	α	Mn4	3.82	3.81	3.82	3.85
		O4	-0.08	-0.12	-0.13	-0.15
		O5	-0.01	-0.02	-0.01	-0.02
		N	0.00	0.00	0.00	-0.01
	β	Mn1	-2.93	-2.94	-2.94	-2.94
	β	Mn2	-2.93	-2.94	-2.95	-2.95
	α	Mn3	2.86	2.85	2.85	2.83
	α	Mn4	3.89	3.86	3.87	3.89
		O4	0.15	0.14	0.14	0.15
		O5	-0.02	-0.01	-0.01	-0.01
		N	0.00	0.00	0.00	-0.01
	α	Mn1	2.93	2.93	2.92	2.92
	α	Mn2	2.92	2.93	2.93	2.93
	α	Mn3	2.83	2.80	2.80	2.80
sextet	β	Mn4	-3.84	-3.81	-3.82	-3.85
		O4	0.06	0.10	0.11	0.13
		O5	0.03	0.03	0.03	0.04
		N	0.00	0.00	0.00	0.01
octet	α	Mn1	2.94	2.94	2.94	2.94
	α	Mn2	2.94	2.95	2.95	2.94

	β	Mn3	-2.77	-2.74	-2.74	-2.74
	α	Mn4	3.82	3.81	3.82	3.84
		O4	-0.08	-0.12	-0.13	-0.15
		O5	0.03	0.01	0.01	0.01
		N	0.00	0.00	0.00	-0.01
	α	Mn1	2.94	2.93	2.92	2.92
	β	Mn2	-2.93	-2.94	-2.94	-2.94
	α	Mn3	2.87	2.88	2.88	2.86
	α	Mn4	3.88	3.86	3.87	3.89
		O4	0.14	0.14	0.14	0.14
		O5	0.01	0.01	0.01	0.01
		N	0.00	0.00	0.00	-0.01
	β	Mn1	-2.92	-2.93	-2.93	-2.92
	α	Mn2	2.93	2.93	2.93	2.93
	α	Mn3	2.90	2.90	2.90	2.87
	α	Mn4	3.88	3.86	3.87	3.89
		O4	0.14	0.12	0.13	0.13
		O5	-0.01	-0.01	-0.01	-0.01
		N	0.00	0.00	0.00	-0.01
14-et	α	Mn1	2.94	2.93	2.93	2.92
	α	Mn2	2.92	2.93	2.93	2.93
	α	Mn3	2.90	2.92	2.92	2.90
	α	Mn4	3.88	3.86	3.87	3.89
		O4	0.13	0.12	0.12	0.12
		O5	0.03	0.03	0.03	0.03

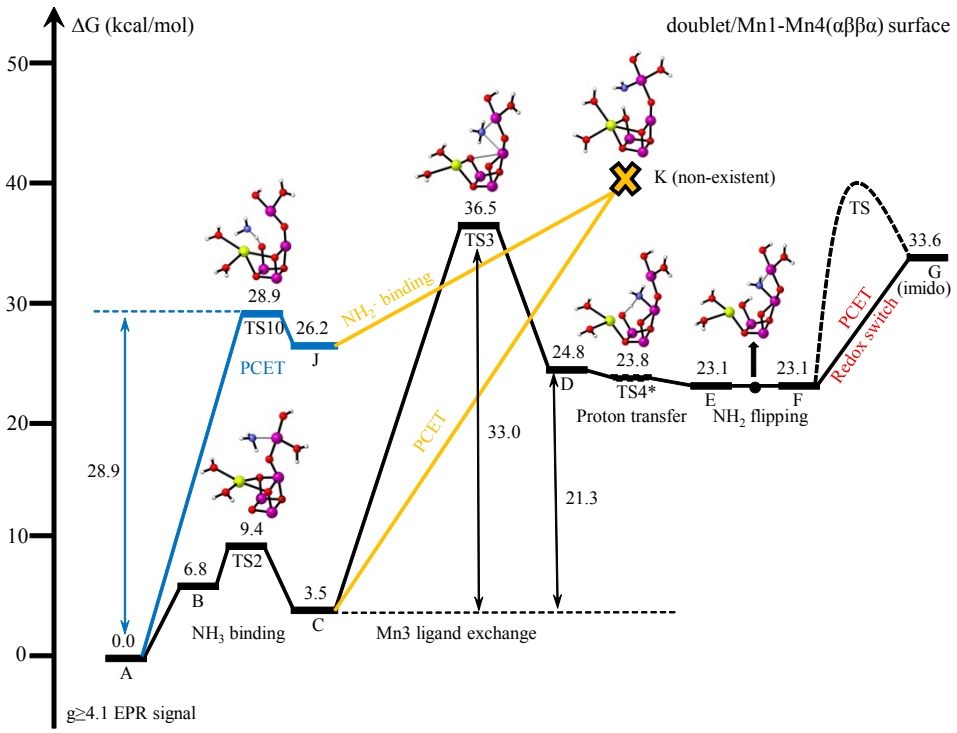
		N	0.00	0.00	0.00	-0.01
			TS3	D	TS4*	E
	α	Mn1	2.78	2.80	2.89	2.94
	β	Mn2	-2.92	-2.94	-2.95	-2.94
	β	Mn3	-2.84	-2.86	-2.90	-2.86
	α	Mn4	3.84	3.82	3.83	3.86
		O4	-0.13	-0.09	-0.08	-0.13
		O5	0.24	0.21	0.09	0.00
		N	0.05	0.07	0.10	0.00
	β	Mn1	-2.78	-2.80	-2.89	-2.93
	α	Mn2	2.91	2.92	2.93	2.92
	β	Mn3	-2.80	-2.82	-2.85	-2.80
doublet	α	Mn4	3.84	3.82	3.83	3.86
		O4	-0.14	-0.11	-0.10	-0.15
		O5	-0.24	-0.21	-0.09	0.00
		N	0.04	0.05	0.06	0.00
	β	Mn1	-2.78	-2.81	-2.89	-2.93
	β	Mn2	-2.93	-2.93	-2.94	-2.93
	α	Mn3	2.88	2.89	2.91	2.90
	α	Mn4	3.86	3.86	3.87	3.86
		O4	0.12	0.00	0.10	0.08
		O5	-0.25	-0.21	-0.10	-0.02
		N	0.00	-0.07	-0.07	0.01
sextet	α	Mn1	2.78	2.80	2.89	2.95

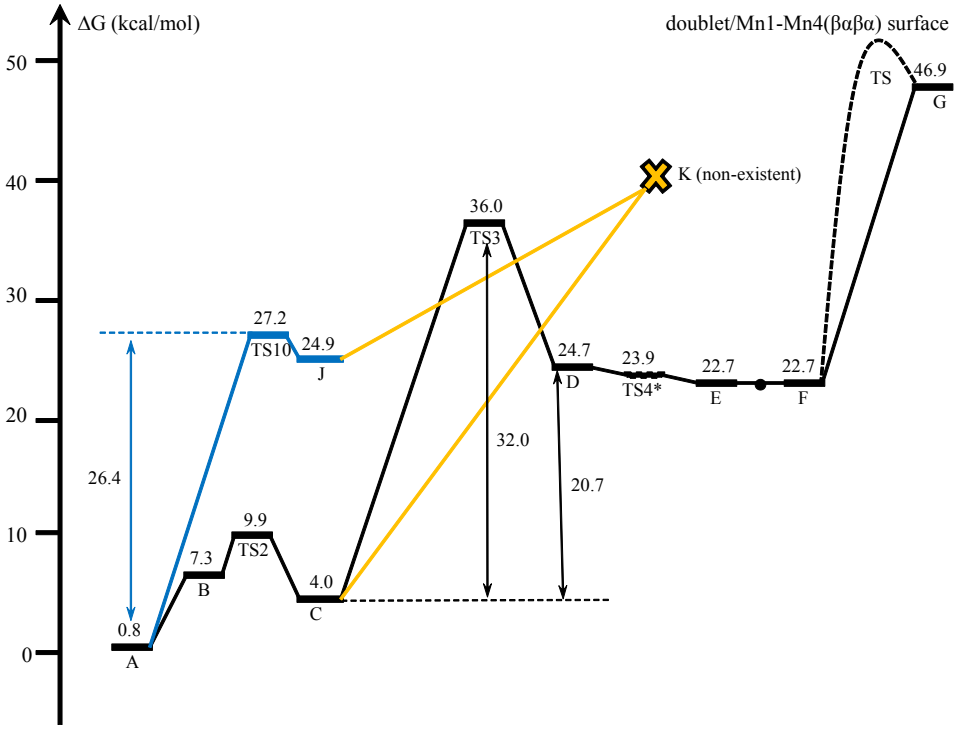
	α	Mn2	2.94	2.95	2.96	2.95
	α	Mn3	2.86	2.86	2.89	2.86
	β	Mn4	-3.84	-3.82	-3.83	-3.86
		O4	0.13	0.10	0.09	0.14
		O5	0.28	0.23	0.10	0.01
		N	-0.01	-0.05	-0.05	0.00
	α	Mn1	2.78	2.81	2.89	2.95
	α	Mn2	2.93	2.94	2.94	2.93
	β	Mn3	-2.79	-2.82	-2.86	-2.80
	α	Mn4	3.84	3.83	3.83	3.86
		O4	-0.14	-0.10	-0.09	-0.14
		O5	0.25	0.22	0.10	0.00
		N	0.05	0.07	0.10	0.00
	α	Mn1	2.79	2.81	2.89	2.93
	β	Mn2	-2.91	-2.92	-2.92	-2.91
octet	α	Mn3	2.89	2.89	2.90	2.89
	α	Mn4	3.86	3.86	3.87	3.86
		O4	0.12	0.12	0.11	0.09
		O5	0.23	0.21	0.10	0.03
		N	0.02	-0.04	-0.03	0.03
	β	Mn1	-2.78	-2.81	-2.88	-2.92
	α	Mn2	2.92	2.94	2.95	2.95
	α	Mn3	2.93	2.93	2.95	2.94
	α	Mn4	3.86	3.86	3.87	3.86
		O4	0.11	0.10	0.09	0.07

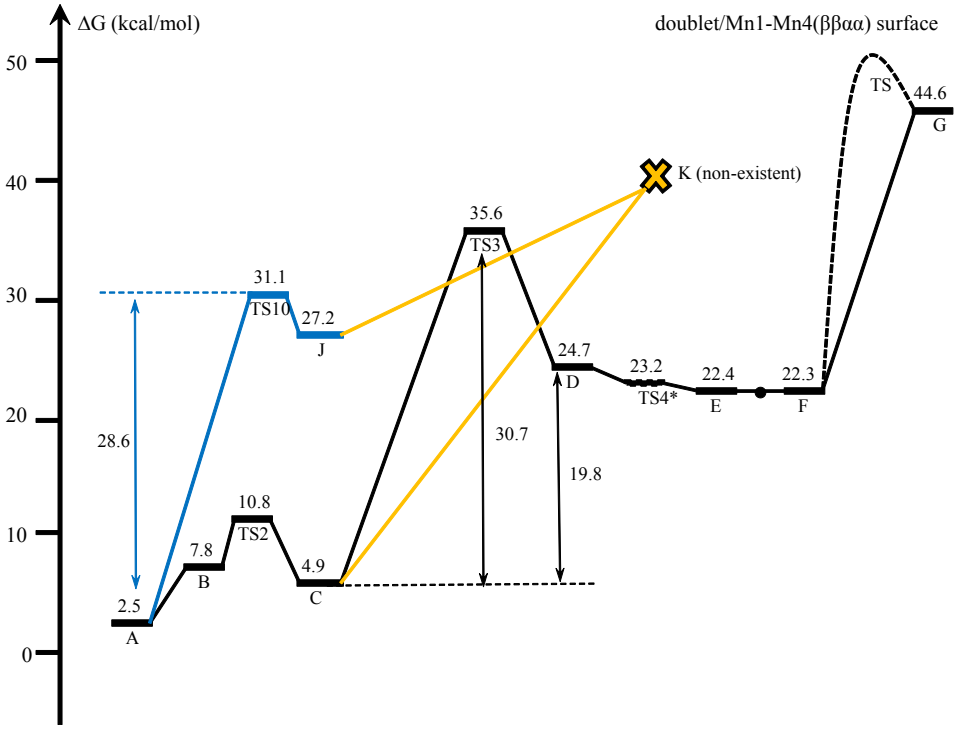
		O5	-0.23	-0.20	-0.09	-0.02
		N	0.00	-0.07	-0.07	0.01
14-et	α	Mn1	2.79	2.81	2.90	2.95
	α	Mn2	2.94	2.95	2.96	2.96
	α	Mn3	2.95	2.94	2.95	2.94
	α	Mn4	3.86	3.86	3.87	3.86
		O4	0.11	0.11	0.10	0.08
		O5	0.25	0.23	0.12	0.04
		N	0.02	0.00	-0.03	0.04
			F	G	TS10	J
doublet	α	Mn1	2.90	3.90	2.92	2.93
	β	Mn2	-2.92	-2.92	-2.94	-2.94
	β	Mn3	-2.88	-2.98	-3.64	-3.82
	α	Mn4	3.80	2.97	3.82	3.83
		O4	0.12	-0.01	0.02	0.04
		O5	0.01	0.00	0.14	-0.03
		N	0.01	0.01	0.69	1.08
	β	Mn1	-2.91	-2.00	-2.98	-2.93
	α	Mn2	2.92	2.98	2.89	2.88
	β	Mn3	-2.87	-2.95	-3.62	-3.81
	α	Mn4	3.80	2.97	3.82	3.84
		O4	0.11	-0.01	0.01	0.03
		O5	0.01	0.00	0.21	0.00
		N	0.01	0.01	0.69	1.08

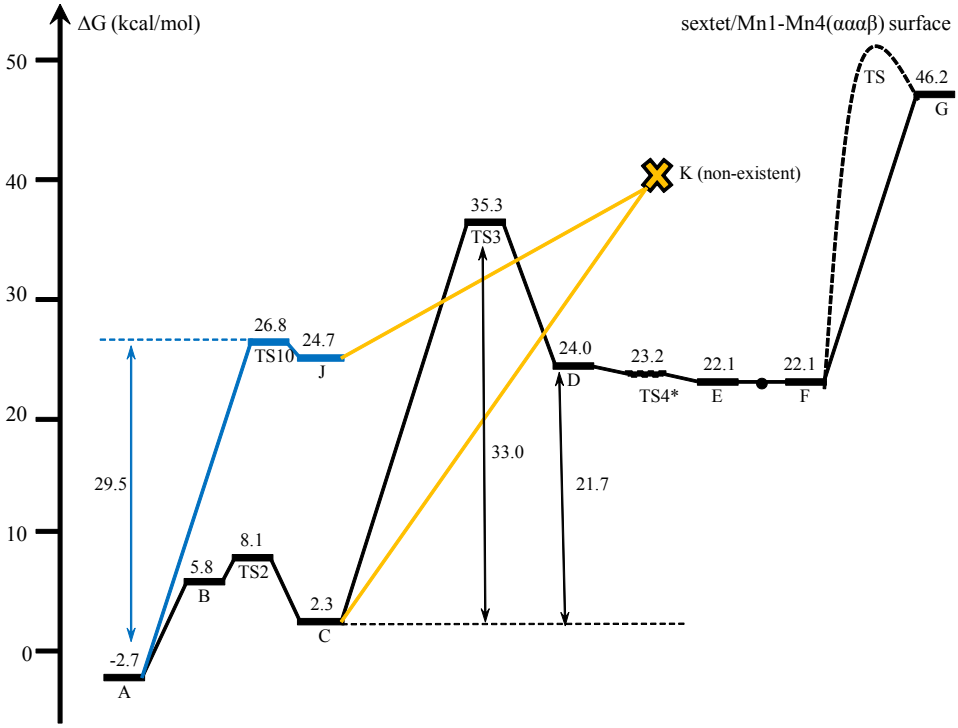
	β	Mn1	-2.91	-2.00	-2.92	-2.92
	β	Mn2	-2.92	-2.95	-2.88	-2.87
	α	Mn3	2.87	3.02	3.65	3.85
	α	Mn4	3.80	3.04	3.89	3.90
		O4	0.12	0.11	0.10	0.09
		O5	0.01	0.00	-0.11	0.02
		N	0.00	-0.25	-0.70	-1.07
	α	Mn1	2.92	2.01	2.99	2.95
	α	Mn2	2.92	2.96	2.95	2.94
	α	Mn3	2.87	2.98	3.67	3.84
sextet	β	Mn4	-3.79	-2.97	-3.82	3.84
		O4	0.11	0.01	-0.02	-0.04
		O5	0.01	0.00	-0.19	0.00
		N	0.01	0.00	-0.72	-1.08
	α	Mn1	2.91	3.90	2.93	2.93
	α	Mn2	2.91	2.97	2.89	2.88
	β	Mn3	-2.87	-2.96	-3.60	-3.80
	α	Mn4	3.80	2.97	3.82	3.83
		O4	0.11	0.00	0.01	0.04
octet		O5	-0.01	0.01	0.15	-0.02
		N	0.00	0.01	0.67	1.08
	α	Mn1	2.91	3.90	2.98	2.94
	β	Mn2	-2.91	-2.90	-2.88	-2.87
	α	Mn3	2.88	3.02	3.69	3.86
	α	Mn4	3.80	3.04	3.88	3.89

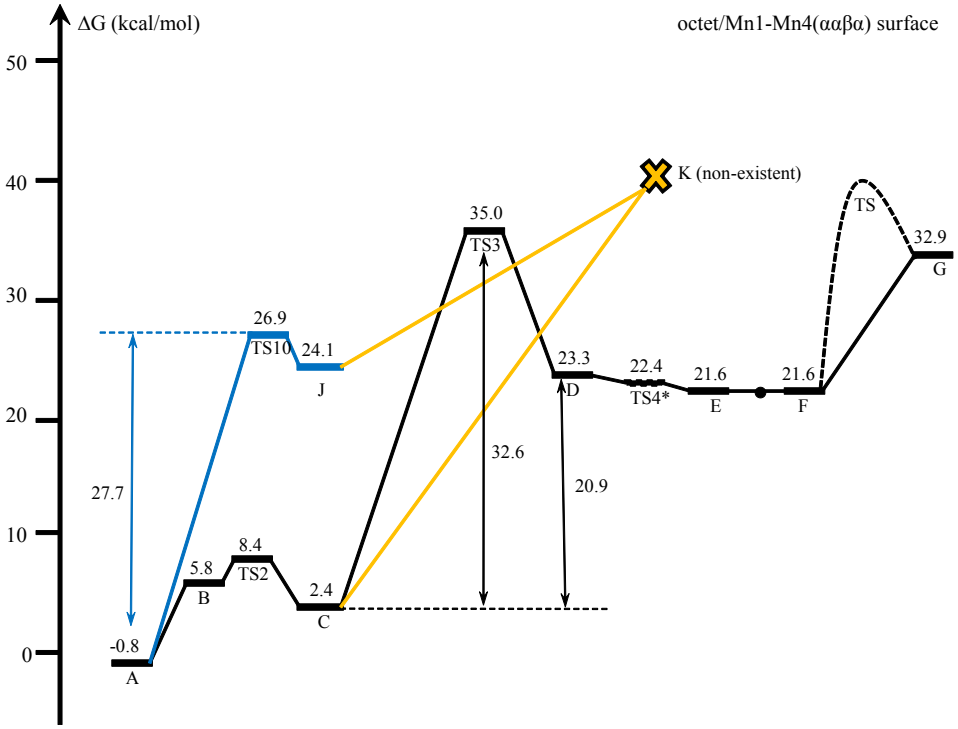
		O4	0.11	0.10	0.11	0.11
		O5	0.01	0.00	-0.21	0.00
		N	0.00	-0.25	-0.69	-1.08
	β	Mn1	-2.91	-2.04	-2.91	-2.92
	α	Mn2	2.92	3.01	2.94	2.94
	α	Mn3	2.88	2.93	3.71	3.87
	α	Mn4	3.80	2.96	3.88	3.89
		O4	0.10	0.13	0.09	0.09
		O5	0.01	-0.02	-0.13	0.03
		N	0.00	-0.17	-0.69	-1.08
	α	Mn1	2.92	3.91	2.99	2.95
	α	Mn2	2.92	3.00	2.94	2.94
	α	Mn3	2.88	3.05	3.73	3.88
14-et	α	Mn4	3.80	3.04	3.88	3.89
		O4	0.10	0.10	0.10	0.09
		O5	0.01	0.00	-0.18	0.03
		N	0.00	-0.25	-0.72	-1.08

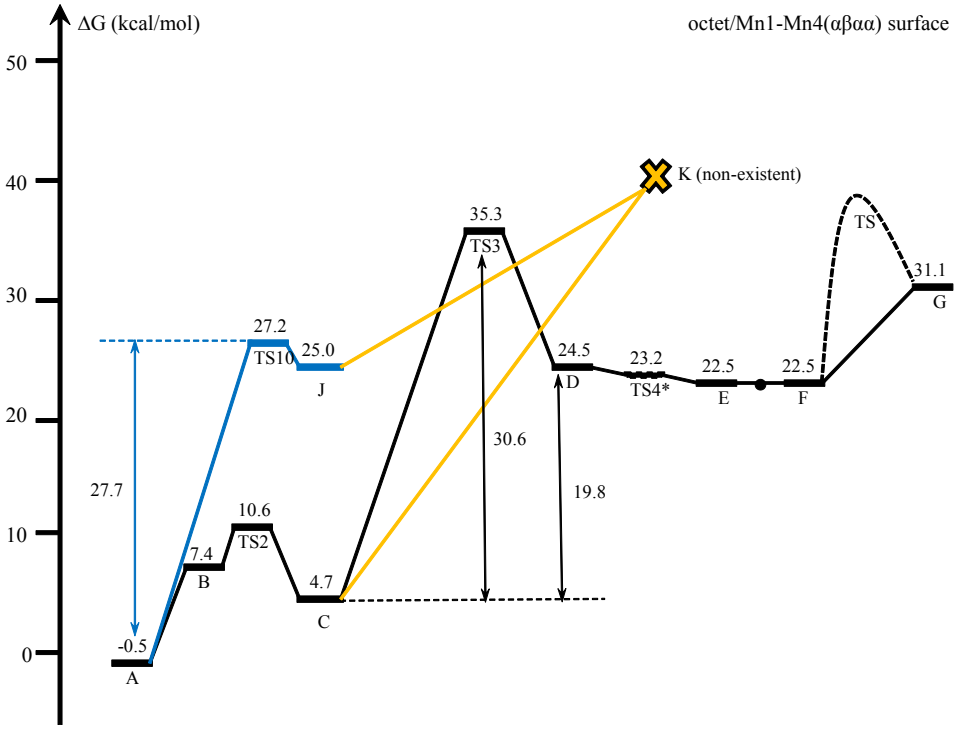

ΔG (kcal/mol)
doublet/Mn1-Mn4(αββα) surface
50
40
30
20
10
0
28.9
TS10
26.2
J
NH2 binding
PCET
K (non-existent)
36.5
TS3
TS
33.6
G
(imido)
PCET
Redox switch
24.8
D
23.8
TS4*
23.1
E
23.1
F
Proton transfer
NH2 flipping
33.0
21.3
28.9
9.4
TS2
6.8
B
3.5
C
0.0
A
NH3 binding
Mn3 ligand exchange
g≥4.1 EPR signal


ΔG (kcal/mol)
doublet/Mn1-Mn4(βαβα) surface
50
40
30
20
10
0
TS
46.9
G
K (non-existent)
36.0
TS3
27.2
TS10
24.9
J
24.7
D
23.9
TS4*
22.7
E
22.7
F
32.0
20.7
26.4
9.9
TS2
7.3
B
4.0
C
0.8
A


ΔG (kcal/mol)
doublet/Mn1-Mn4(ββαα) surface
50
40
30
20
10
0
TS
44.6
G
K (non-existent)
35.6
TS3
31.1
TS10
27.2
J
24.7
D
23.2
TS4*
22.4
E
22.3
F
28.6
30.7
19.8
10.8
TS2
7.8
B
4.9
C
2.5
A


ΔG (kcal/mol)
sextet/Mn1-Mn4(αααβ) surface
50
40
30
20
10
0
TS
46.2
G
K (non-existent)
35.3
TS3
26.8
TS10
24.7
J
24.0
D
23.2
TS4*
22.1
E
22.1
F
29.5
33.0
21.7
8.1
TS2
5.8
B
2.3
C
-2.7
A


ΔG (kcal/mol)
octet/Mn1-Mn4(ααβα) surface
50
40
30
20
10
0
K (non-existent)
35.0
TS3
TS
32.9
G
26.9
TS10
24.1
J
23.3
D
22.4
TS4*
21.6
E
21.6
F
32.6
20.9
27.7
8.4
5.8
TS2
B
2.4
C
-0.8
A


ΔG (kcal/mol)
octet/Mn1-Mn4(αβαα) surface
50
40
30
20
10
0
K (non-existent)
35.3
TS3
TS
31.1
G
27.2
TS10
25.0
J
24.5
D
23.2
TS4*
22.5
E
22.5
F
30.6
19.8
27.7
10.6
7.4
TS2
B
4.7
C
-0.5
A

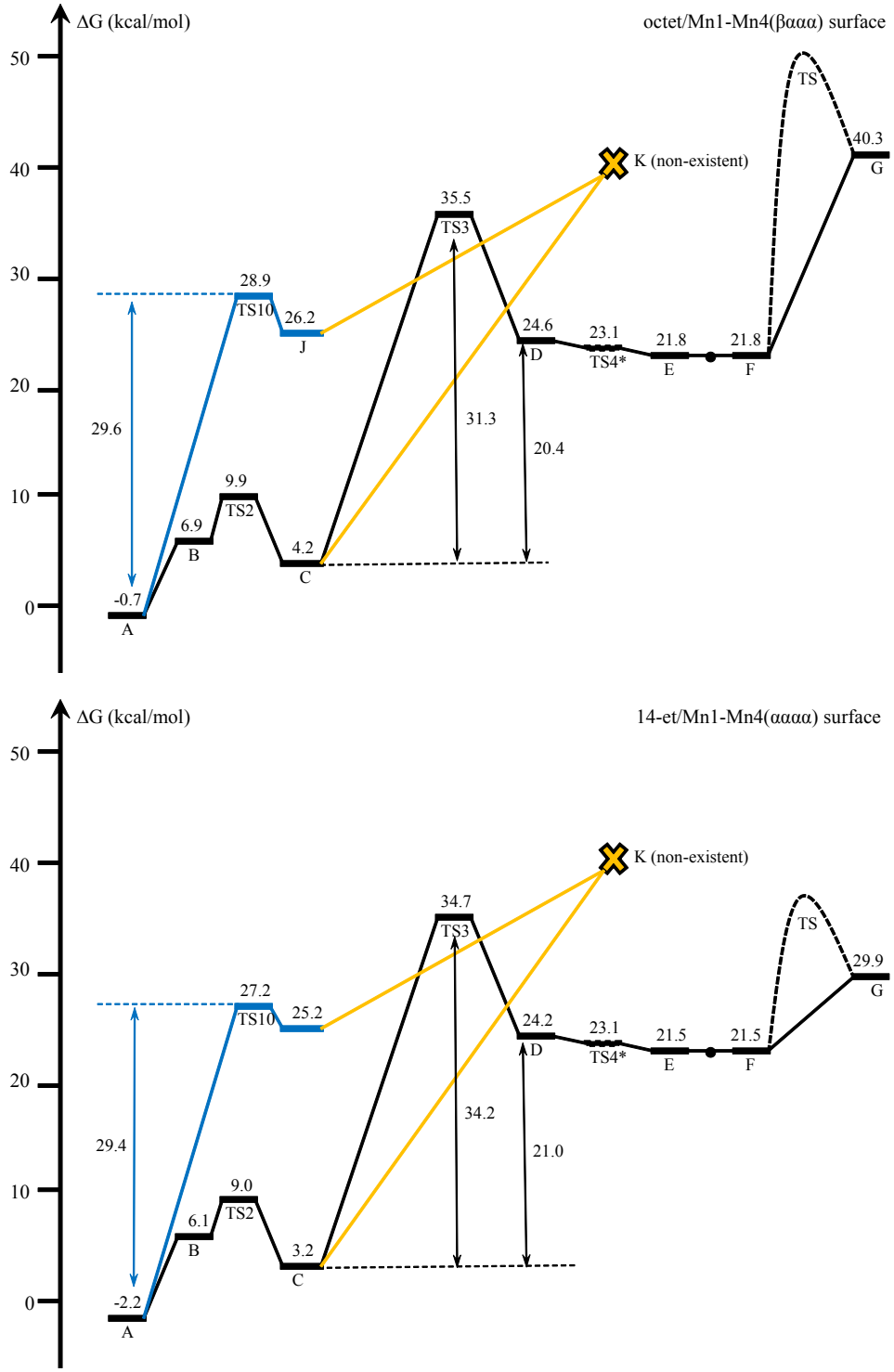


Figure SIIIa. Free energy profiles for the O5 substitution scheme with the closed-

cubane structure as reactant for all spin states.

Because of the structure similarities among all the spin states, cartesian coordinates and 3D images are shown in the example of doublet/Mn1-Mn4(αββα), similarly hereinafter.

The Cartesian coordinates for A to G and TS2 to TS10:

A:

Ca	-2.66359000	-0.60544200	0.76217000	H	-1.25799800	1.19068600	5.44443500	C	2.18311800	-2.08957400	-1.23752200
Mn	0.27760500	0.92645600	1.32840300	C	-2.08702200	-0.75134300	5.96355000	O	1.37816000	-3.05939300	-0.98774600
Mn	-1.21019700	2.22165900	-0.51692800	H	-1.87030500	-1.81087700	5.75854200	O	0.75469800	2.83545700	1.91161300
Mn	-0.02919600	-0.13326700	-1.30856600	H	-3.07918900	-0.56030400	5.53573300	C	0.27074200	3.87247600	1.34888600
Mn	-0.53599700	-3.22208300	-1.30097500	C	-2.10429200	-0.51229500	7.47708000	O	-0.48377600	3.90071500	0.32546100
O	-1.41555100	1.53642000	1.15522800	H	-1.12528000	-0.72478300	7.92959800	C	0.62772400	5.20768400	1.99411200
O	0.54061000	1.51177400	-0.40667400	H	-2.35680400	0.53137400	7.71187500	H	1.66856600	5.14030500	2.33667000
O	-1.67543100	0.63042200	-1.21732900	H	-2.84607200	-1.15323200	7.97086600	H	0.01704600	5.27492000	2.90837800
O	-0.12443600	-0.67164100	0.50453600	N	2.31785100	0.57097500	1.52133100	C	0.40007800	6.43212900	1.10639500
O	-0.63340200	-1.60254900	-2.05779600	C	3.02275700	-0.43297500	2.15437500	H	0.65584400	7.34979300	1.65136100
O	-5.12556100	-1.01127600	1.18769300	H	2.51906400	-1.24767300	2.66308500	H	1.02016200	6.38790100	0.20228000
H	-5.37019300	-0.13166000	0.83104800	C	4.36971300	-0.22319100	1.96733900	H	-0.64521300	6.49609400	0.78595700
H	-5.19544500	-1.62089000	0.42606100	N	4.45882400	0.94688200	1.22032300	O	-4.20747000	1.30446900	0.17839300
O	-2.24150200	-2.93056400	1.59966400	H	5.30602900	1.25992700	0.74116300	C	-4.07058100	2.44711900	-0.30384700
H	-1.74787800	-2.77338800	2.42317200	C	3.20614500	1.37659300	0.95587900	O	-2.94338800	2.99234000	-0.63632500
H	-1.72134700	-3.62592600	1.11189100	H	2.96670300	2.23410100	0.34468700	C	-5.27720000	3.33235500	-0.55956200
O	-0.62198400	-4.51418400	0.04232400	C	5.55665700	-1.02050300	2.44233800	H	-5.37428300	3.51039900	-1.63822700
H	0.28543200	-4.70125100	0.34243100	H	5.74334600	-0.82767800	3.50950900	H	-6.18863500	2.86174000	-0.18090900
O	-0.19201200	-4.15937500	-3.41816900	H	5.29104600	-2.08473800	2.37755200	H	-5.13058500	4.30803700	-0.08142500
H	-1.14745400	-4.37314000	-3.45099800	C	6.89001400	-0.76616200	1.68880100	O	-0.70714600	2.81936100	-2.35847600
H	-0.12676500	-3.29307600	-3.86518300	H	7.32575700	0.19040400	1.99763000	C	-0.10020200	2.07036700	-3.19107800
O	-3.63628400	-2.13306200	-0.90876200	H	7.60329000	-1.55402900	1.96747100	O	0.28668200	0.87010400	-2.99947500
C	-3.47182300	-3.09990500	-1.67677500	C	6.71950800	-0.68686700	0.17303900	C	0.17614700	2.66332300	-4.56518500
O	-2.34888500	-3.71158700	-1.87367200	O	6.68190100	0.40453500	-0.40997800	H	0.86624900	1.99534200	-5.09421800
C	-4.63781300	-3.66671700	-2.48425300	N	6.53882100	-1.86317400	-0.48248700	H	-0.77915600	2.64626900	-5.11440200
H	-4.41591200	-3.46557200	-3.54381200	H	6.53090400	-2.71942200	0.05815400	C	0.71372800	4.10219600	-4.51862500
H	-4.61336200	-4.75975000	-2.37799700	C	6.07089000	-1.90955000	-1.87209100	H	1.65966500	4.11539300	-3.95632800
C	-6.00683600	-3.10198400	-2.10834400	H	6.67866100	-1.20500600	-2.44969200	H	0.00851600	4.72528200	-3.95460400
H	-6.02987800	-2.01221400	-2.22655800	H	6.27426400	-2.91967200	-2.24947400	C	0.93718600	4.68419400	-5.91822900
H	-6.26127700	-3.33805800	-1.06675200	C	4.58188800	-1.54940400	-2.02242100	H	1.65831700	4.08538700	-6.49213900
H	-6.78887900	-3.53157100	-2.74695600	H	4.42905400	-0.51642100	-1.69308400	H	1.32494300	5.70963500	-5.86231900
O	0.04815300	0.38091300	3.15940800	H	4.32874700	-1.57825600	-3.09199100	H	-0.00045100	4.71281000	-6.49105500
C	-1.04786900	-0.02602600	3.72695800	C	3.65625100	-2.48563900	-1.24067000	N	0.83088200	-2.83530300	2.76195200
O	-2.02954100	-0.50711600	3.12990600	H	3.72076900	-3.51947400	-1.60493200	H	0.51927900	-2.20291200	2.01790300
C	-1.05684500	0.12507200	5.24431600	H	3.95132000	-2.50784100	-0.17993500	H	0.48795000	-3.76640300	2.52379900
H	-0.03912800	-0.05558300	5.61712600	O	1.88005400	-0.88469800	-1.43248900	H	0.35885200	-2.54771700	3.61952400

B:

Ca	2.14591700	0.69904200	-1.57526300	H	0.17155500	5.84269000	-1.41343300	C	-2.22097800	-2.54882400	-0.86195400
Mn	-0.45476800	1.91019400	0.37387800	C	1.31390200	5.60169200	-3.25704900	O	-1.54023500	-3.26629400	-1.67024100
Mn	1.48447000	0.74139500	1.83558700	H	1.37330200	4.87737900	-4.08117900	O	-0.71643900	3.04124400	2.05279600
Mn	0.05463300	-0.88659100	0.12567300	H	2.29516000	5.58252700	-2.76063500	C	0.00798300	2.90142100	3.09704600
Mn	0.41610400	-3.34744600	-2.03475400	C	1.04530800	7.00493200	-3.81249900	O	0.92085300	2.03730100	3.27956100
O	1.32342500	2.07157800	0.64032200	H	0.08422900	7.04593000	-4.34401800	C	-0.25440300	3.89772800	4.22156600
O	-0.36038000	0.44082300	1.52125200	H	1.01035500	7.75328900	-3.00840500	H	-1.34325400	4.01112800	4.31196200
O	1.78205800	-0.42415800	0.51436800	H	1.82936800	7.30971800	-4.51768500	H	0.11349500	4.87044900	3.85951700
O	-0.25859700	0.62404800	-0.89880700	N	-2.50973900	1.84060600	0.21934000	C	0.38853900	3.54092300	5.56205800
O	0.65304500	-1.72589500	-1.27963600	C	-3.24474900	1.58840500	-0.92176400	H	0.16590100	4.31439300	6.30815900
O	3.93145600	2.18408400	-2.58819700	H	-2.77580700	1.44730100	-1.88761800	H	0.01262900	2.58208100	5.93951000
H	4.44914700	2.19111800	-1.75570300	C	-4.57438700	1.50169800	-0.58838300	H	1.47608400	3.45280100	5.46561400
H	3.33991800	2.96428100	-2.53913900	N	-4.62649400	1.72088200	0.78504200	O	4.06390900	1.27152400	-0.00619400
O	1.67348100	0.31748000	-4.03637900	H	-5.42550900	1.46201200	1.36724200	C	4.23921700	1.29980400	1.23041400
H	2.27832800	0.84357100	-4.58760900	C	-3.36282400	1.89874500	1.23214800	O	3.34067400	1.05802400	2.13467800
H	2.12202100	-0.55452100	-3.91828200	H	-3.09091600	2.05310900	2.26591700	C	5.59933700	1.65758000	1.80520100
O	0.10061500	-4.68100600	-3.21980400	C	-5.77931200	1.26503200	-1.45828300	H	6.35797200	1.67247600	1.01764600
H	-0.83418500	-4.94980800	-3.16115400	H	-6.08015400	2.20051400	-1.95404400	H	5.87835900	0.94341600	2.58819300
O	0.77136100	-4.45638900	-0.07499800	H	-5.47479100	0.58593600	-2.26582300	H	5.54137400	2.64866100	2.27467800
H	1.73601500	-4.56932300	-0.16008800	C	-7.03328000	0.70278600	-0.73698900	O	1.37604300	-0.87793900	3.07528600
H	0.63927000	-3.76432500	0.62068200	H	-7.51140200	1.48646200	-0.13840600	C	0.89146000	-1.99401500	2.73467400
O	3.14410300	-1.40055800	-2.63574300	H	-7.76018700	0.38544800	-1.49716500	O	0.31687800	-2.27108500	1.61454300
C	3.28900900	-2.61276900	-2.32940400	C	-6.70202300	-0.43458300	0.22478600	C	0.94630500	-3.13358500	3.74462000
O	2.36469900	-3.50439100	-2.32463700	O	-6.54138300	-0.22497900	1.43366500	H	-0.07449900	-3.23968700	4.14726300
C	4.69461800	-3.10322400	-1.98132200	N	-6.53323000	-1.66433300	-0.33128100	H	1.14190500	-4.06466000	3.19335300
H	5.22181300	-3.23085600	-2.93999000	H	-6.63276700	-1.75330400	-1.33509600	C	1.95057600	-2.94246000	4.88572300
H	5.20690500	-2.28112300	-1.46545900	C	-5.93997800	-2.77882100	0.41141700	H	1.72791300	-2.00218400	5.40561400
C	4.75422000	-4.39986200	-1.17203800	H	-6.35776100	-2.75135600	1.42289900	H	2.95899400	-2.82389400	4.46405500
H	4.24324600	-5.21491500	-1.69629000	H	-6.27053800	-3.70973000	-0.06716800	C	1.93206300	-4.11337700	5.87445100
H	4.27830200	-4.27420300	-0.18882600	C	-4.40481100	-2.70651600	0.48411200	H	0.94146100	-4.23099500	6.33611500
H	5.79530800	-4.69888700	-0.99583800	H	-4.11369900	-1.77849000	0.98851800	H	2.65909800	-3.95890600	6.68198000
O	-0.47526300	3.41265800	-0.83349500	H	-4.05113200	-3.53649800	1.11339500	H	2.18074400	-5.06265400	5.37921900
C	0.42910400	3.74787200	-1.69724200	C	-3.72980700	-2.77573200	-0.89193800	N	-1.69094000	-0.18788500	-3.52261000
O	1.37574800	3.02579700	-2.07649100	H	-4.13058700	-1.98101100	-1.54132500	H	-1.00912600	0.07670700	-4.23817300
C	0.23800000	5.15093100	-2.26639600	H	-3.92272200	-3.73338000	-1.39053500	H	-1.78208400	-1.20414200	-3.59640700
H	-0.75727700	5.17424900	-2.73651500	O	-1.79252000	-1.65993200	-0.07067200	H	-1.20505600	-0.02348900	-2.63441400

TS2:

Ca	-2.26690300	-0.52411200	-1.48093000	H	-0.36423700	3.76312000	0.66418600	C	-1.75737600	-6.83929400	-3.91449400
Mn	0.30988900	-1.97670000	0.30940600	O	-3.18325900	1.65084600	-2.45052300	H	-0.81880200	-6.95301800	-4.47501400
Mn	-1.44408800	-0.67236300	1.87899700	C	-3.17740100	2.88251900	-2.18059100	H	-1.76648100	-7.60565800	-3.12683700
Mn	0.04167900	0.86009700	0.11793700	O	-2.16648000	3.66578200	-2.25465300	H	-2.58457900	-7.05817900	-4.60203800
Mn	-0.21437800	3.37408100	-2.00488300	C	-4.50375000	3.53191300	-1.78260600	N	2.36848300	-2.06380700	0.11030000
O	-1.45819100	-1.99113000	0.65052300	H	-5.04037500	3.73569400	-2.72284300	C	3.10204000	-1.91362000	-1.04542000
O	0.40157800	-0.53366200	1.48209100	H	-5.09551800	2.77248200	-1.25650000	H	2.61499000	-1.86766000	-2.00951800
O	-1.70223700	0.53472200	0.59327600	C	-4.37893000	4.81794500	-0.96346300	C	4.43688300	-1.82165400	-0.72977300
O	0.17710900	-0.66085800	-0.93926200	H	-3.78172100	5.56632600	-1.49578900	N	4.49015900	-1.93775800	0.65472600
O	-0.56171200	1.77157300	-1.23078200	H	-3.89973300	4.62322400	0.00730100	H	5.30710200	-1.67880700	1.21527400
O	-4.21180800	-1.85473400	-2.42252700	H	-5.36859400	5.24497300	-0.75720800	C	3.22672900	-2.06035100	1.11927000
H	-4.68448900	-1.83132900	-1.56380800	O	0.17413700	-3.44882500	-0.93466500	H	2.95847000	-2.12454000	2.16343500
H	-3.68029600	-2.67810800	-2.41171000	C	-0.79553400	-3.69489300	-1.75655300	C	5.64390300	-1.64702900	-1.61456300
O	-1.96674200	-0.11467900	-3.97406500	O	-1.69968500	-2.89379000	-2.07598100	H	5.87556200	-2.59087600	-2.13083000
H	-2.62785000	-0.60052900	-4.49661800	C	-0.74713300	-5.09804200	-2.35603600	H	5.38132200	-0.93136200	-2.40609400
H	-2.37284600	0.76877300	-3.78457800	H	0.22949100	-5.20389900	-2.85324100	C	6.94312500	-1.18051600	-0.90668300
O	0.15553600	4.71994900	-3.15245600	H	-0.72212800	-5.80928100	-1.51678000	H	7.36041800	-1.99467900	-0.30350000
H	1.11848000	4.86932400	-3.16434300	C	-1.88526000	-5.43072100	-3.32350200	H	7.68605100	-0.93232600	-1.67699000
O	-0.50780800	4.47793700	-0.00274600	H	-1.90390800	-4.68533500	-4.13071300	C	6.72138400	-0.00659300	0.04492600
H	-1.47285800	4.60143900	-0.05886800	H	-2.84677700	-5.33651300	-2.79820100	O	6.56817700	-0.18948600	1.26016600

N	6.63923400	1.22599700	-0.51933800	O	-0.93716200	-2.04717600	3.27487600	C	-0.56826900	1.97964900	2.78284300
H	6.73188600	1.30265400	-1.52481400	C	0.09218500	-4.03488600	4.12266600	O	-0.02870300	2.22811600	1.63984500
C	6.15195700	2.38967500	0.22798100	H	1.16180400	-4.28357200	4.13649200	C	-0.47386500	3.10160000	3.80968900
H	6.60800500	2.35009800	1.22242300	H	-0.41819700	-4.94632600	3.77371200	H	0.57896800	3.13676900	4.13454000
H	6.52417200	3.28784200	-0.28100900	C	-0.41272900	-3.63187300	5.50861400	H	-0.64928400	4.05206100	3.28511600
C	4.61945700	2.42117000	0.36030900	H	-0.24077900	-4.44345600	6.22716800	C	-1.40064400	2.95665000	5.02076900
H	4.28698500	1.51891400	0.88590500	H	0.10416300	-2.73588000	5.87398700	H	-1.20180500	1.99589400	5.51236500
H	4.34873400	3.27858700	0.99396000	H	-1.48445900	-3.40706800	5.48630800	H	-2.44315200	2.90946600	4.67512500
C	3.89650200	2.52639500	-0.98935600	O	-4.14884500	-0.96780200	0.16696500	C	-1.23224100	4.10809100	6.01822700
H	4.21935900	1.70435000	-1.64745800	C	-4.26445200	-0.99189000	1.41077900	H	-0.20446300	4.15461900	6.40532100
H	4.13076100	3.46829500	-1.49911800	O	-3.30478100	-0.83637200	2.26936700	H	-1.90574200	3.98799400	6.87647000
O	1.93369400	1.45577200	-0.17336700	C	-5.62060600	-1.23546600	2.05119900	H	-1.45447900	5.07901200	5.55336300
C	2.37812200	2.40132200	-0.89326100	H	-6.41431900	-1.19091300	1.30019900	N	1.10143600	0.59870600	-3.70311500
O	1.71210600	3.25421500	-1.55923400	H	-5.80294700	-0.49697600	2.84021600	H	1.76165400	0.03304500	-4.24083600
O	0.54207600	-3.16945700	1.95439600	H	-5.62175200	-2.22552100	2.52624500	H	0.18360900	0.43813100	-4.12621300
C	-0.11997800	-2.98896900	3.03280800	O	-1.13228100	0.90352100	3.13316600	H	1.03343500	0.17864000	-2.77144900

C:

Ca	2.19914300	0.82567900	-1.50411000	H	0.24039500	5.93961000	-1.33242400	C	-2.32140400	-2.49714300	-0.95784000
Mn	-0.48052400	1.95131500	0.31879000	C	1.45748000	5.74362500	-3.13307500	O	-1.63838000	-3.30229100	-1.64221500
Mn	1.35672800	0.66407600	1.80454000	H	1.54684100	5.04346100	-3.97507200	O	-0.78616700	3.02949400	2.03390500
Mn	-0.05089700	-0.84306200	-0.05096200	H	2.41614300	5.69941100	-2.59563400	C	-0.11334500	2.82086500	3.10112500
Mn	0.45023000	-3.30266000	-2.21028200	C	1.22699800	7.16585400	-3.65648500	O	0.76182700	1.92024300	3.28472300
O	1.28618700	2.05994300	0.66075100	H	0.29030000	7.23362900	-4.22759200	C	-0.39096000	3.77882700	4.25598000
O	-0.47427500	0.43962200	1.40162400	H	1.16406200	7.89002700	-2.83222900	H	-1.47501700	3.95286000	4.28692000
O	1.68588900	-0.44151800	0.44712900	H	2.04389400	7.48335800	-4.31744800	H	0.05440800	4.74351700	3.96620400
O	-0.26748400	0.72956900	-1.00384300	N	-2.53967600	1.93170300	0.11094000	C	0.14617200	3.32337400	5.61321500
O	0.57201700	-1.65617900	-1.45511000	C	-3.24891800	1.66835300	-1.04003900	H	-0.07667100	4.07379800	6.38257800
O	4.02172000	2.30652500	-2.42166500	H	-2.73837500	1.54363100	-1.98485500	H	-0.30727900	2.37281200	5.92019000
H	4.50946700	2.29420300	-1.57142400	C	-4.58734600	1.58110100	-0.74003900	H	1.23047700	3.17321200	5.57602800
H	3.44679000	3.09875900	-2.39202400	N	-4.66844900	1.81301900	0.62917100	O	4.04029400	1.33669000	0.16156100
O	1.94944600	-0.05228700	-3.93889800	H	-5.48247800	1.56455100	1.19691100	C	4.14243500	1.27338800	1.40493500
H	2.45314300	0.42080400	-4.62332800	C	-3.41520600	1.99763500	1.10233300	O	3.19951500	0.94002600	2.23019900
H	2.59537500	-0.71494400	-3.52488200	H	-3.16541300	2.16198600	2.14003900	C	5.45690300	1.61855700	2.08496900
O	0.36662100	-4.90243300	-3.07210200	C	-5.77865500	1.32420800	-1.62482400	H	6.26499500	1.67938300	1.35050000
H	0.31518400	-5.61310800	-2.40733400	H	-6.05036000	2.23878500	-2.17374500	H	5.69478500	0.87380100	2.85266800
O	0.91250700	-4.32806700	-0.35644600	H	-5.47786800	0.59555000	-2.39032700	H	5.35338600	2.58742600	2.59189200
H	1.87725600	-4.17224100	-0.49270400	C	-7.05909000	0.82245200	-0.90524500	O	1.15704600	-0.99339400	2.96610200
H	0.62776200	-3.70231200	0.35827700	H	-7.52489200	1.64050300	-0.34431800	C	0.67440300	-2.08674900	2.55231900
O	3.50873200	-1.20361100	-2.27971100	H	-7.78127000	0.49791800	-1.66693800	O	0.14528900	-2.30556900	1.39947300
C	3.56279600	-2.35786300	-1.73610800	C	-6.77688000	-0.29030100	0.10211600	C	0.68147900	-3.27483600	3.50746500
O	2.76356300	-3.31293800	-1.96070500	O	-6.64156600	-0.04130800	1.30689100	H	-0.37040500	-3.46732400	3.77383400
C	4.72063300	-2.56875600	-0.75734300	N	-6.62125000	-1.54016900	-0.40835300	H	1.00351700	-4.15845200	2.93647600
H	5.64665900	-2.44903100	-1.33942600	H	-6.69536600	-1.65734700	-1.41150100	C	1.53005300	-3.09497900	4.76965500
H	4.70147600	-1.72075300	-0.05887500	C	-6.03456400	-2.63383200	0.37228600	H	1.18688300	-2.20339700	5.31002200
C	4.72466000	-3.90189900	-0.01038400	H	-6.44187300	-2.55921200	1.38547600	H	2.57043900	-2.89061500	4.48038100
H	4.70698400	-4.74872600	-0.70653800	H	-6.38404800	-3.57757700	-0.06602900	C	1.47244200	-4.32365400	5.68419800
H	3.85257500	-3.99325500	0.65178100	C	-4.49732400	-2.57968200	0.42005700	H	0.44429600	-4.52850300	6.01494800
H	5.62040900	-3.99111800	0.61805800	H	-4.18489000	-1.64292600	0.89538200	H	2.08735300	-4.17681500	6.58142700
O	-0.43557200	3.50966600	-0.83376500	H	-4.14652600	-3.39797800	1.06623600	H	1.84019100	-5.22393500	5.17182400
C	0.48650000	3.85049300	-1.67198200	C	-3.84080400	-2.69426500	-0.96246200	N	0.20498600	-2.44703500	-4.13573400
O	1.42610400	3.12169300	-2.06225300	H	-4.24473800	-1.90907100	-1.62200000	H	0.53073800	-3.13439300	-4.81702900
C	0.33604300	5.27447000	-2.20330400	H	-4.05449300	-3.66282300	-1.43059700	H	0.70165200	-1.55044600	-4.24010000
H	-0.63789200	5.32599400	-2.71489100	O	-1.90463700	-1.50101400	-0.27082200	H	-0.79493800	-2.29895100	-4.27864100

TS3:

Ca	-2.63938900	0.80762700	-1.24627600	Mn	0.83289800	1.29257800	0.45927700	O	0.20405700	-0.59728800	0.88945900
Mn	-0.89279400	-1.77721500	-0.23602200	Mn	1.71338100	3.33440000	-1.59037900	O	-0.90596900	1.55059900	0.75693900
Mn	-1.31519800	0.05676700	1.76403300	O	-2.24147400	-0.78641500	0.51944300	O	-0.79655300	-0.84728700	-1.66581900

O	1.21050000	2.94894600	0.13518600	H	-6.67733100	-5.19514900	-2.29577900	C	-1.29920500	-2.70099200	2.59448900
O	-5.09972000	0.84558300	-1.69121400	H	-6.77819900	-4.78542300	-4.01867800	O	-1.50307700	-1.50201800	2.97637700
H	-5.30105400	1.11715000	-0.77111700	N	0.75528400	-2.89708900	-0.79135000	C	-1.53754700	-3.80203800	3.62350200
H	-5.19345400	-0.12941100	-1.70792600	C	1.46982200	-2.77358500	-1.96379300	H	-0.82186000	-4.60821100	3.41623200
O	-2.39386600	-0.07135100	-3.65515700	H	1.06560900	-2.20556600	-2.78979000	H	-2.53164400	-4.21871500	3.39599900
H	-3.15526800	-0.68052000	-3.63091500	C	2.66657000	-3.43964000	-1.84332200	C	-1.47308800	-3.34819500	5.08294100
H	-1.67864800	-0.61369600	-3.23396200	N	2.64584800	-3.99120200	-0.56776800	H	-1.68395100	-4.18993800	5.75502500
O	2.23984100	3.64818000	-3.30055400	H	3.47791500	-4.35173900	-0.09117000	H	-0.47930600	-2.95460400	5.33196400
H	3.20363600	3.51210100	-3.35608500	C	1.49299200	-3.62647100	0.03491300	H	-2.20098500	-2.55365900	5.27812300
O	2.17774600	5.37515700	-0.62148800	H	1.21854000	-3.87328600	1.04930400	O	-3.97990300	1.57462300	0.67417700
H	1.89523400	5.02922800	0.24994400	C	3.80652800	-3.59647500	-2.81673100	C	-3.87814700	1.44023900	1.91833600
H	1.35908700	5.74885300	-1.00788100	H	3.51776300	-4.27884500	-3.63028200	O	-2.89788000	0.88580100	2.53978500
O	-1.65555900	2.81251700	-2.07138400	H	3.98458500	-2.62279200	-3.29473100	C	-4.97265100	1.97371300	2.82885800
C	-1.24823500	3.99875200	-1.94801200	C	5.13913000	-4.12831100	-2.22748500	H	-4.57213700	2.80674400	3.42112800
O	-0.01901200	4.35389700	-1.92797300	H	5.03361500	-5.18197000	-1.94463800	H	-5.28661200	1.19559900	3.53437700
C	-2.29582600	5.10653300	-1.84750900	H	5.90535700	-4.07841500	-3.01327900	H	-5.82816100	2.32406600	2.24445100
H	-2.91782100	5.02998500	-2.75132600	C	5.59221400	-3.38509400	-0.97191800	O	-0.29555800	0.81416700	3.36919000
H	-2.95854800	4.83695400	-1.01188300	O	5.31597900	-3.80931000	0.15821300	C	0.86726600	1.26376900	3.29639800
C	-1.75213000	6.52493000	-1.67864600	N	6.26251000	-2.21847200	-1.16255500	O	1.52371100	1.46750600	2.20480900
H	-1.09113700	6.79723500	-2.51002800	H	6.44118100	-1.91337900	-2.11122500	C	1.61975200	1.64570800	4.56110500
H	-1.18092600	6.62300400	-0.74626300	C	6.53154500	-1.28939500	-0.06014300	H	2.67778700	1.39144600	4.41201300
H	-2.57479900	7.25061800	-1.64326900	H	6.79770500	-1.89587000	0.81122600	H	1.58095200	2.74538100	4.62415700
O	-2.18398800	-3.01912900	-0.98111700	H	7.40813300	-0.68971000	-0.33735200	C	1.06200000	1.01397600	5.84107000
C	-3.32955300	-2.71863700	-1.49129000	C	5.32496900	-0.39605500	0.27744200	H	1.09842100	-0.08078200	5.74875100
O	-3.75120000	-1.56069700	-1.72995600	H	4.46722400	-1.03350300	0.51900100	H	0.00065400	1.27506400	5.93726400
C	-4.20855200	-3.93155600	-1.79356400	H	5.55933700	0.17508700	1.18735800	C	1.83535200	1.46042300	7.08653000
H	-3.55600700	-4.79490900	-1.97516700	C	4.94979300	0.56612800	-0.85408700	H	2.89687300	1.18263700	7.02262200
H	-4.76003000	-4.15717800	-0.86555200	H	4.89865300	0.01711600	-1.80962600	H	1.42348000	0.99619100	7.99166800
C	-5.19648600	-3.72644300	-2.94761800	H	5.70369900	1.35161100	-0.99099100	H	1.78541500	2.55039500	7.21891700
H	-4.63830800	-3.48942200	-3.86633200	O	2.68496100	0.62071700	-0.07663400	N	0.76436600	1.22921900	-2.17582500
H	-5.82128100	-2.84906900	-2.73478100	C	3.58623900	1.24194600	-0.71225300	H	0.35603400	0.28774600	-1.95341400
C	-6.08142500	-4.95432300	-3.18740900	O	3.45886700	2.35375000	-1.32083800	H	1.50660900	1.09827100	-2.86622500
H	-5.47892500	-5.84039400	-3.43129900	O	-0.94042800	-3.05964000	1.43561500	H	-0.00231300	1.75075700	-2.62054900

D:

Ca	-2.49769900	1.18434100	-1.26173200	C	-1.42556300	5.28605800	-1.88511800	N	2.01402500	-4.26959000	-0.56964700
Mn	-1.26893200	-1.69199800	-0.27511100	H	-2.02519600	5.25764600	-2.80670900	H	2.81742800	-4.68465700	-0.08618100
Mn	-1.26351900	0.22089500	1.71380300	H	-2.13479000	5.09411900	-1.06617000	C	0.89361100	-3.79772400	0.01926700
Mn	1.04959000	1.06301700	0.37070600	C	-0.75065000	6.64684900	-1.71561500	H	0.61449200	-3.97172400	1.04742700
Mn	2.39910700	3.23168000	-1.47719100	H	-0.03871900	6.83933100	-2.52664500	C	3.18722500	-4.05366200	-2.83802600
O	-2.36446800	-0.45292900	0.48808600	H	-0.20345100	6.70218700	-0.76547900	H	2.81947000	-4.66543100	-3.67509600
O	0.08330100	-0.70330100	0.80629200	H	-1.49944100	7.44908900	-1.71652700	H	3.50064700	-3.09837900	-3.28359200
O	-0.63265600	1.60947000	0.67775200	O	-2.79198900	-2.67701800	-0.94982100	C	4.43257600	-4.77369900	-2.26093500
O	-1.07955500	-0.85284700	-1.76531800	C	-3.86059100	-2.16387600	-1.46082500	H	4.17148800	-5.79384000	-1.95614400
O	1.69798400	2.66894100	0.10310000	O	-4.05532100	-0.94972000	-1.70966200	H	5.17974600	-4.85546800	-3.06230000
O	-4.91301900	1.67591900	-1.68356900	C	-4.95768300	-3.18893800	-1.74695500	C	5.02878500	-4.08982100	-1.03118400
H	-5.04216700	1.98496000	-0.76165200	H	-4.48790500	-4.17016800	-1.88909400	O	4.69494500	-4.42131000	0.11459300
H	-5.18512300	0.73447500	-1.68808900	H	-5.56052700	-3.26830600	-0.82692500	N	5.90537200	-3.07689900	-1.25955400
O	-2.51553500	0.32021000	-3.67377900	C	-5.86379500	-2.82759600	-2.92982900	H	6.14271800	-2.84564600	-2.21595400
H	-3.38328200	-0.12391400	-3.63942300	H	-5.25317000	-2.74041600	-3.84167000	C	6.39432000	-2.21660400	-0.17615000
H	-1.91472000	-0.37139400	-3.29318500	H	-6.30039900	-1.83505100	-2.75752800	H	6.60447700	-2.86472400	0.68087400
O	3.07483800	3.67857000	-3.10072200	C	-6.97566700	-3.85803000	-3.15384700	H	7.34261900	-1.77471600	-0.50783100
H	3.94382600	3.25187000	-3.21443400	H	-6.56180700	-4.85565900	-3.35637500	C	5.37946000	-1.13533200	0.23304700
O	3.01142200	5.00285100	-0.22460300	H	-7.62350600	-3.94223500	-2.26992700	H	4.43602400	-1.62335600	0.49991400
H	2.55260700	4.62458700	0.55530000	H	-7.60897300	-3.58005500	-4.00635100	H	5.74437000	-0.64056100	1.14431100
H	2.37684800	5.64043100	-0.60582700	N	0.20160200	-3.05719800	-0.83653900	C	5.12815100	-0.08970200	-0.85880700
O	-1.00236600	2.93771100	-2.06668700	C	0.91399200	-3.04131000	-2.01719700	H	5.04068100	-0.58307900	-1.84167400
C	-0.48734800	4.08285100	-1.94065700	H	0.54570100	-2.48304000	-2.86665200	H	5.95945600	0.62078700	-0.95094700
O	0.76836300	4.32211800	-1.88077000	C	2.06290500	-3.78293100	-1.87011500	O	2.90341700	0.20727000	-0.02450100

C	3.83422400	0.71025100	-0.70657300	O	-3.64659600	2.21005000	0.64577200	H	1.81969900	2.42513300	4.67315200
O	3.79086200	1.80074300	-1.38372300	C	-3.55918600	2.04207100	1.88945000	C	1.16777100	0.68851600	5.80718600
O	-1.47743300	-2.92581400	1.39563200	O	-2.68981200	1.31826600	2.49465700	H	1.14229500	-0.40323700	5.67713400
C	-1.75173600	-2.50314700	2.55882900	C	-4.53772500	2.75067200	2.81361900	H	0.12155300	1.00920200	5.88582800
O	-1.73160300	-1.28905300	2.93567700	H	-3.99400200	3.49743600	3.40683200	C	1.93146000	1.04242800	7.08778300
C	-2.16498500	-3.54696900	3.59235600	H	-4.97519900	2.03347600	3.51783900	H	2.97662500	0.70531500	7.03963600
H	-1.55509400	-4.44310500	3.41644300	H	-5.32512800	3.24830800	2.24023900	H	1.46986900	0.57184000	7.96545500
H	-3.19662200	-3.83554400	3.33608300	O	-0.17795100	0.78287500	3.31365300	H	1.94184500	2.12823300	7.25905800
C	-2.08402800	-3.08456200	5.04779900	C	1.05279400	1.04598800	3.26523200	N	0.82296200	0.83456900	-1.63157300
H	-2.42139400	-3.88251300	5.72186200	O	1.74103300	1.12303600	2.19399200	H	0.17643400	-0.01377600	-1.75218900
H	-1.05571800	-2.81762500	5.32220300	C	1.79440400	1.32823900	4.56302200	H	1.70056000	0.68452700	-2.13021300
H	-2.70811700	-2.19990500	5.21321700	H	2.83748700	1.01316600	4.42823800	H	0.31639500	1.65010700	-2.02253600

TS4:

Ca	-2.54779700	1.15684400	-1.19408200	H	-5.04335400	-3.78933100	-1.10217800	O	3.69891200	2.07620900	-1.27009400
Mn	-1.14493700	-1.72318900	-0.33149200	C	-5.87893800	-2.82937300	-2.86705300	O	-1.34777900	-3.05739200	1.21018000
Mn	-1.26568100	0.08757700	1.72234600	H	-5.50797400	-2.34972300	-3.78473000	C	-1.64397800	-2.71865900	2.40159400
Mn	1.00790200		1.11167000	H	-6.40661100	-2.04521200	-2.30702500	O	-1.67916900	-1.53604300	2.85329200
0.39655200				C	-6.85394800	-3.95504900	-3.22972300	C	-2.00282100	-3.85406900	3.35527100
Mn	2.16071700	3.35927300	-1.34089900	H	-6.35814300	-4.73889200	-3.81927100	H	-1.28651800	-4.66835600	3.17922700
O	-2.32672500	-0.59372800	0.44751100	H	-7.26647300	-4.43075700	-2.32887300	H	-2.97643200	-4.24108400	3.01657800
O	0.10590500	-0.76277700	0.77301900	H	-7.69664800	-3.57522200	-3.82179500	C	-2.05931700	-3.46347200	4.83224800
O	-0.71354200	1.53849400	0.75756000	N	0.39440800	-2.98244400	-0.96459500	H	-2.34225800	-4.32914500	5.44487300
O	-0.95063600	-0.75568800	-1.80015000	C	1.10890200	-2.87237200	-2.13904000	H	-1.08647500	-3.09801200	5.18314400
O	1.57140800	2.76181200	0.28286300	H	0.72301600	-2.28322900	-2.95910300	H	-2.78937200	-2.66418900	4.99955700
O	-4.98525700	1.51585200	-1.61818200	C	2.28689700	-3.57302400	-2.02611400	O	-3.77570300	1.96914200	0.76263400
H	-5.14991000	1.75301700	-0.68115500	N	2.25474300	-4.13126000	-0.75435000	C	-3.66807600	1.74579100	1.99493400
H	-5.20232000	0.56354900	-1.69361900	H	3.07551500	-4.53316600	-0.28890100	O	-2.74927500	1.04702100	2.55739300
O	-2.47838200	0.44478600	-3.65491800	C	1.11435900	-3.73856500	-0.14633300	C	-4.67747100	2.34638300	2.96053400
H	-3.30596900	-0.07191600	-3.64364000	H	0.84134500	-3.98014100	0.86973600	H	-4.17828800	3.11250700	3.56821300
H	-1.81714700	-0.21847800	-3.33578500	C	3.42296500	-3.74523800	-3.00254400	H	-5.04573000	1.57602600	3.64774300
O	2.71592200	3.81174600	-3.00898700	H	3.08705500	-4.33954800	-3.86522900	H	-5.51057600	2.80296100	2.41848500
H	3.60970600	3.45112500	-3.15483100	H	3.68538900	-2.75685900	-3.40658700	O	-0.20988100	0.58853100	3.33590600
O	2.78072500	5.15580700	-0.09673100	C	4.70397700	-4.42363100	-2.45340800	C	1.01683300	0.89731000	3.30848300
H	2.41417800	4.73988400	0.71163000	H	4.49846900	-5.47034600	-2.20060800	O	1.70346700	1.05402400	2.25163900
H	2.05949100	5.72622100	-0.42917700	H	5.45760500	-4.42476300	-3.25284700	C	1.72471700	1.13018800	4.63454500
O	-1.21722800	3.05042700	-1.88474700	C	5.25511200	-3.76879300	-1.18744600	H	2.80289800	1.01445400	4.46742600
C	-0.73584100	4.20107600	-1.70280200	O	4.93442600	-4.17507300	-0.06202200	H	1.56001100	2.18948400	4.89262900
O	0.51244500	4.46966800	-1.61402300	N	6.07309100	-2.69780800	-1.35987900	C	1.23089100	0.23508000	5.77879800
C	-1.70574500	5.37670700	-1.60742700	H	6.29736900	-2.40508500	-2.30254700	H	1.39310000	-0.81875300	5.50732200
H	-2.29148300	5.37300400	-2.53831400	C	6.49835900	-1.85771500	-0.23450600	H	0.14636100	0.36068700	5.88563200
H	-2.42120300	5.13066400	-0.80873200	H	6.73444700	-2.52880100	0.59765200	C	1.93684800	0.54323800	7.10344400
C	-1.07006700	6.74607300	-1.36910500	H	7.42393600	-1.34923000	-0.53334400	H	3.02372400	0.39995300	7.02335500
H	-0.35415000	6.99310100	-2.16175000	C	5.41824800	-0.85362600	0.20337700	H	1.57288100	-0.11053200	7.90662200
H	-0.53609900	6.77413200	-0.41036200	H	4.50244300	-1.40496700	0.44195400	H	1.76222800	1.58277000	7.41518400
H	-1.84010400	7.52768000	-1.34529300	H	5.74604600	-0.37258200	1.13587200	N	0.74492700	0.99233900	-1.55806300
O	-2.58446300	-2.73223300	-1.16015200	C	5.11581400	0.21561000	-0.85212800	H	-0.03780800	-0.01903000	-1.69961900
C	-3.67900500	-2.25268000	-1.64836600	H	5.04863700	-0.24889900	-1.85058100	H	1.59734700	0.84673500	-2.10060900
O	-3.94757800	-1.03811000	-1.80908800	H	5.91256000	0.96704400	-0.91984200	H	0.21286400	1.79500700	-1.93233200
C	-4.69183600	-3.32910700	-2.03944000	O	2.87036000	0.35788700	-0.03617600				
H	-4.14746900	-4.12475300	-2.56755400	C	3.78679200	0.94828000	-0.67166500				

E:

Ca	-2.75442300	0.78677300	-1.15925700	O	0.25590300	-0.72620100	0.74061300	H	-5.31647500	-0.21081900	-1.56571200
Mn	-0.84469100	-1.83334600	-0.26803200	O	-0.84645800	1.47630400	0.79644400	O	-2.61034400	0.11851700	-3.63548500
Mn	-1.17774800	-0.01797700	1.73523200	O	-0.79078900	-0.75799300	-1.78767400	H	-3.28927500	-0.57994000	-3.56870500
Mn	0.94148000	1.35484000	0.37966800	O	1.26031100	3.06023100	0.44096800	H	-1.78685600	-0.36429000	-3.39769700
Mn	1.53396300	3.53369100	-1.34235000	O	-5.23218100	0.76030700	-1.48212600	O	1.90982000	3.92649300	-3.07448100
O	-2.16529700	-0.88300900	0.48183400	H	-5.40195800	0.96457400	-0.53875700	H	2.86699600	3.80009500	-3.21147800

O	1.81965600	5.53535700	-0.48603200	N	2.81132700	-3.80746400	-0.81796900	H	-0.49824400	-4.76393400	3.15441900
H	1.69991000	5.27126700	0.44865100	H	3.68282200	-4.12295600	-0.37594400	H	-2.23263400	-4.64213000	2.95641800
H	0.91924700	5.80135100	-0.78319500	C	1.64988500	-3.54952100	-0.18047600	C	-1.50518100	-3.74392200	4.80495000
O	-1.87838800	2.85394300	-1.84503800	H	1.43200900	-3.82986200	0.83887200	H	-1.64076300	-4.65695400	5.39845600
C	-1.60116500	4.07653600	-1.62895500	C	3.88229400	-3.27032100	-3.08111900	H	-0.62029100	-3.21687400	5.18126800
O	-0.42772900	4.53578300	-1.50079200	H	3.60356800	-3.89265900	-3.94432800	H	-2.36961900	-3.09102700	4.96782200
C	-2.77875500	5.04747300	-1.53589300	H	4.01797500	-2.25414000	-3.47814100	O	-4.00651400	1.37285900	0.86159000
H	-3.36638300	4.92011900	-2.45661800	C	5.24349400	-3.79655200	-2.55760800	C	-3.80707700	1.20891400	2.08984600
H	-3.42614800	4.68648100	-0.72222500	H	5.17307800	-4.86627600	-2.32900900	O	-2.75749200	0.68665000	2.61871300
C	-2.40515700	6.51414200	-1.32340700	H	5.98343100	-3.68406800	-3.36179700	C	-4.85031500	1.66909000	3.09440300
H	-1.76110100	6.87841600	-2.13278500	C	5.71963800	-3.10742700	-1.27866400	H	-4.47892200	2.56876400	3.60296900
H	-1.86591900	6.65290500	-0.37785500	O	5.47640200	-3.59013300	-0.16309500	H	-5.00553200	0.90135200	3.86046600
H	-3.30538800	7.14163600	-1.29316500	N	6.37277700	-1.92728700	-1.42724800	H	-5.79302100	1.90667900	2.59314400
O	-2.10086900	-3.00886900	-1.19692700	H	6.52319500	-1.57260600	-2.36356400	O	-0.16701200	0.56509400	3.32470300
C	-3.27872100	-2.72280000	-1.63690800	C	6.66305500	-1.05033500	-0.28654400	C	1.02797000	0.98682900	3.27849800
O	-3.75258000	-1.56758600	-1.76395400	H	6.96078900	-1.69652600	0.54515000	O	1.67348500	1.21805400	2.21265600
C	-4.10528600	-3.94821800	-2.02327400	H	7.52511800	-0.42808500	-0.55926400	C	1.73745600	1.26486400	4.59382200
H	-3.46785200	-4.59675100	-2.64173200	C	5.45765700	-0.18811000	0.12692300	H	2.81774700	1.20389900	4.41123900
H	-4.28252800	-4.51651600	-1.09652400	H	4.61327400	-0.84573100	0.36143100	H	1.52452300	2.31814300	4.84098800
C	-5.42912700	-3.64339500	-2.72891700	H	5.71248500	0.34004900	1.05703800	C	1.30716300	0.35904600	5.75449400
H	-5.23245500	-3.05382200	-3.63611100	C	5.04041000	0.82459000	-0.94472400	H	1.51623300	-0.68852100	5.49103300
H	-6.04700500	-3.00626900	-2.08102900	H	4.96359200	0.31987600	-1.92290300	H	0.21972600	0.43195400	5.87990200
C	-6.20179800	-4.91547600	-3.09530200	H	5.78452300	1.62175800	-1.06501000	C	2.01959400	0.71647100	7.06328600
H	-5.61835800	-5.55691100	-3.77051300	O	2.78524400	0.77363400	-0.15069500	H	3.11062500	0.62570500	6.96552900
H	-6.44119500	-5.50826200	-2.20132600	C	3.67743500	1.48778200	-0.73112300	H	1.70187400	0.05482300	7.87948400
H	-7.14698500	-4.67438900	-3.59847100	O	3.51779500	2.64208400	-1.20549400	H	1.79944500	1.74962900	7.36703800
N	0.82972600	-2.87320800	-0.97419000	O	-0.87423400	-3.17569800	1.18633600	N	0.69702300	1.63071700	-1.55284800
C	1.49946200	-2.67663700	-2.16421800	C	-1.18012300	-2.89274100	2.40170700	H	-0.03242800	-0.14922800	-1.65383600
H	1.03163000	-2.13816500	-2.97659300	O	-1.35154600	-1.73900600	2.86994900	H	1.26433400	1.16885600	-2.26321900
C	2.75161100	-3.24079200	-2.08385400	C	-1.35236000	-4.09350900	3.32483800	H	-0.22321900	1.94400500	-1.90260700

F:

Ca	-2.71981300	0.87976500	-1.15003100	H	1.11591200	5.78083100	-0.76101000	C	-6.35110500	-4.70707600	-3.14441900
Mn	-0.90767600	-1.82121400	-0.27662300	O	-1.77483800	2.91872900	-1.84062800	H	-5.78705100	-5.35886800	-3.82617200
Mn	-1.18818000	-0.01655000	1.73466700	C	-1.44618300	4.12770100	-1.62921000	H	-6.61103000	-5.30232300	-2.25783200
Mn	0.96771200	1.32166800	0.38373900	O	-0.25382400	4.54110200	-1.50523300	H	-7.28715800	-4.43013500	-3.64624200
Mn	1.65126400	3.48256400	-1.33869500	C	-2.58054500	5.14929300	-1.53738100	N	0.73679200	-2.90821700	-0.98369100
O	-2.20825700	-0.83197700	0.47515400	H	-3.16945800	5.04964300	-2.46072900	C	1.41413200	-2.71827700	-2.17046100
O	0.22871500	-0.76367900	0.74798500	H	-3.24618100	4.81460800	-0.72729300	H	0.96012400	-2.16468100	-2.98048600
O	-0.81540700	1.46848200	0.78464200	C	-2.14524700	6.59811000	-1.32005800	C	2.65442700	-3.30779000	-2.08964400
O	-0.82086200	-0.73978500	-1.77928600	H	-1.48299300	6.93621000	-2.12606400	N	2.69908600	-3.88270500	-0.82681300
O	1.32274900	3.02390500	0.44814500	H	-1.60465500	6.71178700	-0.37187400	H	3.56340800	-4.21588800	-0.38377800
O	-5.19654700	0.91714700	-1.47799400	H	-3.01792700	7.26348500	-1.29181900	C	1.54081700	-3.60513800	-0.19140600
H	-5.36430300	1.11897600	-0.53384100	O	-2.19586800	-2.95475000	-1.21519600	H	1.31501700	-3.88612700	0.82609300
H	-5.30360100	-0.05136100	-1.56842000	C	-3.36177100	-2.62542900	-1.65747800	C	3.78640400	-3.35485000	-3.08469100
O	-2.60131500	0.21316400	-3.62839600	O	-3.79687300	-1.45426800	-1.77618300	H	3.49627400	-3.96583500	-3.95224000
H	-3.30465500	-0.46094000	-3.56188000	C	-4.22658100	-3.81959400	-2.05842600	H	3.94448300	-2.33936300	-3.47518000
H	-1.79627800	-0.30037400	-3.39212500	H	-3.60931300	-4.48092100	-2.68381600	C	5.13507700	-3.91303900	-2.56226600
O	2.05034800	3.87965400	-3.06050100	H	-4.42294300	-4.39264500	-1.13851900	H	5.04030400	-4.98154100	-2.33661300
H	3.00864200	3.75221600	-3.18805300	C	-5.53898700	-3.46465100	-2.76195500	H	5.87748200	-3.81537700	-3.36611400
O	2.00542300	5.49157100	-0.45532400	H	-5.32222500	-2.87085700	-3.66176300	C	5.62687800	-3.23842700	-1.28160000
H	1.86554400	5.21929700	0.47381400	H	-6.13736900	-2.81591500	-2.10731500	O	5.36782200	-3.71481100	-0.16693300
N	6.31396700	-2.07727600	-1.42781900	H	5.73114400	0.19286200	1.07316400	O	-0.98948900	-3.16857900	1.17312900
H	6.47877500	-1.72722400	-2.36341000	C	5.06611300	0.71386100	-0.92166500	C	-1.27903200	-2.87998200	2.38952200
C	6.63519800	-1.21436300	-0.28480500	H	4.97789400	0.22194300	-1.90541600				
H	6.91828100	-1.87253900	0.54266600	H	5.82857300	1.49477700	-1.03312100	O	-1.41442400	-1.72004000	2.85817900
H	7.51359200	-0.61618600	-0.55923200	O	2.81208200	0.70993100	-0.12390700	C	-1.48066800	-4.07317100	3.31577500
C	5.45763800	-0.31985600	0.13973800	C	3.71854300	1.40450000	-0.70092300	H	-0.64162500	-4.76324200	3.14848600
H	4.59518500	-0.95432300	0.37206100	O	3.58559100	2.56777500	-1.16733300	H	-2.37239800	-4.60278500	2.94726400

C	-1.62748500	-3.71654800	4.79483500	H	-5.73207200	2.06134700	2.60589100	H	0.21420800	0.41600400	5.88607900
H	-1.78414900	-4.62489800	5.39029900	O	-0.16354600	0.54400800	3.32864300	C	2.02070000	0.65320800	7.06981200
H	-0.73161100	-3.20834200	5.17099400					H	3.10885200	0.53204900	6.97285400
H	-2.47746900	-3.04427800	4.95515100	C	1.03834000	0.94328400	3.28393600	H	1.68439300	0.00240200	7.88728000
O	-3.95966000	1.48594500	0.87250200	O	1.68851900	1.16675200	2.21863500	H	1.82911600	1.69272800	7.37120400
C	-3.76810400	1.30626500	2.09972800	C	1.75506900	1.20363100	4.59907100	N	0.74871900	1.56764200	-1.56500300
O	-2.73839100	0.74391700	2.62682300	H	2.83333300	1.11206400	4.41703000	H	-0.05502500	-0.13503300	-1.64361800
C	-4.79599900	1.79652300	3.10597800	H	1.57225200	2.26316200	4.84365600	H	1.31706400	1.08974800	-2.26287400
H	-4.39799500	2.68573900	3.61289400	C	1.29927100	0.31274700	5.76140100	H	-0.14615800	1.92437400	-1.93248300
H	-4.97222800	1.03427700	3.87288000	H	1.47931800	-0.74079800	5.50039500				

G:

Ca	-2.71827700	0.75901000	-1.04689100	H	-4.22898800	-4.38162400	-1.52099900	C	3.40040200	1.54728900	-0.67974200
Mn	-0.65296600	-1.90162400	-0.31999300	C	-4.90039300	-3.64949900	-3.45242300	O	3.06672800	2.61085100	-1.32168100
Mn	-1.25921200	-0.21796700	1.75611700	H	-4.45714700	-3.19477300	-4.35174400	O	-0.63397800	-3.40021500	1.24542100
Mn	0.71796500	1.36399500	0.55747100	H	-5.58403200	-2.89765300	-3.03550000	C	-1.06852400	-3.10302600	2.39744200
Mn	1.29206400	3.36254800	-1.29663000	C	-5.68587100	-4.90518600	-3.84657000	O	-1.36160100	-1.93437000	2.80735700
O	-2.08755200	-1.03297100	0.36799900	H	-5.02882200	-5.66303100	-4.29541800	C	-1.26635800	-4.25297300	3.38434400
O	0.28532000	-0.64606600	0.82365400	H	-6.16815600	-5.36294600	-2.97157400	H	-0.33928500	-4.84421800	3.37664400
O	-1.05988200	1.40522500	0.91619900	H	-6.47196500	-4.67049700	-4.57597600	H	-2.03383900	-4.90812100	2.94475600
O	-0.58128700	-0.44905000	-2.17654400	N	1.12673000	-2.74695900	-1.00848200	C	-1.65016600	-3.83965900	4.80503800
O	1.11483600	3.09482000	0.51640700	C	1.82701800	-2.52213100	-2.17624400	H	-1.77936700	-4.72598700	5.44023000
O	-5.17888400	0.54347800	-1.57683400	H	1.37196000	-1.99586400	-3.00320400	H	-0.87847900	-3.20303700	5.25389700
H	-5.38627700	0.69197800	-0.62745400	C	3.09722400	-3.03484600	-2.05772300	H	-2.58572200	-3.26922100	4.80958900
H	-5.13841500	-0.42849200	-1.69068700	N	3.14180100	-3.59641000	-0.78784300	O	-4.18533200	1.06733600	0.85511100
O	-2.79224300	0.46522600	-3.61152700	H	4.00974700	-3.86731000	-0.31524100	C	-4.02349700	0.79955400	2.07802900
H	-3.34041100	1.05747500	-4.15245300	C	1.95033100	-3.38677900	-0.18717100	O	-2.96583000	0.31584100	2.60566900
H	-3.29516100	-0.37215900	-3.48512400	H	1.70172200	-3.68177700	0.82195900	C	-5.15142500	1.09983300	3.05292200
O	1.51265700	3.81487500	-3.04413500	C	4.24618700	-3.04155700	-3.03348300	H	-4.99648200	2.10647700	3.46541800
H	2.39657000	3.50991200	-3.31950800	H	4.02612700	-3.72422100	-3.86795100	H	-5.14422800	0.39061200	3.88617000
O	2.05440200	5.31189900	-0.51308500	H	4.32249000	-2.04012000	-3.48062400	H	-6.11884300	1.08504500	2.54082000
H	1.89242900	5.00668200	0.40609300	C	5.62645300	-3.45155200	-2.45933400	O	-0.40308800	0.41778800	3.42643400
H	1.25472500	5.82125500	-0.75093200	H	5.62603200	-4.51498300	-2.19407800	C	0.73397700	0.98478300	3.47638700
O	-2.08561200	2.97434800	-1.65951400	H	6.38023000	-3.31283000	-3.24652700	O	1.41470600	1.33576300	2.47074900
C	-1.62598200	4.13498700	-1.48301600	C	6.00910400	-2.68633000	-1.19357200	C	1.29816400	1.28312000	4.85865400
O	-0.38678400	4.42963300	-1.35677900	O	5.79065600	-3.15721100	-0.06937300	H	2.36231800	1.52396300	4.74602100
C	-2.61615700	5.29452400	-1.42234500	N	6.54521900	-1.45067100	-1.36945000	H	0.79788600	2.19951400	5.21226100
H	-3.21059500	5.24440100	-2.34620300	H	6.67633800	-1.11132900	-2.31423900	C	1.08108000	0.15478200	5.87717000
H	-3.31758300	5.05952100	-0.60823900	C	6.72130100	-0.51372600	-0.25419700	H	1.57679000	-0.75825200	5.51393800
C	-2.00743500	6.68410100	-1.23805700	H	7.11425800	-1.08717200	0.59157200	H	0.00946000	-0.07492300	5.92682200
H	-1.31227900	6.92289800	-2.05195300	H	7.48552400	0.21457700	-0.55441100	C	1.61490500	0.51349400	7.26795500
H	-1.45823500	6.75307200	-0.29086500	C	5.41286500	0.18222000	0.15734600	H	2.69308600	0.72623200	7.24253200
H	-2.79524200	7.44801300	-1.22625500	H	4.68029600	-0.57916700	0.44635400	H	1.45398700	-0.30795100	7.97846000
O	-1.82243800	-3.00314300	-1.51463900	H	5.60731400	0.78498200	1.05575700	H	1.11145100	1.40459000	7.66909700
C	-2.97903800	-2.73482200	-1.98583800	C	4.82524800	1.06996300	-0.94407500	N	0.48454000	1.67553800	-1.34039100
O	-3.47645600	-1.57369200	-2.09000600	H	4.77339700	0.51160200	-1.89338900	H	0.10009200	0.31320500	-2.05774500
C	-3.79334600	-3.94583600	-2.43562800	H	5.44907600	1.95202200	-1.13819200	H	-0.47122100	2.04998500	-1.47400600
H	-3.09355700	-4.70095300	-2.81716200	O	2.66624600	0.87109400	0.07829600	H	-0.94084000	-0.39989900	-3.08252800

TS10:

Ca	2.58409100	-0.65776500	-0.88777600	O	5.02386900	-1.10241000	-1.42677800	H	0.10946700	-3.51536900	3.78574500
Mn	-0.29566500	1.05911900	-1.36373400	H	5.29126400	-0.24894600	-1.02449300	O	3.56803600	-2.20252900	0.75089300
Mn	1.23880400	2.08094300	0.62488900	H	5.09465800	-1.75267700	-0.70008200	C	3.47706600	-3.12994500	1.57804500
Mn	-0.04405200	-0.25982300	1.43637400	O	2.37695400	-2.98323000	-1.77691500	O	2.38684800	-3.76604900	1.85566400
Mn	0.56666600	-3.30801100	1.28667300	H	2.08791900	-2.96204400	-2.70332500	C	4.69703600	-3.60447200	2.36376600
O	1.40463100	1.50728000	-1.12911500	H	1.82034500	-3.66439000	-1.30934000	H	4.52553000	-3.31610300	3.41244100
O	-0.52226100	1.42898800	0.42713800	O	0.72073400	-4.47363800	-0.19597600	H	4.69478000	-4.70275700	2.35222100
O	1.66047000	0.46064200	1.22490000	H	-0.14182800	-4.87614800	-0.39739100	C	6.02977300	-3.04514800	1.86805400
O	0.04922700	-0.74384700	-0.74983900	O	0.22842300	-4.37862300	3.34160700	H	6.03049000	-1.94915400	1.89423900
O	0.57118900	-1.76950400	2.17455700	H	1.19352800	-4.53706800	3.39409300	H	6.23530800	-3.36263000	0.83715100

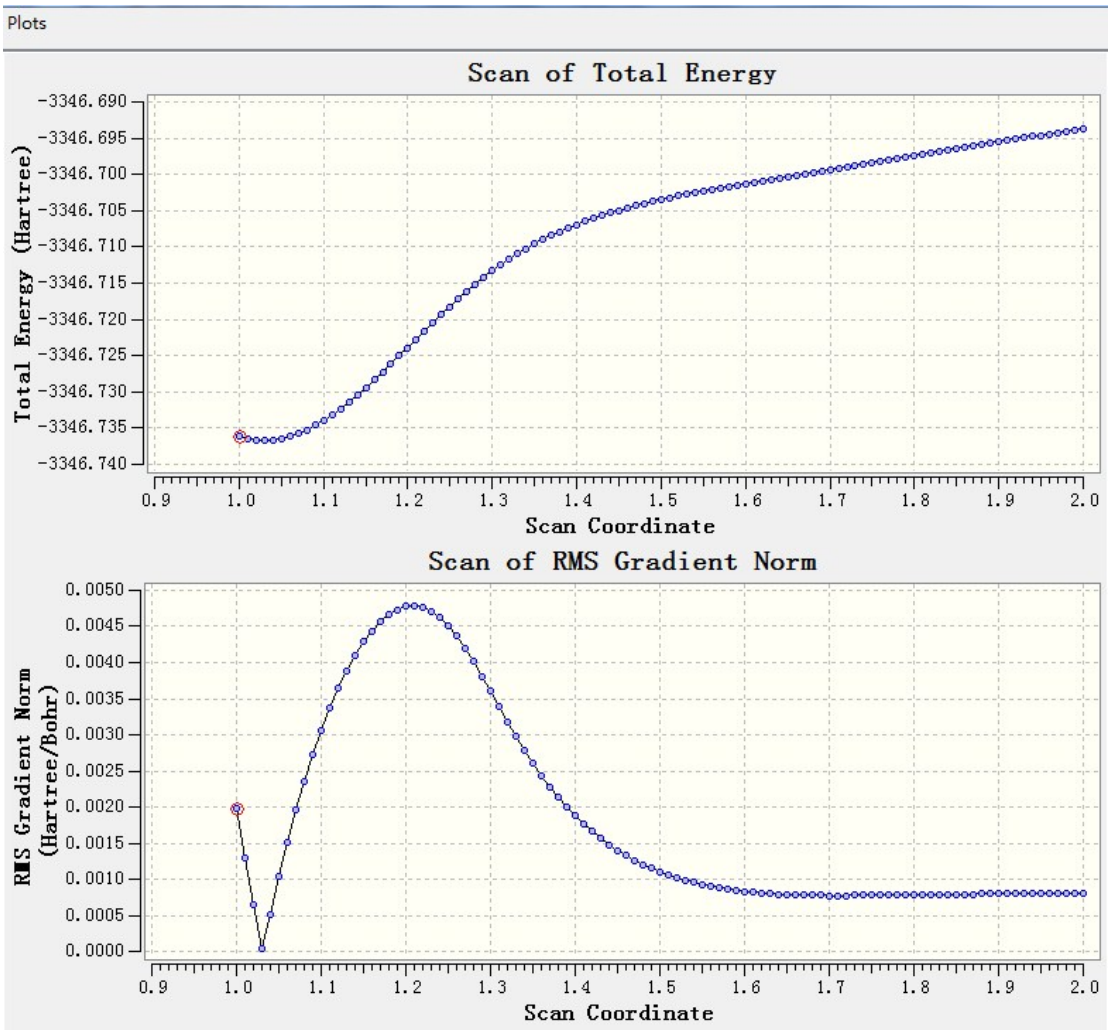
H	6.85528400	-3.40260200	2.49637700	H	-7.38370600	0.51788700	-1.72808600	H	-0.58531300	6.45518000	0.08417300
O	-0.11093000	0.61774400	-3.23627600	H	-7.71985100	-1.19974800	-1.96887800	H	0.98665800	6.46770800	-0.72296400
C	0.93884900	0.12222400	-3.82252600	C	-6.73761900	-0.66300300	-0.10022100	O	4.19595100	1.16076800	-0.25735500
O	1.88021700	-0.46023000	-3.25120200	O	-6.66243500	0.31766400	0.65240200	C	4.10153700	2.27028600	0.30884800
C	0.94558900	0.30827100	-5.33729100	N	-6.55441200	-1.93056500	0.34950500	O	3.00278000	2.81207000	0.72067900
H	-0.08515600	0.20595900	-5.70425900	H	-6.59139200	-2.69287700	-0.31587400	C	5.34103300	3.10328400	0.58592100
H	1.21740800	1.36172800	-5.51622700	C	-6.09914000	-2.20873400	1.71681800	H	5.53079000	3.11439700	1.66736600
C	1.90600100	-0.61935700	-6.08758100	H	-6.72127200	-1.62025900	2.40003300	H	6.21008000	2.68621600	0.06936700
H	1.61899200	-1.66602200	-5.90327700	H	-6.29473800	-3.27062400	1.91193900	H	5.17529300	4.14051700	0.27357000
H	2.91345000	-0.50510900	-5.66792200	C	-4.61739600	-1.86668400	1.95145800	O	0.81449700	2.74706300	2.40629700
C	1.92420000	-0.34847500	-7.59580200	H	-4.46857800	-0.79293600	1.79891400	C	0.13281400	2.11101400	3.29424800
H	0.92847900	-0.48420500	-8.04136200	H	-4.38705200	-2.06974000	3.00739700	O	-0.37395700	0.96666600	3.16256600
H	2.24439400	0.68070500	-7.81084800	C	-3.66375800	-2.65599500	1.04869300	C	-0.04269400	2.84132200	4.62000600
H	2.61587300	-1.02663400	-8.11214600	H	-3.73337800	-3.73600200	1.23022300	H	-0.73806600	2.26054100	5.23772300
N	-2.36170000	0.74866400	-1.50855200	H	-3.92637200	-2.49103600	-0.00838500	H	0.93629200	2.83015600	5.12512100
C	-3.13171300	-0.08657200	-2.28811400	O	-1.92262800	-1.04819200	1.40599900	C	-0.51626100	4.29567700	4.46448300
H	-2.67779500	-0.75204100	-3.00757200	C	-2.19698800	-2.25553400	1.16423700	H	-1.48560400	4.30560600	3.94286400
C	-4.45569000	0.05880300	-1.94328200	O	-1.36222500	-3.20289400	0.94678800	H	0.19103700	4.82978500	3.81766300
N	-4.46486900	1.03093000	-0.94896700	O	-0.70764900	2.93127300	-1.80277400	C	-0.65031100	5.01251200	5.81207700
H	-5.27238000	1.25091300	-0.36024200	C	-0.18350100	3.92722200	-1.17933800	H	-1.37089800	4.50367700	6.46775600
C	-3.19001000	1.40106900	-0.70381800	O	0.56742700	3.86948900	-0.17004600	H	-0.99344800	6.04683400	5.67838600
H	-2.88525700	2.09522000	0.06596000	C	-0.52617700	5.29452000	-1.76013500	H	0.31263300	5.04618000	6.34103000
C	-5.68321100	-0.65110300	-2.45476200	H	-1.60751900	5.30623900	-1.95413900	N	-0.86507600	-2.48546400	-2.23099200
H	-5.92342100	-0.31146100	-3.47333800	H	-0.04891500	5.33598800	-2.75122700	H	-0.54557600	-1.44714500	-1.32840700
H	-5.43938900	-1.71890400	-2.54961000	C	-0.09491400	6.47972500	-0.89642600	H	-0.39269100	-3.30464700	-1.82190200
C	-6.96798700	-0.48775700	-1.60135900	H	-0.35886000	7.42400500	-1.38950500	H	-0.37722800	-2.30837500	-3.11915300

J:

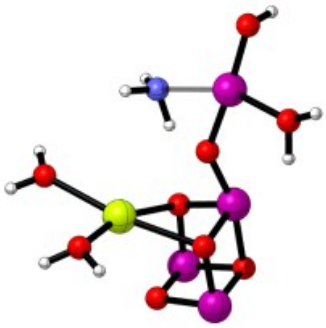
Ca	-2.56952600	-0.87043500	0.83800500	O	0.12667600	0.15533400	3.32324200	C	6.15199300	-1.62544300	-2.11740600
Mn	0.24360900	0.83482700	1.52395100	C	-0.88525800	-0.47669400	3.84524800	H	6.74921200	-0.90549000	-2.68741300
Mn	-1.34441400	2.09111600	-0.29193100	O	-1.85535900	-0.94061800	3.21970600	H	6.37353300	-2.62842800	-2.50298600
Mn	0.01092900	0.00096500	-1.53938800	C	-0.80363400	-0.60888700	5.36400300	C	4.65765000	-1.28995400	-2.27264700
Mn	-0.43863300	-3.06971300	-1.75885700	H	0.24384600	-0.79673200	5.63874000	H	4.48307400	-0.26236200	-1.93818200
O	-1.46620000	1.26351000	1.36193300	H	-1.04114100	0.38601000	5.77547600	H	4.41377800	-1.31670800	-3.34431900
O	0.43196800	1.46917300	-0.21731800	C	-1.73874200	-1.66540900	5.95921600	C	3.74357300	-2.24926100	-1.50547900
O	-1.72011500	0.56686300	-1.13854900	H	-1.48422200	-2.65154400	5.54272200	H	3.83315900	-3.27887500	-1.87514700
O	-0.07089100	-0.88003300	0.75551000	H	-2.76568300	-1.45791600	5.63300300	H	4.03301600	-2.26942200	-0.44245700
O	-0.52799300	-1.45087200	-2.47401700	C	-1.66695300	-1.71618800	7.48922300	O	1.93414200	-0.67245400	-1.62320100
O	-4.98904200	-1.51770400	1.24271900	H	-0.65079400	-1.95077700	7.83725200	C	2.26186000	-1.88448500	-1.51442600
H	-5.28747600	-0.62192100	0.97500600	H	-1.95306400	-0.75232200	7.93347300	O	1.47085600	-2.87884400	-1.34918400
H	-5.04093800	-2.05439300	0.42847600	H	-2.34232800	-2.48176300	7.89283100	O	0.62531400	2.64184200	2.20376100
O	-2.07836000	-3.22140700	1.46321500	N	2.32069100	0.55535000	1.59374500	C	0.05344100	3.70001000	1.74731800
H	-1.57227200	-3.14302600	2.28999000	C	3.12326000	-0.36977500	2.22394800	O	-0.72472100	3.76533100	0.76024400
H	-1.50326500	-3.72534100	0.82279300	H	2.69665200	-1.12795900	2.86623500	C	0.37232400	4.97861100	2.51449400
O	-0.52132400	-4.44069000	-0.43201600	C	4.43883500	-0.13909200	1.88687200	H	1.45818900	4.99840500	2.68108300
H	-1.14996000	-5.13489600	-0.69628100	N	4.40532500	0.97361400	1.05471000	H	-0.07635600	4.85870600	3.51251800
O	-0.00550300	-3.68997900	-3.99877600	H	5.20121600	1.31940800	0.51163900	C	-0.11907500	6.26226300	1.84564400
H	-0.94754700	-3.91413800	-4.13491700	C	3.11796400	1.34456000	0.88836300	H	0.13035000	7.13298100	2.46554100
H	0.01905300	-2.72127900	-4.15507800	H	2.78131900	2.14037100	0.23965500	H	0.34296900	6.39788500	0.86034200
O	-3.40411600	-2.28217300	-1.02317600	C	5.69614600	-0.88482200	2.25941100	H	-1.20434300	6.23861000	1.69844800
C	-3.31672800	-3.03375100	-2.01150500	H	5.92272800	-0.73740700	3.32578600	O	-4.26462000	0.92898800	0.46517600
O	-2.21967100	-3.59942600	-2.40916600	H	5.50022700	-1.96108000	2.14624300	C	-4.21660200	2.11954900	0.08327900
C	-4.53677000	-3.35491100	-2.86987500	C	6.97301500	-0.51052200	1.46183400	O	-3.14635000	2.76055700	-0.24258600
H	-4.38174200	-2.84026100	-3.83086900	H	7.34239200	0.47221400	1.77453100	C	-5.49268500	2.93357900	-0.04982100
H	-4.51512000	-4.42854300	-3.10068800	H	7.75540800	-1.24411000	1.70067800	H	-5.71455200	3.07829500	-1.11560300
C	-5.87373900	-2.94268800	-2.25539500	C	6.75392200	-0.41854500	-0.04909800	H	-6.33159800	2.41861100	0.42699800
H	-5.89497100	-1.86633300	-2.04831500	O	6.64188900	0.67937800	-0.61106800	H	-5.35495600	3.92648100	0.39246100
H	-6.06193000	-3.47745800	-1.31476300	N	6.61624100	-1.58751700	-0.72460300	O	-1.00605300	3.08237100	-1.93202700
H	-6.69991400	-3.17403100	-2.93921500	H	6.68957300	-2.45765000	-0.21208700	C	-0.31978200	2.66851700	-2.94126500

O	0.25090900	1.55380400	-3.03786600	H	1.18176200	5.01986000	-3.20091200	H	-0.74517200	6.13191100	-5.34167700
C	-0.23100900	3.65072000	-4.10337000	H	-0.50723200	5.43033900	-2.91687300	N	1.26150500	-3.33980500	1.57822800
H	0.46034800	3.23526700	-4.84634900	C	0.24021300	6.04009600	-4.86327300	H	0.49466000	-1.58024000	1.16290300
H	-1.22913500	3.69439800	-4.56741000	H	0.95110700	5.70383000	-5.63123200	H	0.79753900	-3.98214300	0.90568700
C	0.19197100	5.06715200	-3.68053300	H	0.54832300	7.04311100	-4.53978200	H	2.12655600	-3.82618000	1.86204300

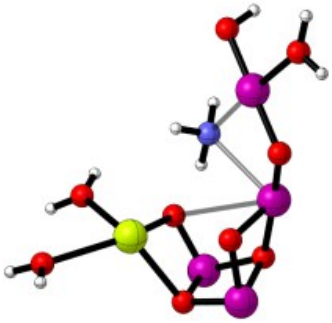
Relaxed PES scan plots for step9:



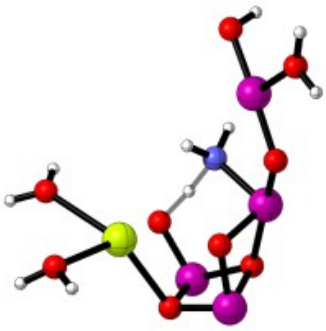
3D image for TSs (All the amino acid ligands are not shown for clarity, the same below):



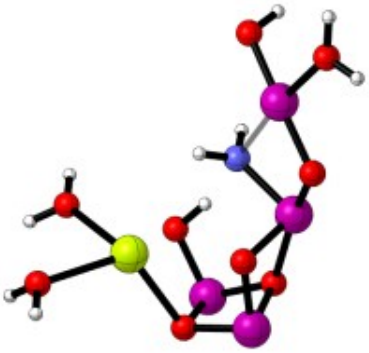
TS2



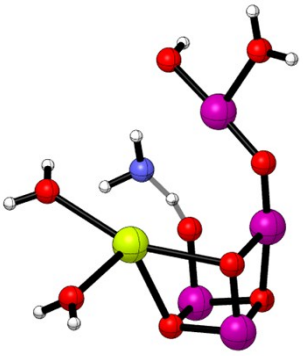
TS3



TS4

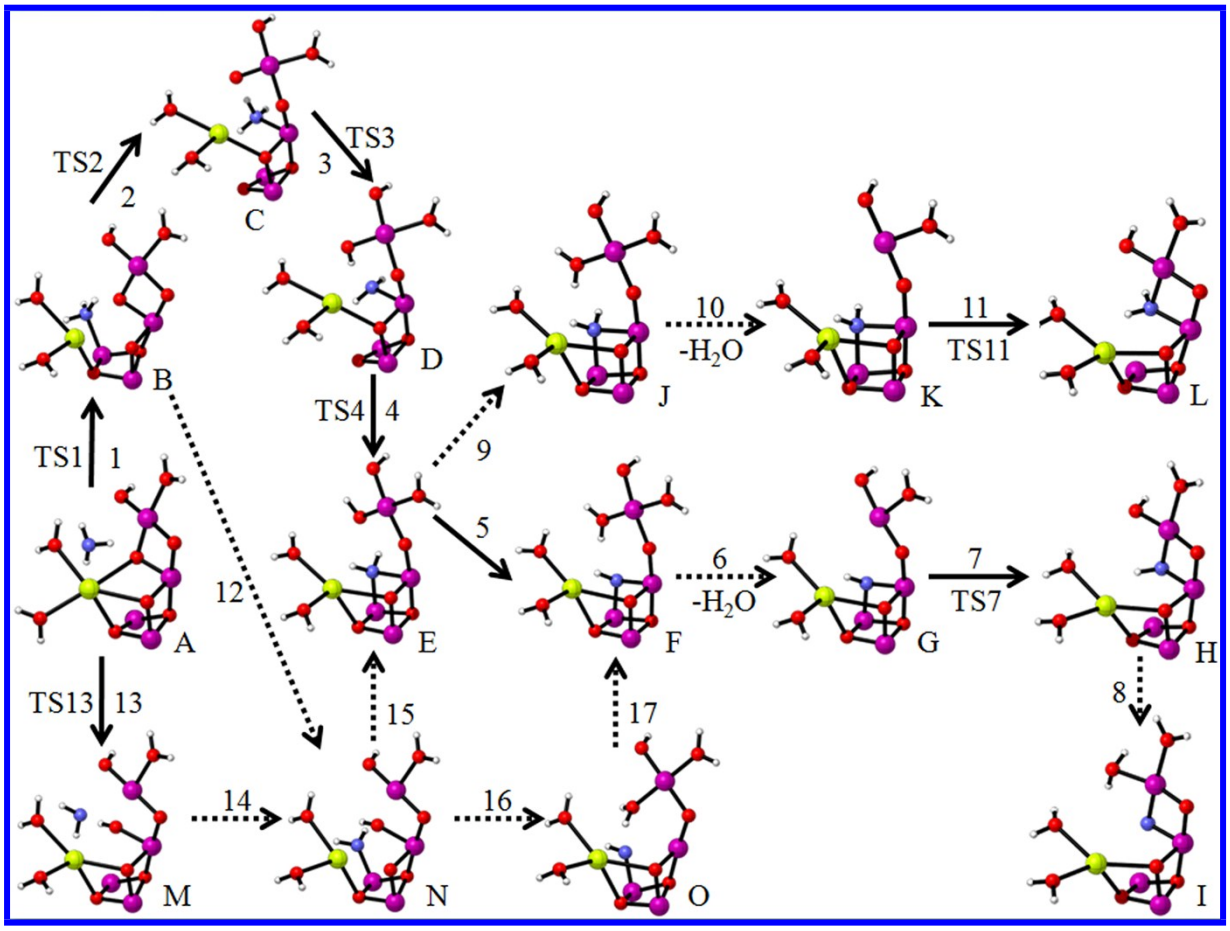


$TS_{E\text{-}F}$:



TS10

IIIb. Open-cubane structure as reactant



Scheme S2. Here are specific annotations for each step: 1: NH_3 binding to Mn1; 2: Mn3 ligand exchange between NH_3 and O5; 3: PT from NH_3 to O5; 4: NH_2^- flipping and binding to Mn1; 5: PCET of PT from NH_2^- to $O5H^-$ and ET from Mn4 to Mn1; 6&10: $O5H_2$ ligand dissociating; 7: NH^{2-} ligand shifting to Mn4; 8: PT from NH^{2-} to W2; 9: PCET of PT from elsewhere to $O5H^-$ and ET from Mn4 to Mn1; 11: NH_2^- ligand shifting to Mn4; 12: PCET of PT from NH_3 to O5 and ET from Mn1 to Mn4; 13: PCET of PT from NH_3 to O5 and ET from N to Mn4; 14: $NH_2\cdot$ binding to Mn1 and ET from Mn1 to N; 15: Mn3 ligand exchange between NH_2^- and $O5H^-$; 16: PCET of PT

from NH_2 to O5H$^-$and ET from N to Mn3; 17: NH$^{\cdot -}$ binding to Mn3 and ET from Mn3 to N.

Table SIIIb. Gibbs free energies and Mulliken spin populations for the O5 substitution scheme with the open-cubane structure as reactant:

Spin states	Spin topology (Mn1-Mn4)	Gibbs Free energy (a.u.)			
		A	TS1	B	TS2
doublet	αααβ	-3347.6332	-3347.6269	-3347.6290	-3347.5799
	αβαβ	-3347.6336	-3347.6293	-3347.6320	-3347.5833
	αββα	-3347.6341	-3347.6294	-3347.6320	-3347.5831
sextet	βααα	-3347.6345	-3347.6299	-3347.6325	-3347.5832
octet	αααβ	-3347.6337	-3347.6292	-3347.6311	-3347.5822
	αaβα	-3347.6358	-3347.6289	-3347.6309	-3347.5823
	αβαα	-3347.6343	-3347.6298	-3347.6325	-3347.5832
14-et	αααα	-3347.6361	-3347.6290	-3347.6311	-3347.5816
		C	TS3	D	TS4
doublet	αααβ	-3347.6165	-3347.6105	-3347.6060	\
	αβαβ	-3347.6184	-3347.6163	-3347.6095	-3347.5953
	αββα	-3347.6180	-3347.6165	-3347.6095	-3347.5957
sextet	βααα	-3347.6188	-3347.6148	-3347.6089	-3347.5947
octet	αααβ	-3347.6170	-3347.6158	-3347.6090	-3347.5943
	αaβα	-3347.6182	-3347.6150	-3347.6093	-3347.5943
	αβαα	-3347.6193	-3347.6146	-3347.6092	-3347.5943
14-et	αααα	-3347.6173	-3347.6136	-3347.6078	-3347.5926
		E	F	G	TS7

	ααββ	\	-3347.5657	\	\
doublet	αβαβ	-3347.5978	-3347.5699	\	\
	αββα	-3347.5973	-3347.6099	-3271.2003	-3271.1771
sextet	βααα	-3347.5958	-3347.5668	\	\
	αααβ	-3347.6076	-3347.5721	\	\
octet	ααβα	-3347.6073	-3347.6114	-3271.2034	-3271.1774
	αβαα	-3347.5962	-3347.6104	-3271.1926	-3271.1794
14-et	αααα	-3347.6061	-3347.6124	-3271.1946	-3271.1796

		H	K	TS11	L
	ααββ	\	\	\	\
doublet	αβαβ	\	\	\	\
	αββα	-3271.1918	-3271.6568	-3271.6241	-3271.6387
sextet	βααα	\	\	\	\
	αααβ	\	\	\	\
octet	ααβα	-3271.1914	-3271.6585	-3271.6249	-3271.6394
	αβαα	-3271.1811	-3271.6563	-3271.6259	-3271.6392
14-et	αααα	-3271.1798	-3271.6579	-3271.6258	-3271.6385

		TS13	M
	ααββ	-3347.5967	-3347.6072
doublet	αβαβ	-3347.6036	-3347.6085
	αββα	-3347.6038	-3347.6084
sextet	βααα	-3347.6015	-3347.6102
	αααβ	-3347.6032	-3347.6084

octet	ααβα	-3347.6032	-3347.6078
	αβαα	-3347.5999	-3347.6100
14-et	αααα	-3347.6022	-3347.6092

Spin states	Spin topology (Mn1-Mn4)		Mulliken spin density			
			A	TS1	B	TS2
doublet	α	Mn1	3.86	3.90	3.90	3.88
	α	Mn2	2.97	2.97	2.98	2.95
	β	Mn3	-2.88	-2.88	-2.88	-2.78
	β	Mn4	-2.87	-2.86	-2.86	-2.78
		O4	-0.14	-0.13	-0.13	-0.19
		O5	-0.05	-0.06	-0.07	-0.20
		N	0.00	0.00	0.05	0.03
	α	Mn1	3.87	3.90	3.89	3.89
	β	Mn2	-2.90	-2.90	-2.88	-2.87
	α	Mn3	2.88	2.87	2.88	2.73
	β	Mn4	-2.83	-2.83	-2.82	-2.75
		O4	-0.01	-0.01	-0.02	0.17
		O5	-0.08	-0.09	-0.10	-0.19
		N	0.00	0.00	0.04	0.01
	α	Mn1	3.86	3.89	3.89	3.88
	β	Mn2	-2.91	-2.92	-2.90	-2.87
	β	Mn3	-2.88	-2.89	-2.89	-2.77
	α	Mn4	2.84	2.84	2.82	2.76

		O4	0.02	0.03	0.03	-0.15
		O5	0.08	0.09	0.10	0.19
		N	0.00	0.00	0.04	0.04
	β	Mn1	-3.86	-3.89	-3.89	-3.88
	α	Mn2	2.91	2.92	2.91	2.87
	α	Mn3	2.90	2.90	2.90	2.83
sextet	α	Mn4	2.87	2.87	2.87	2.78
		O4	0.13	0.13	0.12	0.18
		O5	0.05	0.06	0.07	0.20
		N	0.00	0.00	-0.04	-0.03
	α	Mn1	3.88	3.91	3.91	3.89
	α	Mn2	2.98	2.99	2.99	2.94
	α	Mn3	2.90	2.90	2.90	2.78
	β	Mn4	-2.83	-2.83	-2.82	-2.75
		O4	-0.02	-0.02	-0.03	0.16
		O5	-0.08	-0.08	-0.09	-0.19
		N	0.00	0.00	0.05	0.01
octet	α	Mn1	3.86	3.90	3.90	3.88
	α	Mn2	2.97	2.97	2.98	2.95
	β	Mn3	-2.86	-2.87	2.87	-2.73
	α	Mn4	2.84	2.84	2.83	2.76
		O4	0.02	0.02	0.03	-0.17
		O5	0.08	0.09	0.10	0.19
		N	0.00	0.01	0.00	0.05
	α	Mn1	3.87	3.90	3.89	3.89

	β	Mn2	-2.90	-2.90	-2.88	-2.87
	α	Mn3	2.89	2.88	2.89	2.78
	α	Mn4	2.88	2.87	2.87	2.78
		O4	0.14	0.14	0.13	0.20
		O5	0.05	0.06	0.07	0.20
		N	0.00	0.01	0.04	0.02
14-et	α	Mn1	3.87	3.91	3.91	3.89
	α	Mn2	2.98	2.99	2.99	2.95
	α	Mn3	2.92	2.91	2.91	2.83
	α	Mn4	2.88	2.87	2.87	2.78
		O4	0.14	0.14	0.13	0.19
		O5	0.05	0.06	0.07	0.20
		N	0.00	0.01	0.05	0.03
			C	TS3	D	TS4
doublet	α	Mn1	3.87	3.87	3.87	\
	α	Mn2	2.95	2.95	2.95	\
	β	Mn3	-2.81	-2.89	-2.92	\
	β	Mn4	-2.72	-2.87	-2.89	\
		O4	-0.16	-0.11	-0.10	\
		O5	-0.25	-0.09	-0.04	\
		N	0.04	0.06	0.07	\
	α	Mn1	3.87	3.88	3.88	3.87
	β	Mn2	-2.89	-2.89	-2.89	-2.87
	α	Mn3	2.78	2.85	2.88	2.80

	β	Mn4	-2.71	-2.84	-2.85	-2.84
		O4	0.18	0.09	0.02	0.02
		O5	-0.23	-0.06	-0.02	-0.02
		N	-0.06	-0.09	-0.07	0.05
	α	Mn1	3.87	3.87	3.87	3.85
	β	Mn2	-2.89	-2.89	-2.90	-2.87
	β	Mn3	-2.81	-2.87	-2.91	-2.81
	α	Mn4	2.72	2.84	2.85	2.84
		O4	-0.16	-0.08	-0.01	-0.01
		O5	0.23	0.07	0.02	0.02
		N	0.06	0.09	0.09	0.03
	β	Mn1	-3.87	-3.87	-3.89	-3.86
	α	Mn2	2.89	2.89	2.91	2.87
	α	Mn3	2.85	2.92	2.91	2.87
sextet	α	Mn4	2.72	2.86	2.87	2.88
		O4	0.15	0.11	0.12	0.12
		O5	0.25	0.09	0.07	0.03
		N	-0.05	-0.06	-0.04	-0.02
	α	Mn1	3.88	3.88	3.89	3.87
	α	Mn2	2.95	2.96	2.96	2.95
	α	Mn3	2.83	2.89	2.92	2.84
octet	β	Mn4	-2.71	-2.84	-2.85	-2.83
		O4	0.16	0.08	0.02	0.10
		O5	-0.23	-0.06	-0.02	-0.02
		N	-0.07	-0.09	-0.07	0.06

	α	Mn1	3.87	3.87	3.88	3.85
	α	Mn2	2.95	2.95	-2.88	2.95
	β	Mn3	-2.77	-2.85	2.92	-2.79
	α	Mn4	2.71	2.85	2.89	2.84
		O4	-0.17	-0.08	0.11	-0.02
		O5	0.23	0.06	0.04	0.02
		N	0.05	0.09	-0.05	0.04
	α	Mn1	3.87	3.88	3.88	3.87
	β	Mn2	-2.89	-2.89	-2.88	-2.87
	α	Mn3	2.81	2.89	2.92	2.87
	α	Mn4	2.72	2.87	2.89	2.88
		O4	0.17	0.12	0.11	0.13
		O5	0.25	0.09	0.04	0.03
		N	-0.05	-0.05	-0.05	0.05
	α	Mn1	2.88	3.88	3.89	3.87
	α	Mn2	2.95	2.96	2.96	2.95
	α	Mn3	2.87	2.94	2.97	2.91
14-et	α	Mn4	2.72	2.86	2.89	2.88
		O4	0.16	0.11	0.10	0.13
		O5	0.25	0.09	0.04	0.03
		N	-0.05	-0.06	-0.05	-0.01
			E	F	G	TS7
	α	Mn1	\	3.01	\	\
doublet	α	Mn2	\	2.96	\	\
	β	Mn3	\	-2.89	\	\

	β	Mn4	\	-1.94	\	\
		O4	\	-0.19	\	\
		O5	\	0.01	\	\
		N	\	0.01	\	\
	α	Mn1	3.87	3.03	\	\
	β	Mn2	-2.87	-2.96	\	\
	α	Mn3	2.88	2.87	\	\
	β	Mn4	-2.83	-1.88	\	\
		O4	0.01	0.11	\	\
		O5	0.00	0.01	\	\
		N	-0.03	-0.23	\	\
	α	Mn1	3.85	3.03	3.04	3.56
	β	Mn2	-2.86	-2.95	-2.94	-2.94
	β	Mn3	2.83	-2.85	-2.91	-2.92
	α	Mn4	-2.83	3.83	3.84	3.58
		O4	0.00	-0.13	-0.04	-0.08
		O5	0.01	0.02	\	\
		N	0.09	0.00	-0.03	-0.18
	β	Mn1	-3.85	-3.01	\	\
	α	Mn2	2.86	2.95	\	\
	α	Mn3	2.88	2.93	\	\
sextet	α	Mn4	2.88	1.93	\	\
		O4	0.13	0.18	\	\
		O5	0.02	-0.01	\	\
		N	-0.06	-0.01	\	\

	α	Mn1	3.91	3.04	\	\
	α	Mn2	2.93	2.95	\	\
	α	Mn3	2.94	2.91	\	\
	β	Mn4	-2.79	-1.88	\	\
		O4	-0.07	0.10	\	\
		O5	-0.03	0.02	\	\
		N	-0.13	-0.23	\	\
octet	α	Mn1	3.90	3.03	3.03	3.62
	α	Mn2	2.93	2.96	2.95	2.97
	β	Mn3	-2.87	-2.81	-2.87	-2.90
	α	Mn4	2.79	3.83	3.84	3.53
		O4	0.06	-0.14	-0.06	-0.08
		O5	0.03	0.02	\	\
		N	0.07	0.00	-0.01	-0.18
14-et	α	Mn1	3.87	3.04	3.07	3.60
	β	Mn2	-2.86	-2.95	-2.95	-2.93
	α	Mn3	2.93	2.95	2.99	2.95
	α	Mn4	2.89	3.88	3.88	3.62
		O4	0.13	0.14	0.14	0.14
		O5	0.02	0.02	\	\
		N	-0.01	-0.24	-0.22	-0.43
	α	Mn1	3.91	3.04	3.04	3.67
	α	Mn2	2.93	2.96	2.95	2.97
	α	Mn3	2.99	2.99	2.99	2.97
	α	Mn4	2.84	3.88	3.88	3.54

		O4	0.18	0.13	0.13	0.13
		O5	0.03	0.02	\	\
		N	-0.12	-0.23	-0.16	-0.41
			H	K	TS11	L
	α	Mn1	\	\	\	\
	α	Mn2	\	\	\	\
	β	Mn3	\	\	\	\
	β	Mn4	\	\	\	\
		O4	\	\	\	\
		O5	\	\	\	\
		N	\	\	\	\
doublet	α	Mn1	\	\	\	\
	β	Mn2	\	\	\	\
	α	Mn3	\	\	\	\
	β	Mn4	\	\	\	\
		O4	\	\	\	\
		O5	\	\	\	\
		N	\	\	\	\
	α	Mn1	3.86	2.96	3.65	3.86
	β	Mn2	-2.92	-2.95	-2.93	-2.94
	β	Mn3	-2.93	-2.79	-2.80	-2.86
	α	Mn4	2.96	3.81	3.50	2.96
		O4	-0.02	-0.10	-0.06	0.03
		O5	\	\	\	\

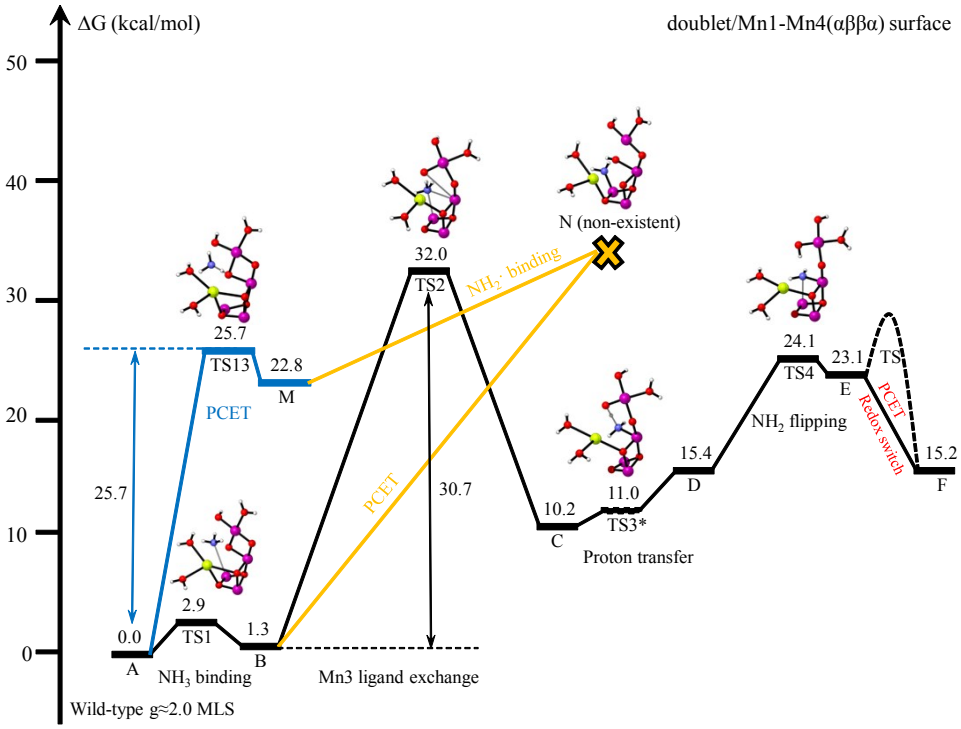
		N	0.00	-0.03	-0.33	-0.08
	β	Mn1	\	\	\	\
	α	Mn2	\	\	\	\
	α	Mn3	\	\	\	\
sextet	α	Mn4	\	\	\	\
		O4	\	\	\	\
		O5	\	\	\	\
		N	\	\	\	\
	α	Mn1	\	\	\	\
	α	Mn2	\	\	\	\
	α	Mn3	\	\	\	\
	β	Mn4	\	\	\	\
		O4	\	\	\	\
		O5	\	\	\	\
		N	\	\	\	\
	α	Mn1	3.86	2.97	3.67	3.86
octet	α	Mn2	2.96	2.96	2..97	2.98
	β	Mn3	-2.91	-2.75	-2.77	-2.83
	α	Mn4	2.98	3.81	3.49	2.96
		O4	-0.02	-0.12	-0.07	0.02
		O5	\	\	\	\
		N	-0.01	-0.03	-0.33	-0.09
	α	Mn1	3.88	2.97	-3.63	3.87
	β	Mn2	-2.93	-2.95	-2.93	-2.92
	α	Mn3	2.95	2.87	2.82	2.88

	α	Mn4	3.07	3.88	3.52	2.98
		O4	0.15	0.18	0.16	0.17
		O5	\	\	\	\
		N	-0.19	-0.15	-0.35	-0.17
	α	Mn1	3.87	2.98	3.66	3.87
	α	Mn2	2.98	2.96	2.97	2.99
	α	Mn3	2.97	2.92	2.86	2.91
14-et	α	Mn4	3.09	3.88	3.51	2.98
		O4	0.14	0.17	0.15	0.17
		O5	\	\	\	\
		N	-0.20	-0.15	-0.34	-0.17

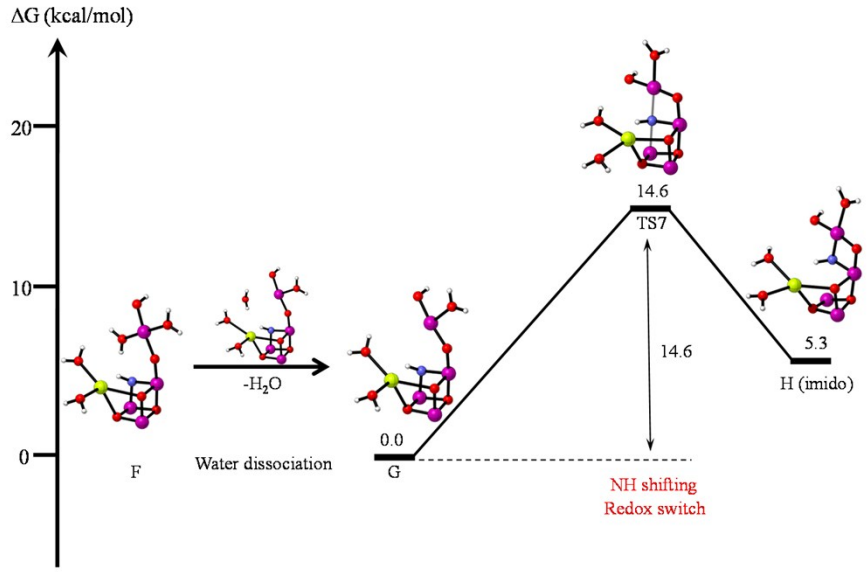
			TS13	M
	α	Mn1	3.87	3.87
	α	Mn2	2.97	2.97
	β	Mn3	-2.90	-2.87
	β	Mn4	-3.79	-3.91
		O4	-0.08	-0.10
		O5	0.20	-0.01
doublet		N	0.71	1.08
	α	Mn1	3.88	3.88
	β	Mn2	-2.91	-2.91
	α	Mn3	2.84	2.85
	β	Mn4	-3.85	-3.88
		O4	0.13	0.10

		O5	0.19	-0.04
		N	0.75	0.07
	α	Mn1	3.87	3.87
	β	Mn2	-2.91	-2.91
	β	Mn3	-2.86	-2.87
	α	Mn4	3.83	3.89
		O4	-0.11	-0.08
		O5	-0.17	0.05
		N	-0.74	-1.07
	β	Mn1	-3.87	-3.87
	α	Mn2	2.91	2.91
	α	Mn3	2.93	2.91
sextet	α	Mn4	3.80	3.91
		O4	0.07	0.08
		O5	-0.20	0.01
		N	-0.72	-1.08
	α	Mn1	3.88	3.88
	α	Mn2	2.97	2.97
	α	Mn3	2.89	2.89
	β	Mn4	-3.82	-3.88
octet		O4	0.11	0.08
		O5	0.17	-0.04
		N	0.75	1.08
	α	Mn1	3.87	3.87
	α	Mn2	2.97	2.97

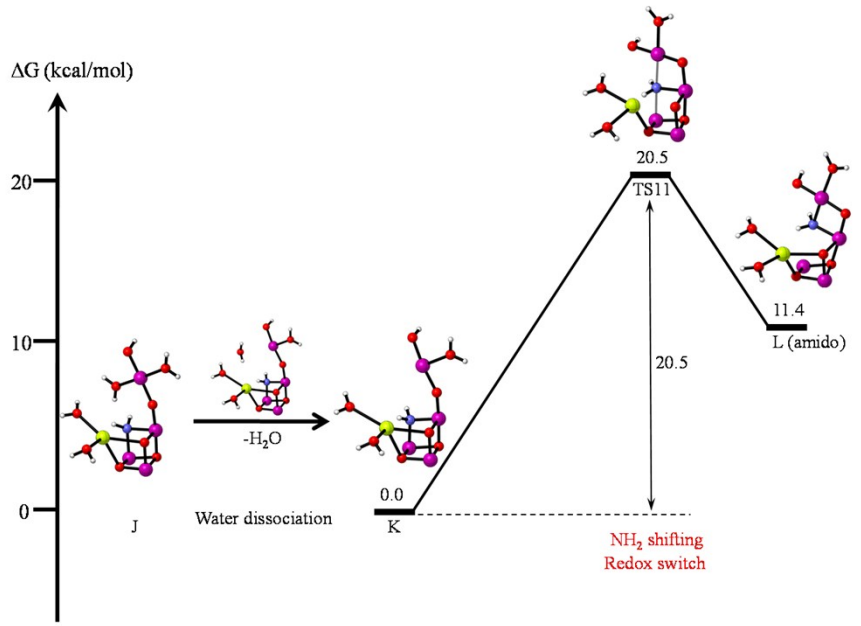
	β	Mn3	-2.82	-2.83
	α	Mn4	3.84	3.89
		O4	-0.12	-0.09
		O5	-0.18	0.06
		N	-0.74	-1.07
	α	Mn1	3.88	3.88
	β	Mn2	-2.91	-2.90
	α	Mn3	2.91	2.88
	α	Mn4	3.81	3.91
		O4	0.09	0.10
		O5	-0.20	0.02
		N	-0.71	-1.08
	α	Mn1	3.88	3.88
	α	Mn2	2.97	2.97
	α	Mn3	2.96	2.93
14-et	α	Mn4	3.82	3.91
		O4	0.08	0.09
		O5	-0.20	0.02
		N	-0.72	-1.08

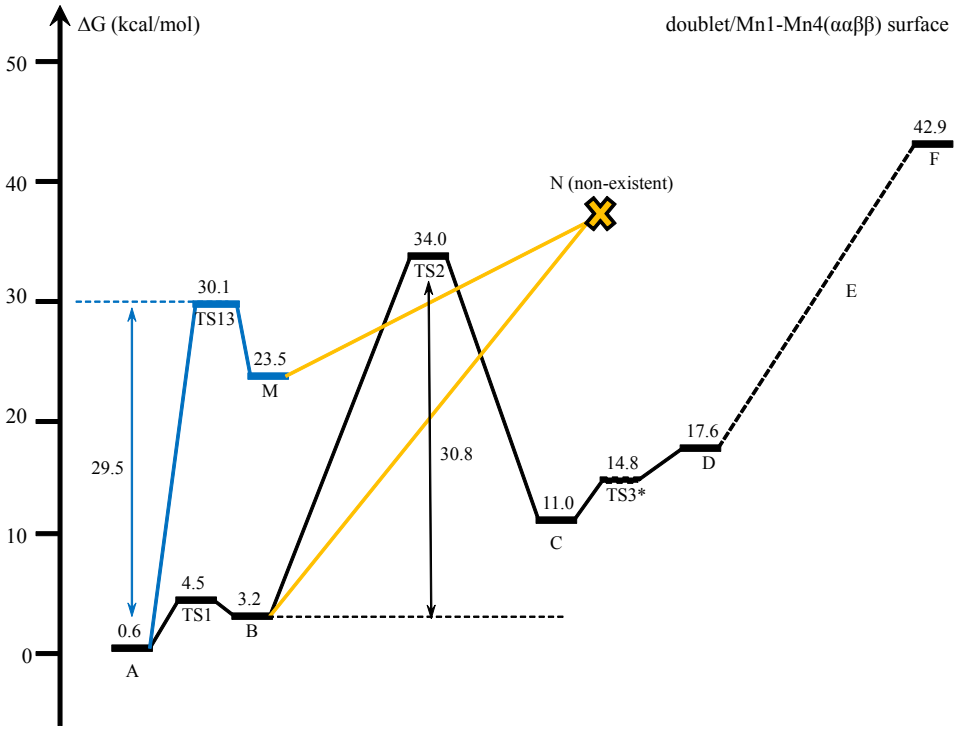


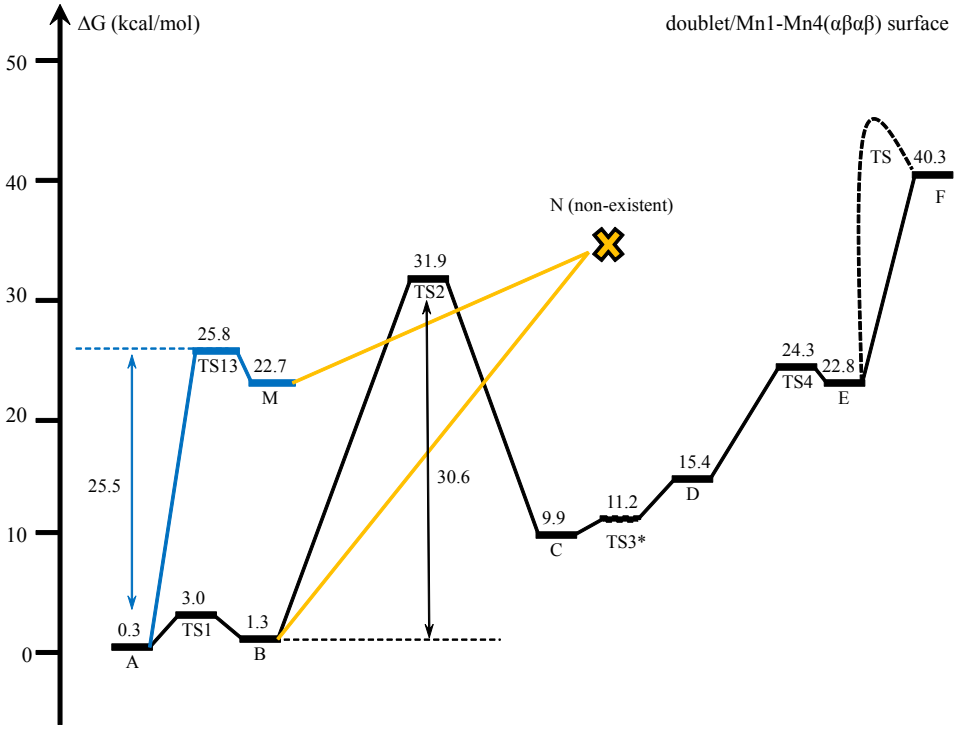
doublet/Mn1-Mn4(αββα) surface

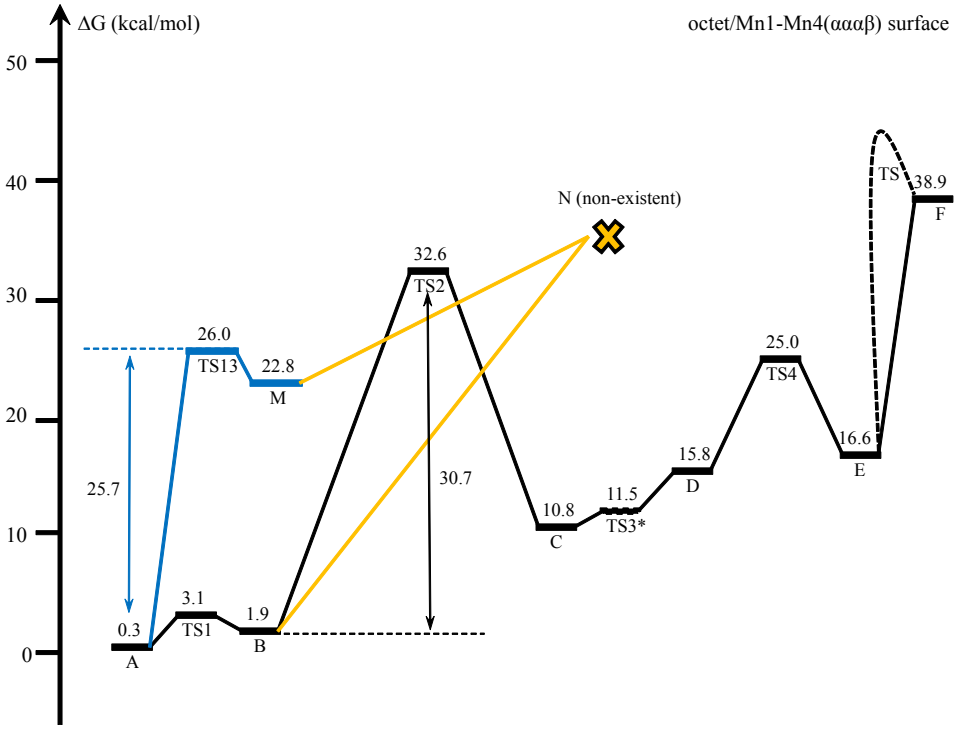


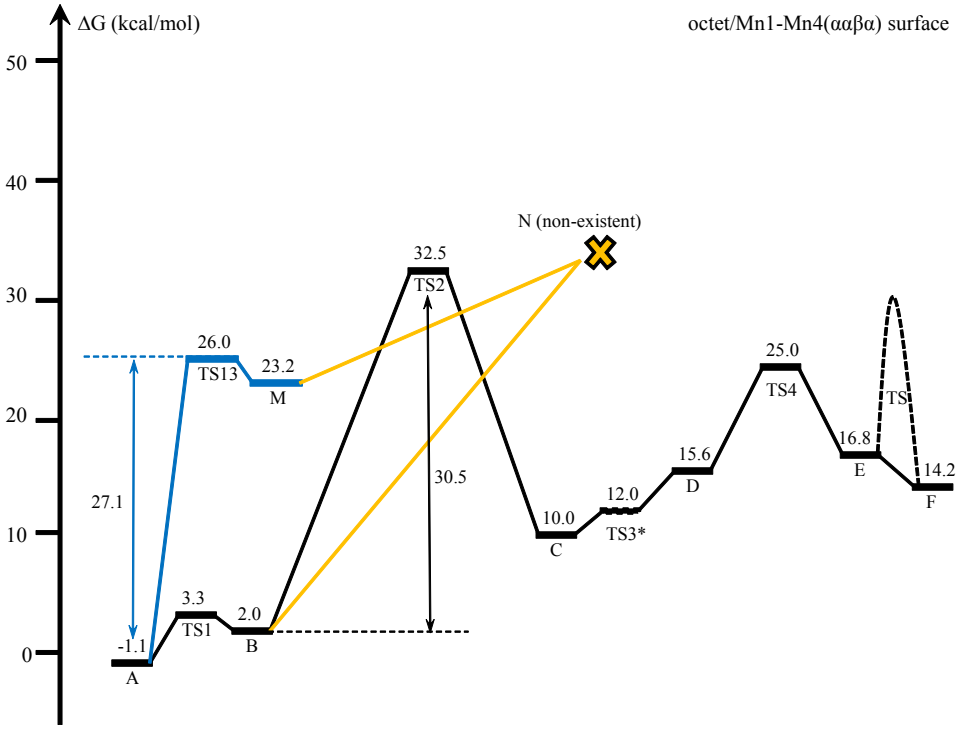
doublet/Mn1-Mn4(αββα) surface

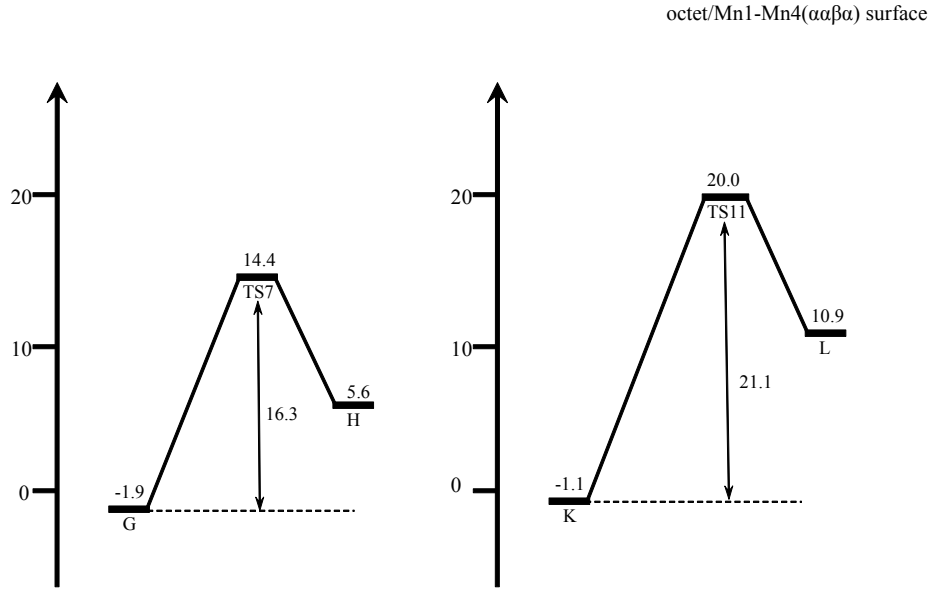


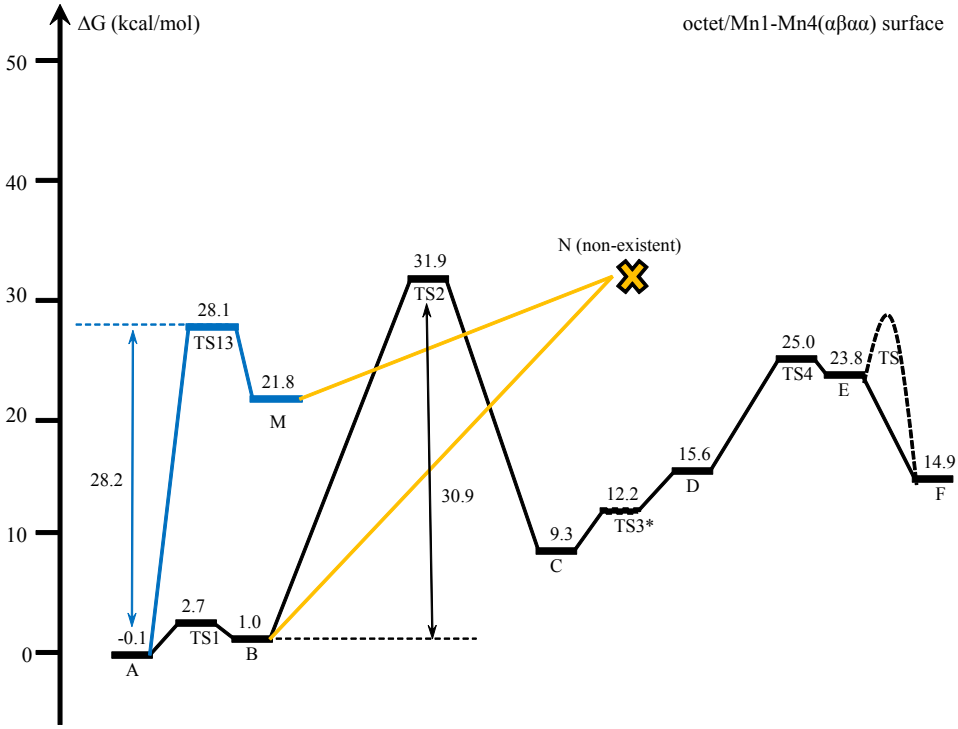


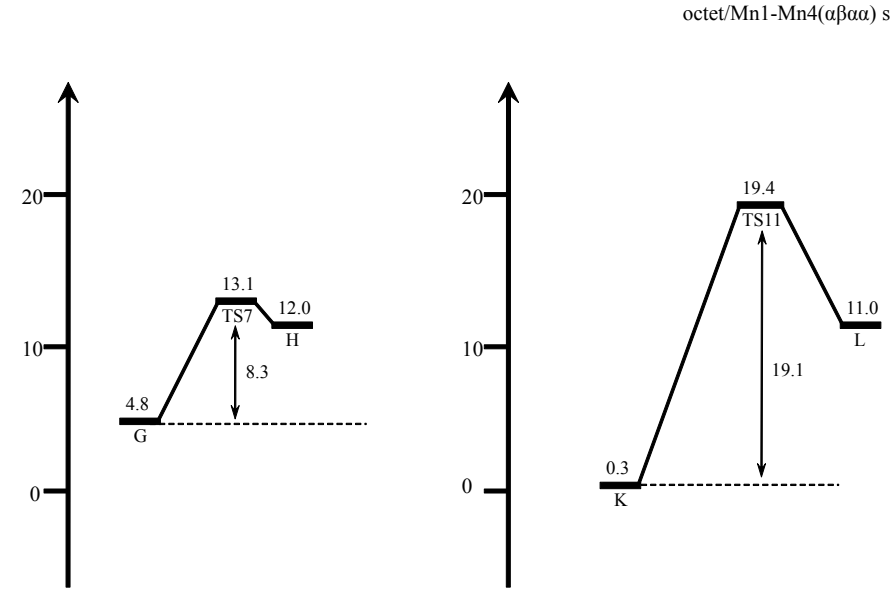

ΔG (kcal/mol)
doublet/Mn1-Mn4(αβαβ) surface
50
40
30
20
10
0
N (non-existent)
TS
40.3
F
31.9
TS2
25.8
TS13
22.7
M
24.3
TS4
22.8
E
25.5
30.6
15.4
D
9.9
11.2
C
TS3*
3.0
TS1
0.3
1.3
A
B


ΔG (kcal/mol)
octet/Mn1-Mn4(αααβ) surface
50
40
30
20
10
0
N (non-existent)
TS
38.9
F
32.6
TS2
26.0
TS13
22.8
M
25.0
TS4
16.6
E
25.7
30.7
15.8
D
10.8
11.5
C
TS3*
3.1
TS1
0.3
1.9
A
B


ΔG (kcal/mol)
octet/Mn1-Mn4(ααβα) surface
50
40
30
20
10
0
N (non-existent)
32.5
TS2
26.0
TS13
23.2
M
25.0
TS4
TS
16.8
E
15.6
D
14.2
F
12.0
TS3*
10.0
C
30.5
27.1
3.3
TS1
2.0
B
-1.1
A


octet/Mn1-Mn4(ααβα) surface
20
10
0
14.4
TS7
16.3
5.6
H
-1.9
G
20
10
0
20.0
TS11
21.1
10.9
L
-1.1
K


ΔG (kcal/mol)
octet/Mn1-Mn4(αβαα) surface
50
40
30
20
10
0
N (non-existent)
31.9
TS2
28.1
TS13
21.8
M
28.2
30.9
25.0
TS4
23.8
E
TS5
15.6
D
14.9
F
12.2
TS3*
9.3
C
2.7
TS1
1.0
B
-0.1
A


octet/Mn1-Mn4(αβαα) surface
20
10
0
13.1
TS7
12.0
H
8.3
4.8
G
20
10
0
19.4
TS11
11.0
L
19.1
0.3
K

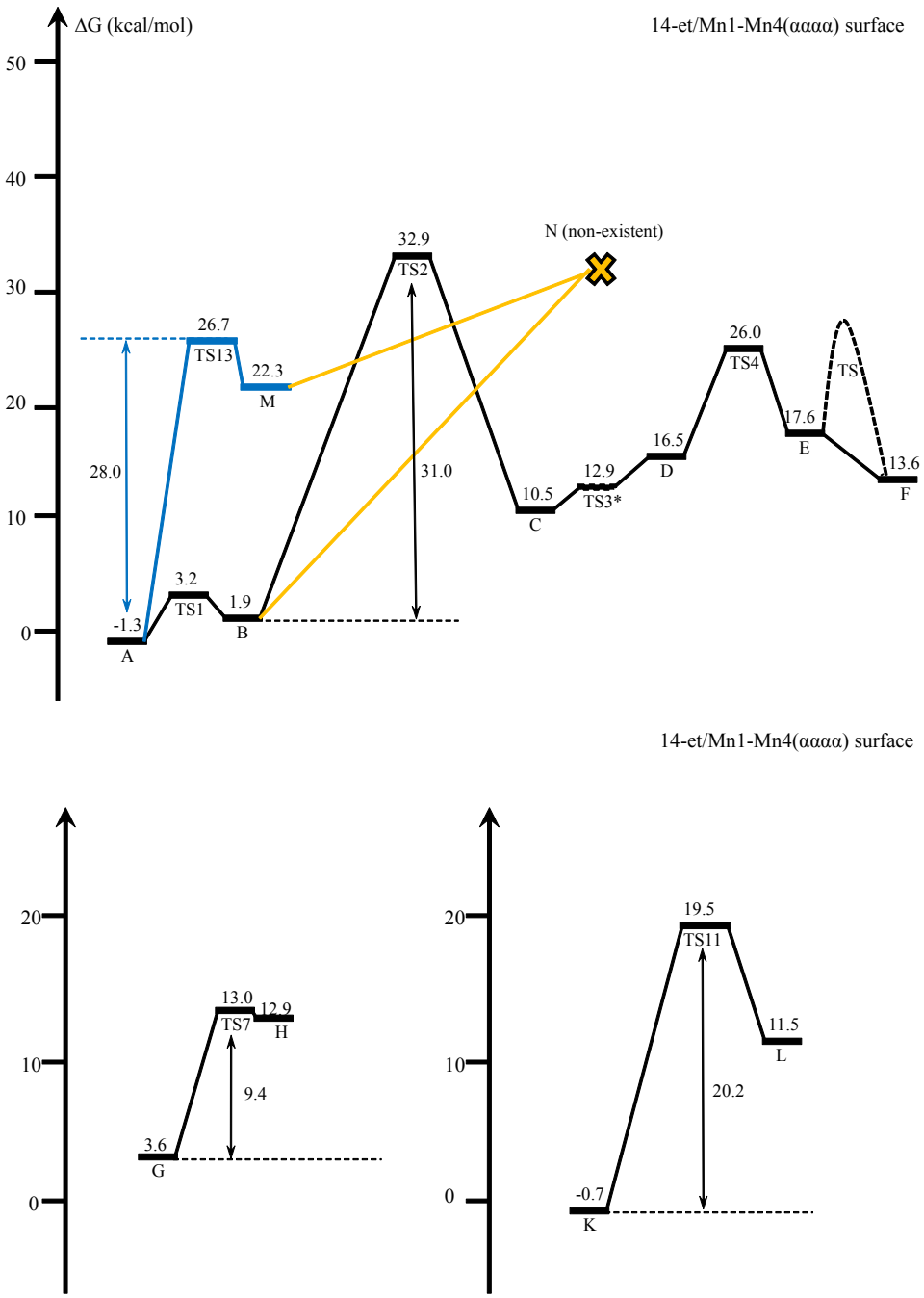


Figure SIIIb. Free energy profiles for the O5 substitution scheme with the open-cubane structure as reactant for all spin states.

The Cartesian coordinates for A to M and TS1 to TS13:

A:

Ca	2.88738400	-0.13216800	-0.20642900	H	2.34769100	5.14512700	-1.39449000	C	-2.14764200	-1.99448200	-1.51428900
Mn	-0.05622100	1.86006500	-0.06902400	C	4.14765900	4.44920200	-2.41342400	O	-1.20539500	-2.52134500	-2.21777900
Mn	0.70480800	0.62448500	2.25164800	H	4.42085900	3.64652400	-3.11231300	O	-0.85398100	3.32134300	1.24183900
Mn	-0.24049500	-1.40824300	0.65156300	H	4.70489000	4.24996000	-1.48622000	C	-0.64891700	3.23098000	2.48630100
Mn	0.59517700	-2.76449400	-1.53728000	C	4.57057400	5.80769100	-2.98377200	O	-0.05030900	2.27059600	3.08013700
O	1.44895700	1.55673400	0.89368700	H	4.05414600	6.02089400	-3.93036400	C	-1.14235300	4.34815300	3.40105100
O	-0.71177500	0.45638000	1.02236500	H	4.33447700	6.62458000	-2.28757700	H	-0.26201700	4.72662000	3.94084400
O	1.23562800	-0.99328700	1.58686700	H	5.65026900	5.83765800	-3.17911900	H	-1.77353500	3.87691300	4.16799800
O	0.69201200	-1.08135400	-0.95870600	N	-1.64386300	1.88795900	-1.40799300	C	-1.88288100	5.48053800	2.69047500
O	0.03440600	-3.11119500	0.14700800	C	-3.00010300	1.99607300	-1.15032700	H	-2.19477700	6.24552500	3.41334500
O	5.20562900	0.82848500	-0.47981400	H	-3.38379000	1.94020300	-0.14104800	H	-1.24642900	5.95733100	1.93585300
H	5.28120900	1.01131100	0.47942600	C	-3.67849400	2.14900100	-2.33557400	H	-2.77788500	5.10776200	2.17809800
H	4.86481400	1.64940000	-0.88993800	N	-2.68892700	2.11208200	-3.31464100	O	3.93368300	0.52950300	1.94356900
O	3.27415400	-0.82222500	-2.61326900	H	-2.83536400	2.19895000	-4.31259200	C	3.47892800	0.74759400	3.08808600
H	4.08920300	-1.34665200	-2.68079700	C	-1.47986100	1.95832400	-2.72429900	O	2.22931900	0.76700600	3.41514600
H	2.55150700	-1.41309500	-2.97002300	H	-0.53843800	1.85572200	-3.26925200	C	4.42144700	1.03139000	4.24604000
O	1.23214700	-2.47831900	-3.28264100	C	-5.11953900	2.38010100	-2.68567700	H	4.18261900	0.37268500	5.08911500
H	0.45878000	-2.30823000	-3.84912900	H	-5.26711600	3.43326700	-2.97370800	H	4.27535900	2.06393600	4.58912400
O	0.16553100	-4.88684200	-1.84552900	H	-5.37247400	1.79811200	-3.58772500	H	5.46154900	0.88815700	3.94011900
H	1.10742000	-5.13823000	-1.73133500	C	-6.10654200	2.05434400	-1.54953800	O	-0.34554900	-0.35468700	3.65646400
H	-0.22645400	-4.99903200	-0.95397800	H	-5.91554400	2.69535300	-0.68257000	C	-1.07254300	-1.36077000	3.40663900
O	3.75602700	-2.34958900	-0.01380100	H	-7.12507100	2.28089800	-1.89735600	O	-1.21289800	-1.92213500	2.26644100
C	3.37936500	-3.44398200	-0.46144600	C	-6.06789800	0.61322300	-1.02658000	C	-1.87211700	-1.96104300	4.55002200
O	2.32816400	-3.63824500	-1.19315800	O	-6.00345100	0.36465000	0.17335400	H	-1.55768500	-3.00961100	4.66070900
C	4.23027500	-4.68259400	-0.17426700	N	-6.13203200	-0.36991600	-1.97721300	H	-1.61193200	-1.42630400	5.47069000
H	5.23816400	-4.46186900	-0.55433300	H	-6.19796900	-0.11002700	-2.95201800	C	-3.38972700	-1.90725400	4.29129300
H	4.33452400	-4.72882700	0.91890500	C	-6.04377500	-1.79062100	-1.63581400	H	-3.60590300	-2.42590700	3.34832700
C	3.71773200	-6.01084200	-0.73009500	H	-6.78005000	-2.00394300	-0.85087300	H	-3.69437300	-0.85981500	4.14946000
H	3.62064000	-5.97768700	-1.82265600	H	-6.33440300	-2.35602400	-2.53077400	C	-4.19564500	-2.52966800	5.43580600
H	2.73881100	-6.26930700	-0.30488000	C	-4.65187200	-2.20844700	-1.13665600	H	-3.93184700	-3.58714300	5.57895200
H	4.40975600	-6.82477100	-0.47877900	H	-4.43195000	-1.64637500	-0.22433700	H	-5.27314700	-2.47793100	5.23232400
O	0.88450600	3.00527500	-1.32987200	H	-4.68602600	-3.27283700	-0.86197300	H	-4.00947000	-2.00940000	6.38572000
C	2.14995400	3.03617300	-1.59498900	C	-3.52842400	-1.96642300	-2.15551600	N	1.16571900	0.92824700	-4.25045700
O	2.92748900	2.06486300	-1.47586400	H	-3.64054800	-0.95730300	-2.58239100	H	1.50776400	0.96090700	-5.21358900
C	2.64646700	4.37779900	-2.12422700	H	-3.55122200	-2.68193900	-2.98643200	H	1.97866500	1.13315900	-3.66245500
H	2.06481800	4.60059300	-3.03242200	O	-2.02071000	-1.48779600	-0.37556000	H	0.97869800	-0.05911700	-4.05594200

TS1:

Ca	2.90170500	-0.00585700	-0.23716300	H	2.74384000	-1.67598800	-2.75483700	H	5.13626800	-6.45541000	0.72212500
Mn	-0.09881200	1.91839000	-0.34754800	O	1.77849000	-3.07378000	-2.83449800	O	0.82106500	3.16851500	-1.53443400
Mn	0.57240300	0.81689000	2.07806500	H	1.08828700	-2.98665100	-3.51690700	C	2.07667400	3.12812900	-1.84224500
Mn	-0.20224400	-1.40659700	0.63675700	O	0.57918000	-5.24079900	-1.13879100	O	2.85464900	2.18408600	-1.59089400
Mn	0.91791600	-3.09391000	-1.16639000	H	1.50278200	-5.44425100	-0.87814700	C	2.56995500	4.36170400	-2.59818300
O	1.36590800	1.66570100	0.69400100	H	0.08587200	-5.21460100	-0.29147700	H	2.03160700	4.38445200	-3.55983400
O	-0.74302500	0.50064300	0.74821000	O	3.99265400	-2.10196500	0.08302700	H	2.22388500	5.24879800	-2.04794800
O	1.18266000	-0.83834100	1.62013100	C	3.69672400	-3.30552700	0.02386300	C	4.08070900	4.41702400	-2.83650100
O	0.90547000	-1.33764300	-0.88685700	O	2.59014000	-3.79104500	-0.43925300	H	4.39715700	3.50359500	-3.35798800
O	0.12052500	-3.16231900	0.45520400	C	4.70456200	-4.33636800	0.53403200	H	4.60002400	4.41207800	-1.86666900
O	5.13884500	1.12873300	-0.49143700	H	5.66144100	-4.09799800	0.04911300	C	4.50456500	5.65313300	-3.63773300
H	5.17836700	1.33707900	0.46458000	H	4.85174400	-4.11113400	1.60037800	H	4.02737000	5.66929700	-4.62795900
H	4.73008600	1.90705600	-0.92500300	C	4.33932000	-5.80724400	0.33551600	H	4.22378300	6.58135500	-3.12048300
O	3.26567400	-0.82941500	-2.60463700	H	4.19970300	-6.04400600	-0.72712300	H	5.59117900	5.67323000	-3.79187800
H	4.19501500	-1.07112600	-2.75408200	H	3.41463700	-6.06268200	0.86845500	N	-1.84198700	2.05709400	-1.47967500

C	-3.10011600	1.53713000	-1.23298300	H	-4.12904000	-2.50985700	-0.47568700	C	4.18315000	1.45095500	4.20750300
H	-3.26366900	0.85209400	-0.41162800	H	-4.23121400	-4.05836200	-1.32384000	H	3.90901300	0.85480700	5.08552500
C	-3.98424400	2.02376900	-2.16768500	C	-3.12517300	-2.51639100	-2.39039300	H	4.01284300	2.50484300	4.46396700
N	-3.21676700	2.85000900	-2.98594400	H	-3.35640400	-1.51090500	-2.77330400	H	5.23803300	1.29821200	3.96262700
H	-3.55997100	3.39393600	-3.76761800	H	-2.99199600	-3.19031900	-3.24422300	O	-0.57760200	-0.04695100	3.49081600
C	-1.93920000	2.84428600	-2.53617000	O	-1.82635900	-1.66116700	-0.60216400	C	-1.31804500	-1.04771200	3.26379600
H	-1.11801200	3.40219200	-2.96345500	C	-1.81482600	-2.38552200	-1.62866000	O	-1.35346800	-1.72408900	2.17898000
C	-5.45480900	1.85005200	-2.41263100	O	-0.79840100	-3.01700000	-2.10122700	C	-2.29994500	-1.46225000	4.34346800
H	-5.90611200	2.84317400	-2.56542700	O	-0.91885700	3.48183700	0.88408900	H	-2.38687000	-2.55640600	4.33512300
H	-5.61790800	1.31398400	-3.36359600	C	-0.75705200	3.44791100	2.13319600	H	-1.90568300	-1.14247600	5.31566700
C	-6.22386000	1.16165400	-1.27063400	O	-0.22262000	2.49052000	2.79123200	C	-3.68540600	-0.82688000	4.09714400
H	-6.04674400	1.68676300	-0.32638000	C	-1.22194800	4.63003500	2.97997600	H	-4.04521100	-1.12094500	3.10152600
H	-7.29991700	1.24247000	-1.48584400	H	-0.32982400	5.02218500	3.49035400	H	-3.57558700	0.26723300	4.08405900
C	-5.91884900	-0.31659700	-0.99565100	H	-1.85922200	4.22395400	3.77807400	C	-4.70653400	-1.23396400	5.16413800
O	-5.78481700	-0.73714600	0.14980700	C	-1.93800500	5.73281400	2.20100300	H	-4.85086300	-2.32332400	5.18056800
N	-5.85676400	-1.13828700	-2.08905400	H	-2.22883500	6.55027100	2.87365200	H	-5.68280700	-0.77090000	4.97039000
H	-6.04177100	-0.75357100	-3.00556300	H	-1.29266700	6.14374800	1.41587700	H	-4.38089700	-0.92538500	6.16744100
C	-5.66594500	-2.58527800	-1.96285300	H	-2.84380900	5.34958300	1.71541600	N	0.45236900	0.46057900	-3.11564800
H	-6.41255400	-2.97819300	-1.26001100	O	3.81414000	0.79830900	1.92153900	H	-0.08614500	0.34450100	-3.97556200
H	-5.86874700	-3.02356800	-2.94854800	C	3.30068500	1.07161700	3.02892300	H	1.44317400	0.43662200	-3.36867800
C	-4.26640800	-2.96791700	-1.45962000	O	2.03801700	1.07897400	3.30037200	H	0.30873100	-0.37401600	-2.54123400

B:

Ca	2.92093500	-0.07594200	-0.24018300	H	2.49508000	5.29609100	-1.66517000	C	-1.77792100	-2.50242600	-1.65124700
Mn	-0.03229300	1.83843800	-0.52322400	C	4.18043100	4.50089800	-2.79357700	O	-0.76371500	-3.17538200	-2.06244500
Mn	0.56581400	0.84245200	1.97941600	H	4.36447200	3.68655900	-3.50825800	O	-0.83820700	3.51791500	0.70526500
Mn	-0.19040300	-1.44484600	0.62385100	H	4.77764800	4.26251800	-1.90181000	C	-0.69520800	3.49831700	1.95132100
Mn	0.94240800	-3.22028600	-1.08627500	C	4.65249400	5.83385600	-3.38537000	O	-0.20556900	2.53077400	2.63662400
O	1.40089000	1.63006400	0.58598700	H	4.09712500	6.08343000	-4.30068300	C	-1.12245400	4.70708800	2.78307000
O	-0.71305400	0.47694500	0.63594100	H	4.50691100	6.66023600	-2.67548500	H	-0.21798500	5.08082700	3.28560000
O	1.17445400	-0.84523500	1.60692900	H	5.71919300	5.79942500	-3.64216100	H	-1.77070800	4.33457700	3.58847100
O	0.95195100	-1.46877000	-0.86516800	N	-1.90952500	2.14944300	-1.49598600	C	-1.80511000	5.81895600	1.98740500
O	0.10143900	-3.21769100	0.51351000	C	-3.08536700	1.43377500	-1.36635600	H	-2.06989800	6.65678200	2.64574800
O	5.10968600	1.12057100	-0.54707500	H	-3.10088400	0.50085600	-0.81686400	H	-1.14819500	6.19621400	1.19484100
H	5.16624800	1.34157500	0.40485100	C	-4.10354900	2.10769400	-2.00205300	H	-2.72357700	5.45568700	1.50970700
H	4.67206300	1.88569200	-0.98124100	N	-3.50261200	3.25202200	-2.51816400	O	3.81846500	0.76468900	1.89695900
O	2.99974900	-0.79777800	-2.65899100	H	-3.97565300	3.99158300	-3.02239100	C	3.28412000	1.07709900	2.98557400
H	3.85492700	-0.81180600	-3.11883100	C	-2.18730100	3.24134700	-2.18616500	O	2.01804400	1.11856800	3.22768000
H	2.61228300	-1.72761600	-2.74481100	H	-1.47706700	4.02232200	-2.42359900	C	4.14982800	1.46018400	4.17602100
O	1.83453100	-3.22173100	-2.75017800	C	-5.56501100	1.83766800	-2.22084700	H	3.89146900	0.83205700	5.03695000
H	1.14424700	-3.22285500	-3.43820600	H	-6.08419100	2.80412200	-2.30987900	H	3.94318000	2.49999300	4.46000200
O	0.59943200	-5.36493700	-0.99129900	H	-5.72066500	1.34511500	-3.19616700	H	5.21015900	1.34478100	3.93433800
H	1.51234700	-5.55834500	-0.68885500	C	-6.26185900	1.04431200	-1.09807300	O	-0.62649300	0.03721500	3.40262300
H	0.07410600	-5.30852900	-0.16510600	H	-6.06356800	1.51299000	-0.12874600	C	-1.37838100	-0.95793100	3.19487900
O	4.02093200	-2.16723800	0.00874300	H	-7.34857700	1.10230900	-1.26401100	O	-1.39188300	-1.68103100	2.13909900
C	3.72919900	-3.37302500	0.04617000	C	-5.92415700	-0.44226600	-0.92283200	C	-2.40417400	-1.30746800	4.25687700
O	2.59587900	-3.88832200	-0.30691000	O	-5.85236900	-0.94619300	0.19373900	H	-2.51905200	-2.39864600	4.28678000
C	4.77268200	-4.36654600	0.55726100	N	-5.77693700	-1.18267700	-2.06648800	H	-2.03273500	-0.96041700	5.22879000
H	5.69758500	-4.15126700	0.00449100	H	-5.93545700	-0.74310000	-2.96307200	C	-3.76454400	-0.64780200	3.94300100
H	4.97886500	-4.07913000	1.59867100	C	-5.61879400	-2.63897900	-2.01754200	H	-4.10482700	-0.97208600	2.94984800
C	4.40900000	-5.84827100	0.46494700	H	-6.38681200	-3.05016000	-1.34948800	H	-3.62459500	0.44175100	3.89055500
H	4.21327400	-6.14661700	-0.57309500	H	-5.81035300	-3.02050300	-3.02885200	C	-4.82659800	-0.98519100	4.99432700
H	3.51708900	-6.07680100	1.06185600	C	-4.23706800	-3.07632100	-1.51005800	H	-5.00001700	-2.06899900	5.04967000
H	5.23168700	-6.46871900	0.84305200	H	-4.09392600	-2.63730200	-0.51785200	H	-5.78452800	-0.50651400	4.75266700
O	0.87403200	3.21906300	-1.63337000	H	-4.23786300	-4.16883600	-1.38876600	H	-4.52240100	-0.64433800	5.99398100
C	2.14646500	3.20475900	-1.86171900	C	-3.07638800	-2.65125800	-2.43112500	N	0.30887900	0.57949100	-2.50651200
O	2.90286900	2.22593500	-1.67154600	H	-3.29902700	-1.65578900	-2.84483100	H	-0.10545600	1.13943300	-3.25164500
C	2.69682900	4.51872500	-2.41842400	H	-2.93239600	-3.34726800	-3.26498600	H	1.27320500	0.34701000	-2.77047200
H	2.08028700	4.79198700	-3.28868500	O	-1.79555500	-1.71350100	-0.67117400	H	-0.18558100	-0.30795300	-2.42965200

TS2:

Ca	-2.74193000	-2.16268600	0.15434200	H	3.44025900	-4.97743300	-1.81592600	C	-0.75768300	2.42004100	-1.91770700
Mn	1.90280100	-1.16861700	-0.31607700	C	2.48100100	-5.51931800	-3.69739600	O	-1.75392400	1.85441500	-2.46183900
Mn	0.51269100	-1.27973700	2.00545500	H	2.11426700	-5.00443300	-4.59650500	O	3.59859400	-1.34024500	1.09427300
Mn	-0.74505000	0.65902500	0.44528500	H	1.59721100	-5.97498400	-3.23161700	C	3.38786900	-1.48769300	2.32253800
Mn	-3.34178000	0.87408200	-1.60319500	C	3.48860900	-6.60568600	-4.08896700	O	2.23909800	-1.45838100	2.90387600
O	0.98122800	-2.39081500	0.70188200	H	4.37015800	-6.17574100	-4.58584100	C	4.56180800	-1.72985100	3.26786300
O	1.11082200	0.07919200	0.83959600	H	3.84366900	-7.15799000	-3.20751800	H	4.39209100	-2.71050100	3.73650600
O	-1.12239500	-0.85069400	1.29796500	H	3.04030400	-7.33270800	-4.77846600	H	4.47868800	-0.99818800	4.08386800
O	-2.87272100	-0.74519100	-1.86185900	N	3.00519000	0.32536900	-1.30806000	C	5.93600800	-1.66957900	2.60212600
O	-2.39719600	0.95027300	0.06119800	C	3.08650400	1.67416800	-1.00368400	H	6.72726100	-1.86476900	3.33756300
O	-1.00293200	-3.68538900	-0.61354700	H	2.39475600	2.12621700	-0.30676500	H	6.01790600	-2.41250300	1.80025800
H	-0.26829800	-3.43088100	0.00374400	C	4.12081700	2.24020700	-1.71047800	H	6.11669300	-0.68332000	2.15726000
H	-0.52428500	-3.72964500	-1.46954300	N	4.66139800	1.19231200	-2.45098100	O	-2.14780700	-3.30023100	2.18046000
O	-3.97635900	-3.12753900	-1.79460300	H	5.46136500	1.25317500	-3.06863100	C	-1.33484700	-3.27717800	3.12489100
H	-3.52335400	-3.76682600	-2.36918800	C	3.96901800	0.06173500	-2.17694500	O	-0.23808500	-2.58617900	3.18448600
H	-3.82937600	-2.23686400	-2.21783400	H	4.18763100	-0.91859400	-2.57634100	C	-1.57242400	-4.13419400	4.35792300
O	-4.22037000	1.28204700	-3.12082300	C	4.69333500	3.62518700	-1.79593500	H	-1.51289800	-3.51411700	5.26025300
H	-3.57326500	1.74738900	-3.68422800	H	5.79178000	3.55381200	-1.76410600	H	-0.78082100	-4.89103700	4.43107400
O	-3.80473200	3.01235800	-0.76500900	H	4.46418800	4.06716000	-2.78074400	H	-2.54699600	-4.62611700	4.29917400
H	-4.74558200	2.78609500	-0.63350900	C	4.25588400	4.57535400	-0.66541700	O	0.16131900	0.23809400	3.40357600
H	-3.35523200	2.69405900	0.04869900	H	4.46765100	4.12344100	0.30901700	C	-0.21666900	1.38770700	3.09669300
O	-4.83916600	-1.19277700	0.60387600	H	4.86311600	5.49027900	-0.73485600	O	-0.67161300	1.76945000	1.93775100
C	-5.48279700	-0.23971300	0.12633900	C	2.78194200	5.00194400	-0.62268000	C	-0.11248000	2.51201900	4.10926200
O	-5.05382500	0.61633800	-0.74529300	O	2.15349300	5.01594100	0.43285500	H	-0.95062700	3.20473100	3.96340200
C	-6.93600200	-0.04674400	0.55763000	N	2.23463000	5.40720000	-1.80879300	H	-0.18231000	2.07116100	5.11105300
H	-7.50852500	-0.82799900	0.03361600	H	2.82036700	5.43935300	-2.63239200	C	1.22668700	3.26685300	3.94918700
H	-6.98706100	-0.30301000	1.62356300	C	0.86565000	5.92282100	-1.90828300	H	1.29869200	3.67335100	2.93113200
C	-7.54218700	1.32919300	0.27768600	H	0.74595900	6.74751600	-1.19287800	H	2.05162600	2.54959800	4.06734600
H	-7.50694900	1.56556900	-0.79153200	H	0.75338200	6.33645300	-2.91858600	C	1.36882800	4.39766900	4.97311100
H	-7.00382100	2.11959700	0.81864900	C	-0.20346600	4.85937200	-1.61899900	H	0.56629600	5.13949800	4.85954800
H	-8.58955500	1.36003900	0.60430600	H	-0.04427500	4.50539200	-0.59622300	H	2.32545900	4.92021800	4.84557500
O	2.65903700	-2.45093100	-1.58501300	H	-1.19271400	5.33593600	-1.65341200	H	1.32870100	4.01457900	6.00231800
C	2.10981100	-3.39337900	-2.29457100	C	-0.16657600	3.65524200	-2.58321400	N	-0.04262500	-0.72215800	-1.89200700
O	0.90822700	-3.43039100	-2.62165100	H	0.88232200	3.41812400	-2.81481800	H	0.36240500	-0.02572100	-2.51854300
C	3.07622900	-4.48956300	-2.73418600	H	-0.69626300	3.86012300	-3.51993400	H	0.21549700	-1.65168100	-2.25945000
H	3.96213900	-4.00357400	-3.17133900	O	-0.15836800	2.04978600	-0.85530300	H	-1.07555200	-0.66110400	-2.00742900

C:

Ca	-2.72311300	-2.17919900	0.07335200	H	-4.68205700	2.64331200	-0.07061700	H	1.77866800	-4.26349900	-4.84934200
Mn	2.36087500	-1.21082000	-0.22675900	H	-3.22392900	2.38527900	0.40024500	H	1.21436100	-5.35115000	-3.59462000
Mn	0.67223800	-1.38764400	1.87685000	O	-4.85310600	-1.36893200	0.65151600	C	2.84322300	-6.15381800	-4.77981600
Mn	-0.66701000	0.46212800	0.23053700	C	-5.52580100	-0.39050100	0.27667500	H	3.73898500	-5.81128900	-5.31728800
Mn	-3.49825200	0.85361500	-1.50534900	O	-5.14164800	0.53253500	-0.54682000	H	3.16579700	-6.90779700	-4.04818600
O	1.32446400	-2.46793000	0.59317400	C	-6.95942500	-0.24264200	0.78280900	H	2.19017900	-6.65369100	-5.50681700
O	1.26798600	-0.01039400	0.71595600	H	-7.56041500	-0.94388000	0.18257800	N	3.24210900	0.37061600	-1.27747000
O	-0.91598100	-1.07108900	1.09517000	H	-6.97735200	-0.63205200	1.80837300	C	3.16623100	1.73047000	-1.01666900
O	-3.10719600	-0.73005400	-2.01647400	C	-7.55502000	1.16395400	0.69936500	H	2.48722100	2.11530600	-0.26751000
O	-2.38798500	0.63202100	0.03931200	H	-7.54859500	1.53384300	-0.33168900	C	4.04739100	2.39931600	-1.83338600
O	-0.83964700	-3.51369800	-0.78966900	H	-6.98945700	1.87364800	1.31894600	N	4.65539500	1.40315600	-2.59319500
H	-0.09292700	-3.31278300	-0.16522100	H	-8.59108400	1.16300500	1.06133000	H	5.37781100	1.54720800	-3.28801100
H	-0.36678300	-3.52974500	-1.64765400	O	3.12243000	-2.43401900	-1.56305400	C	4.14990500	0.20290500	-2.22858200
O	-3.98788200	-3.19053700	-1.81861400	C	2.34220000	-3.09688200	-2.36289200	H	4.45463300	-0.75381800	-2.62902500
H	-3.56879900	-3.79361600	-2.45418200	O	1.14276500	-2.81314400	-2.55938700	C	4.41803800	3.84194600	-2.02596900
H	-3.95484800	-2.28694100	-2.24061500	C	3.00586800	-4.27144000	-3.07299400	H	5.50081800	3.89706300	-2.21721700
O	-4.48236800	1.52148100	-2.85293100	H	3.93044900	-3.90005700	-3.54141100	H	3.93943700	4.23208900	-2.93955700
H	-3.86286900	2.05419300	-3.38741000	H	3.34197900	-4.96922800	-2.29008800	C	4.10503900	4.76256500	-0.82927900
O	-3.75329400	2.85441700	-0.28389100	C	2.12122200	-4.98731100	-4.09661700	H	4.50000400	4.32877000	0.09473200

H	4.62666800	5.71766000	-0.99197500	O	3.88193000	-1.29910300	1.23656400	O	0.20147100	0.03035300	3.27131500
C	2.62611800	5.07507500	-0.56115800	C	3.56228800	-1.47972400	2.44640400	C	-0.24629000	1.17313600	2.97924800
O	2.11940200	4.89286900	0.54202900	O	2.37154700	-1.50297900	2.90892000	O	-0.65801900	1.55890100	1.82606600
N	1.92944200	5.60092800	-1.61692900	C	4.66397000	-1.69241500	3.47953100	C	-0.25960100	2.23545000	4.06348000
H	2.43696900	5.83611100	-2.46000600	H	4.48469400	-2.67966000	3.93018100	H	-1.14725500	2.86687500	3.92869100
C	0.54831500	6.08022600	-1.48816100	H	4.49217700	-0.96741300	4.28766000	H	-0.32119900	1.73628700	5.03815500
H	0.49684500	6.79764600	-0.65753900	C	6.08609000	-1.58839700	2.92954800	C	1.01491900	3.10495700	3.99031100
H	0.31308900	6.62142800	-2.41354800	H	6.81862100	-1.76434700	3.72793300	H	1.08630200	3.56312600	2.99444500
C	-0.46153300	4.95400400	-1.22928400	H	6.25651000	-2.32464800	2.13550200	H	1.89328600	2.45319800	4.10432000
H	-0.17827400	4.46684000	-0.29214100	H	6.27418500	-0.59516000	2.50407800	C	1.03173800	4.19281200	5.06894500
H	-1.45467900	5.39972500	-1.08188000	O	-2.05275300	-3.41534100	2.02699700	H	0.17411500	4.87159300	4.96175200
C	-0.52317500	3.89580100	-2.34951000	C	-1.18334200	-3.45560400	2.92036500	H	1.94549900	4.79728000	5.00103900
H	0.49096600	3.74377000	-2.74963500	O	-0.07430500	-2.78359100	2.96257900	H	0.98989400	3.75820700	6.07755100
H	-1.17876800	4.19807200	-3.17337000	C	-1.36301700	-4.38273300	4.11321900	N	-0.41722900	-0.45926900	-1.60730500
O	-0.28480300	2.11469100	-0.82355800	H	-1.27297500	-3.81070400	5.04451400	H	0.10993200	0.17756100	-2.20547400
C	-0.97848500	2.54913700	-1.80208900	H	-0.56210400	-5.13308900	4.11488800	H	0.06179000	-1.36879400	-1.64134200
O	-1.95374500	1.95716000	-2.35843700	H	-2.33543500	-4.88044800	4.06764400	H	-1.37944100	-0.57195400	-2.01095700

TS3:

Ca	-2.82371000	-2.08878800	0.52287300	H	2.62865000	-5.42020800	-2.20037000	C	-0.79962300	2.79275900	-1.69663900
Mn	2.08891300	-1.46587300	-0.34280700	C	1.17094700	-5.57526800	-3.81446100	O	-1.99328900	2.59708600	-2.08466400
Mn	0.64738400	-1.26186900	1.93351000	H	0.73287600	-4.91390400	-4.57506700	O	3.75039500	-1.58006200	0.97905800
Mn	-0.66092900	0.48894400	0.16733400	H	0.33936100	-5.87749000	-3.16342300	C	3.55040200	-1.59383500	2.22612100
Mn	-3.43221100	1.39570500	-1.43268600	C	1.78586300	-6.80962500	-4.48308500	O	2.42182900	-1.43637500	2.80744000
O	1.07818200	-2.53173400	0.72662600	H	2.60165200	-6.53137800	-5.16551700	C	4.73288300	-1.81402700	3.16452900
O	1.24355700	-0.07210700	0.60534100	H	2.20109100	-7.50272000	-3.73803000	H	4.51176700	-2.72575500	3.73886100
O	-0.98280800	-0.91544700	1.22017600	H	1.03661700	-7.35924500	-5.06745000	H	4.71890500	-0.99601300	3.89849500
O	-2.94460000	0.04079800	-2.43108300	N	3.06017000	-0.07345200	-1.55827500	C	6.09021800	-1.91712700	2.46977600
O	-2.39330100	0.78541200	0.01872500	C	3.25352100	1.27302000	-1.29512600	H	6.88541500	-2.08697100	3.20724500
O	-1.19057000	-3.74516100	-0.20289200	H	2.76649100	1.74805200	-0.45432800	H	6.10319500	-2.74415300	1.75044600
H	-0.36958800	-3.48222300	0.29345500	C	4.10655300	1.80112600	-2.23501000	H	6.32358300	-0.99773700	1.91912300
H	-0.83344400	-3.80536100	-1.11547600	N	4.41944800	0.73329100	-3.07283100	O	-2.22525900	-3.00817100	2.63170300
O	-3.62612100	-2.39012600	-1.75686600	H	5.04408000	0.76888200	-3.86896100	C	-1.25174000	-3.03119100	3.41670500
H	-3.21282000	-2.96190300	-2.42414400	C	3.77726300	-0.37264900	-2.63146800	O	-0.09436000	-2.48385900	3.23793600
H	-3.57204900	-1.45428400	-2.13983700	H	3.85790800	-1.35933900	-3.06536100	C	-1.36511600	-3.78488900	4.73344900
O	-4.50140100	2.28090500	-2.58694100	C	4.67969800	3.16724400	-2.48094600	H	-0.65648200	-4.62307400	4.73337100
H	-3.91888700	2.72065700	-3.23394400	H	5.70851700	3.05056800	-2.85471700	H	-2.38150700	-4.16272200	4.87387500
O	-3.73743800	3.00291000	0.11972100	H	4.12576800	3.66668400	-3.29308400	H	-1.08641100	-3.12534200	5.56390300
H	-4.67626400	2.81305800	0.30542200	C	4.73052800	4.08235900	-1.23980200	O	0.38649300	0.27505500	3.20646000
H	-3.22058900	2.44412800	0.74475700	H	5.21173700	3.56137000	-0.40626700	C	-0.02585900	1.42290300	2.85777200
O	-4.90012200	-1.06776300	0.67917100	H	5.35135100	4.95608600	-1.48789500	O	-0.50141200	1.73709800	1.71657600
C	-5.55865200	-0.15421600	0.13758200	C	3.37919200	4.58532900	-0.71511700	C	0.10669800	2.54261400	3.87521500
O	-5.10764000	0.75273900	-0.65859300	O	3.00075100	4.35490000	0.43037200	H	-0.62852400	3.32274900	3.64185400
C	-7.06539400	-0.09192600	0.38913000	N	2.64079800	5.32306500	-1.60101600	H	-0.10946900	2.13614300	4.87179500
H	-7.51566900	-0.79795300	-0.32688800	H	3.05107700	5.55985100	-2.49505300	C	1.53323300	3.13363500	3.85151000
H	-7.24584600	-0.51164600	1.38645000	C	1.37240900	5.95794900	-1.22975400	H	1.76189400	3.49648300	2.83962200
C	-7.70238500	1.29000600	0.22774200	H	1.53062900	6.56179200	-0.32584900	H	2.24890500	2.32850300	4.06928000
H	-7.51144800	1.69486900	-0.77162800	H	1.10659500	6.64061300	-2.04684200	C	1.70292900	4.27163500	4.86311200
H	-7.30205800	2.00119000	0.96418600	C	0.24508800	4.95224800	-0.95798300	H	1.00989600	5.09835200	4.65263200
H	-8.78737300	1.23307500	0.38239800	H	0.55646600	4.31672200	-0.12352100	H	2.72310800	4.67580300	4.83104900
O	2.52540100	-2.83066800	-1.67880000	H	-0.64570800	5.50813700	-0.63352400	H	1.50972800	3.92763200	5.88900800
C	1.63377500	-3.54418000	-2.30180300	C	-0.10560600	4.06269300	-2.16805600	N	-0.65055600	-0.49769000	-1.55441100
O	0.42154700	-3.26110000	-2.36086700	H	0.82490600	3.75371900	-2.66546700	H	0.04578200	-0.04028300	-2.14815500
C	2.19097700	-4.78776700	-2.98866100	H	-0.73853600	4.58512100	-2.89369200	H	-0.39967100	-1.49436900	-1.53607700
H	3.04370800	-4.47387100	-3.61045700	O	-0.10351500	2.04889700	-0.94249500	H	-1.86044000	-0.24444100	-2.06894600

D:

Ca	-2.58493200	-2.36073000	0.29094600	Mn	0.66734100	-1.19656700	1.95149600	Mn	-3.56547800	1.11651400	-1.46808000
Mn	2.22917200	-1.26446600	-0.26094000	Mn	-0.71019700	0.39288800	0.10169400	O	1.26935700	-2.41961400	0.76725100

O	1.20202400	0.04011400	0.63172500	C	2.90426700	-6.62829900	-4.33548100	O	3.82758200	-1.19884300	1.14713400
O	-0.96183000	-1.00178600	1.18065300	H	3.73646700	-6.25721100	-4.95068900	C	3.57008200	-1.24161000	2.38206800
O	-3.05449400	-0.24307000	-2.51647100	H	3.33380500	-7.26604600	-3.55015800	O	2.40391800	-1.20330700	2.90743200
O	-2.47188900	0.56692800	-0.08807300	H	2.27678900	-7.26382400	-4.97377100	C	4.72090500	-1.34781200	3.37802600
O	-0.77631600	-3.85341300	-0.34900800	N	3.12311500	0.21242600	-1.43745700	H	4.56500100	-2.28105300	3.93905500
H	-0.02746000	-3.52614300	0.21856300	C	3.15285900	1.57555600	-1.19256500	H	4.58836500	-0.54035800	4.11185500
H	-0.33675700	-3.87795800	-1.22774900	H	2.56297900	2.00702300	-0.39533000	C	6.11414800	-1.30905500	2.75111100
O	-3.44454300	-2.80579200	-1.95831300	C	4.00534600	2.17898200	-2.08663000	H	6.88539700	-1.40327200	3.52660500
H	-2.92973800	-3.26998800	-2.63919500	N	4.48620700	1.13891300	-2.87838200	H	6.24543200	-2.12547000	2.03151400
H	-3.55172500	-1.87069000	-2.30720100	H	5.15612100	1.22974200	-3.63211400	H	6.28033300	-0.36704200	2.21449900
O	-4.70128200	1.91406800	-2.62617800	C	3.93839000	-0.02328200	-2.45455100	O	-1.99912800	-3.27340100	2.41533700
H	-4.15875100	2.44344600	-3.24007800	H	4.15470300	-1.00204700	-2.85869700	C	-1.11106900	-3.17445100	3.28990200
O	-3.92936300	2.70551900	0.03781600	C	4.44480200	3.59475700	-2.32660400	O	-0.02133800	-2.48095900	3.21990200
H	-4.84675600	2.46137700	0.26589700	H	5.50086300	3.58277900	-2.63706700	C	-1.25102000	-3.94329700	4.59544800
H	-3.35407700	2.21962500	0.67325000	H	3.89205500	4.02065500	-3.18046300	H	-0.44600600	-4.68603300	4.66650800
O	-4.75434300	-1.53998000	0.44936900	C	4.32477400	4.52794800	-1.10402700	H	-2.22054600	-4.44666700	4.64259500
C	-5.50631000	-0.61923500	0.07288300	H	4.80531700	4.07225300	-0.23271400	H	-1.13599700	-3.25878900	5.44428500
O	-5.17740800	0.39107800	-0.66051800	H	4.86606200	5.45816200	-1.33252200	O	0.21778500	0.32592900	3.19002800
C	-6.98388600	-0.67293600	0.46014600	C	2.90039800	4.89687500	-0.66987400	C	-0.27016400	1.43508100	2.80863300
H	-7.45580900	-1.35777200	-0.26226200	O	2.48538900	4.66360100	0.46220500	O	-0.71366800	1.70199100	1.64425700
H	-7.04310100	-1.17211900	1.43529200	N	2.13726600	5.52334900	-1.61863100	C	-0.27621700	2.56557200	3.82394800
C	-7.71700300	0.66997100	0.46258000	H	2.56711800	5.77496100	-2.49927200	H	-1.07582300	3.27091200	3.56452300
H	-7.65681500	1.15214500	-0.51888800	C	0.79203900	6.03024900	-1.33224200	H	-0.48148600	2.14413100	4.81652000
H	-7.28797900	1.35645800	1.20607700	H	0.83818200	6.67190700	-0.44182600	C	1.08568300	3.29320200	3.83772500
H	-8.77479000	0.52840800	0.71801800	H	0.49884200	6.65775000	-2.18347300	H	1.30692400	3.67357200	2.83069700
O	2.92826200	-2.58841600	-1.52071100	C	-0.23639300	4.91833100	-1.08299300	H	1.86999200	2.56249800	4.08064400
C	2.18276200	-3.40216200	-2.21058200	H	0.10016700	4.33896200	-0.21760800	C	1.11463200	4.44530800	4.84719800
O	0.95631700	-3.26429900	-2.37411800	H	-1.19483400	5.38410400	-0.81448800	H	0.35094200	5.20002800	4.61200700
C	2.94139900	-4.56946200	-2.83669900	C	-0.43441700	3.96948000	-2.28379000	H	2.09111300	4.94699900	4.84231400
H	3.79903500	-4.15573000	-3.38962100	H	0.54576200	3.74047200	-2.72448600	H	0.92579200	4.08721900	5.86910000
H	3.38491100	-5.14468000	-2.00885000	H	-1.07779000	4.41113200	-3.05273300	N	-0.57480000	-0.66682000	-1.53538900
C	2.09452900	-5.47380400	-3.73523600	O	-0.27583300	1.96861900	-1.04835500	H	0.02839300	-0.13881200	-2.17178400
H	1.64726400	-4.87041900	-4.53756700	C	-1.02705800	2.65436000	-1.80069000	H	-0.14279800	-1.59348300	-1.44866500
H	1.25215900	-5.87015900	-3.15222200	O	-2.21254000	2.37636800	-2.17399200	H	-2.09620100	-0.45292900	-2.20769200

TS4:

Ca	3.11397000	1.51800400	0.69342600	O	4.66494300	-1.98462600	-0.67938700	H	-3.14736200	-0.94319200	-0.48086000
Mn	-1.36822100	1.81264600	-0.38161000	C	6.74805700	-1.43258100	0.32455100	C	-4.40262300	-0.55564400	-2.28169100
Mn	-0.35022000	1.27683200	2.06010100	H	7.34895200	-0.84885600	-0.39080000	N	-4.31958700	0.54358400	-3.13259800
Mn	0.44423100	-0.67581000	0.22078100	H	6.96907100	-1.01406300	1.31486400	H	-4.91212400	0.71861100	-3.93463300
Mn	2.88802300	-2.21968400	-1.43993500	C	7.12110400	-2.91337700	0.23804200	C	-3.33796300	1.36494500	-2.68849800
O	-0.28688200	2.60857800	0.85794900	H	6.90039300	-3.31688600	-0.75581500	H	-3.06709000	2.31201900	-3.13399500
O	-1.23635000	0.30460000	0.74858700	H	6.56510600	-3.50792600	0.97616800	C	-5.40609200	-1.64667000	-2.51852400
O	1.15793700	0.49700300	1.34718400	H	8.19055100	-3.05089900	0.44196400	H	-6.36109000	-1.18828300	-2.81889800
O	2.75496200	-0.73122900	-2.43729400	O	-1.23327900	3.22740900	-1.76490900	H	-5.09465400	-2.26313600	-3.37866900
O	2.01807700	-1.45610500	-0.01964300	C	-0.17110700	3.74012800	-2.29369700	C	-5.68084300	-2.54401900	-1.29536800
O	2.12100800	3.71502100	0.33624700	O	0.99036400	3.28389700	-2.16068500	H	-5.94601600	-1.92948200	-0.42932300
H	1.21952300	3.54440700	0.72110500	C	-0.41663400	4.99807100	-3.12367600	H	-6.54970300	-3.17807000	-1.52692600
H	1.89655100	3.85434900	-0.60853500	H	-1.25435300	4.79060300	-3.80677200	C	-4.53512200	-3.45669600	-0.83814200
O	3.49784400	1.79101500	-1.70057700	H	-0.79467000	5.76703700	-2.43113300	O	-4.12780200	-3.45026000	0.32048700
H	2.85743800	2.32181300	-2.21342400	C	0.80264700	5.51435000	-3.89200300	N	-4.02354900	-4.29660300	-1.79073800
H	3.49945200	0.88624400	-2.11399000	H	1.16989700	4.72456500	-4.56254700	H	-4.46116300	-4.32403000	-2.70239500
O	3.71643200	-3.25583200	-2.66755200	H	1.61820800	5.71060300	-3.18308500	C	-3.00154100	-5.29971700	-1.47771300
H	3.02392500	-3.61812700	-3.25128900	C	0.49333300	6.78148700	-4.69668800	H	-3.34197800	-5.89305500	-0.61841200
O	2.85843600	-3.89512500	-0.00084500	H	-0.29927600	6.60291000	-5.43724900	H	-2.93466800	-5.97032700	-2.34388700
H	3.81404600	-3.91779000	0.19886300	H	0.15629900	7.59789100	-4.04263400	C	-1.63371900	-4.68808100	-1.14222100
H	2.45576900	-3.29522700	0.66891600	H	1.38082700	7.13357500	-5.23799300	H	-1.76363100	-4.03746100	-0.27203300
O	4.83486900	-0.00028800	0.40373300	N	-2.78016800	0.85014600	-1.60449400	H	-0.95257700	-5.49907600	-0.84837100
C	5.29058400	-1.09441100	0.00958000	C	-3.43038800	-0.34135200	-1.33369900	C	-1.01372100	-3.87536000	-2.29701000

H	-1.80699200	-3.29464500	-2.78926300	H	-5.04221500	4.30239000	1.48203300	H	-0.34372000	-3.56652400	3.53616800
H	-0.53265800	-4.51923600	-3.04138400	H	-5.78512500	2.70018300	1.56637000	H	-0.52511200	-2.35378300	4.83454800
O	-0.48965200	-1.99242200	-0.97977500	O	2.85579600	2.17862700	2.94339500	C	-2.37521000	-2.81542800	3.78747800
C	-0.00865300	-2.86816000	-1.75416500	C	1.89228500	2.37568100	3.71902900	H	-2.69355500	-3.04765900	2.76145200
O	1.20458600	-3.00245700	-2.12512800	O	0.64254200	2.18958200	3.45891700	H	-2.84738000	-1.86063100	4.05759100
O	-3.08110900	2.48431300	0.86834600	C	2.15299300	2.90290000	5.12153100	C	-2.84473200	-3.91973900	4.73993200
C	-3.00237400	2.43520400	2.12072800	H	1.61210500	3.84631400	5.26575200	H	-2.40009400	-4.88960800	4.47571400
O	-2.02706500	1.94909000	2.80845500	H	3.22318200	3.05826100	5.28271300	H	-3.93605500	-4.03229900	4.70187200
C	-4.14444300	2.99011000	2.96973400	H	1.76134600	2.19031400	5.85815300	H	-2.56583000	-3.69722700	5.77959200
H	-3.71577700	3.78760700	3.59435200	O	-0.52568100	-0.33774500	3.27140800	N	0.45117100	0.47758400	-1.34393100
H	-4.44160100	2.19760900	3.67110900	C	-0.41360600	-1.53217100	2.86408700	H	-0.08785200	0.14717300	-2.14216400
C	-5.34103900	3.50196000	2.16888100	O	-0.01434600	-1.90940300	1.70833600	H	0.85907600	1.40087900	-1.51676100
H	-6.11408700	3.89425000	2.84255200	C	-0.84229400	-2.63166000	3.82083700	H	1.91848100	-0.31253600	-2.07410000

E:

Ca	3.07942200	1.56299800	0.73961300	H	-1.00397500	5.75134500	-2.48881400	C	0.04841000	-2.83880500	-1.79953000
Mn	-1.36777200	1.79529100	-0.35542400	C	0.67185000	5.57723700	-3.87234900	O	1.26602700	-2.95136200	-2.16962300
Mn	-0.38460900	1.22379600	2.10259800	H	1.12780500	4.79640100	-4.49701900	O	-3.12099900	2.40339700	0.93379700
Mn	0.45112600	-0.65702000	0.21322300	H	1.43839300	5.86114100	-3.13861100	C	-3.04746500	2.32318100	2.18206600
Mn	2.93693300	-2.14561000	-1.48278600	C	0.30072200	6.78803700	-4.73557200	O	-2.06494800	1.83541700	2.86417200
O	-0.33510400	2.58302000	0.93954800	H	-0.44255400	6.52234300	-5.50086400	C	-4.20042400	2.83380300	3.04468500
O	-1.24538400	0.26120600	0.77160900	H	-0.12705200	7.59702900	-4.12688900	H	-3.78759400	3.62119600	3.69237000
O	1.14502600	0.49342200	1.36500900	H	1.18087700	7.19090700	-5.25306700	H	-4.48536800	2.01701000	3.72291700
O	2.79825300	-0.67468800	-2.53173000	N	-2.81238500	0.86013400	-1.57426200	C	-5.40373500	3.34642200	2.25454900
O	2.05973400	-1.33542800	-0.10855100	C	-3.43724500	-0.34935300	-1.32834100	H	-6.18556400	3.70671200	2.93599200
O	2.04202400	3.73896600	0.40612700	H	-3.13485600	-0.96673200	-0.49334400	H	-5.11681800	4.17019900	1.59061800
H	1.14857100	3.54587900	0.80018900	C	-4.41596100	-0.55759100	-2.27118500	H	-5.83177700	2.55374500	1.62882000
H	1.80135700	3.88286400	-0.53504000	N	-4.36337000	0.56488100	-3.09344900	O	2.80950900	2.16636600	3.00132300
O	3.40946700	1.87003800	-1.65981900	H	-4.96954300	0.75087600	-3.88265000	C	1.84445500	2.32447600	3.78577800
H	2.78258300	2.42092700	-2.16984000	C	-3.39124100	1.39252400	-2.63728300	O	0.59939500	2.11243900	3.52985400
H	3.46991700	0.99393200	-2.12198400	H	-3.14234800	2.35555300	-3.06118300	C	2.10192300	2.83700400	5.19471300
O	3.77682600	-3.19442300	-2.69126300	C	-5.39920900	-1.66300000	-2.52493700	H	1.58937600	3.79756200	5.33191800
H	3.09015700	-3.57318300	-3.27150700	H	-6.36621200	-1.21806500	-2.80658000	H	3.17383500	2.96201300	5.37051100
O	2.90973700	-3.78577500	-0.02988900	H	-5.08361300	-2.25373900	-3.40159700	H	1.67736500	2.13723600	5.92479700
H	3.86268200	-3.81235000	0.18200600	C	-5.64485900	-2.59260900	-1.31975200	O	-0.51039100	-0.44065900	3.27005800
H	2.49460300	-3.20578200	0.64844300	H	-5.91282100	-2.00245600	-0.43775900	C	-0.35037500	-1.61863800	2.83635700
O	4.83770900	0.09565000	0.38576200	H	-6.50436000	-3.23741500	-1.55684000	O	0.06445100	-1.95462200	1.67111100
C	5.31850800	-0.97778800	-0.03323000	C	-4.48069100	-3.49601800	-0.89183200	C	-0.73524500	-2.75668500	3.76700300
O	4.70994600	-1.87298700	-0.73318000	O	-4.07332900	-3.51854500	0.26648900	H	-0.21682400	-3.66984300	3.44912700
C	6.78762900	-1.28398400	0.25912500	N	-3.95323800	-4.29776700	-1.86910700	H	-0.41031600	-2.49933500	4.78380100
H	7.36439500	-0.68733100	-0.46545500	H	-4.39289700	-4.30927700	-2.78014500	C	-2.26315900	-2.97957200	3.75123200
H	7.01472200	-0.86143100	1.24622800	C	-2.92377700	-5.30009500	-1.57925100	H	-2.59165200	-3.18966400	2.72351700
C	7.19124800	-2.75640900	0.16480400	H	-3.26067200	-5.91693800	-0.73522100	H	-2.75498200	-2.04550300	4.05600600
H	6.96408800	-3.16349800	-0.82608000	H	-2.84947700	-5.94877500	-2.46141200	C	-2.68961500	-4.12304600	4.67732000
H	6.65978200	-3.36359300	0.91069600	C	-1.56150400	-4.68605500	-1.22567700	H	-2.22465800	-5.07309400	4.37820300
H	8.26637600	-2.87067800	0.35221600	H	-1.70053600	-4.05183400	-0.34486000	H	-3.77819000	-4.26261800	4.65224100
O	-1.26610900	3.26209800	-1.68411200	H	-0.87673400	-5.49779900	-0.94240400	H	-2.40031600	-3.92375400	5.71885500
C	-0.22808600	3.78323400	-2.25150800	C	-0.94101000	-3.84977400	-2.36328600	N	0.31761000	0.58369500	-1.29725200
O	0.95266900	3.37959700	-2.12241100	H	-1.73679200	-3.26981700	-2.85249400	H	-0.02447100	0.14819200	-2.15370300
C	-0.53525100	4.99263400	-3.13486200	H	-0.44822500	-4.47734000	-3.11387400	H	0.95448100	1.35223300	-1.51408600
H	-1.32185500	4.69514500	-3.84593600	O	-0.44455500	-1.98077500	-1.01527900	H	1.96599000	-0.28021900	-2.18049600

F

Ca	3.02013500	0.66021300	0.63585300	O	-1.04875000	0.46250700	0.85689900	H	3.16707100	3.44783000	0.08421600
Mn	-0.33095800	1.81529000	-0.15663100	O	1.15304700	-0.47932400	1.62707100	O	4.11322500	1.24792800	-1.47516100
Mn	0.09122100	0.79497800	2.31823800	O	2.54151300	-0.74520600	-2.57560600	H	3.64261200	2.03629500	-1.82129300
Mn	0.10802600	-1.07157900	0.26138200	O	1.27297800	-2.26393400	-0.22645700	H	3.89447400	0.50621700	-2.08129000
Mn	1.95660900	-2.85244500	-1.82099800	O	3.46411900	3.09910900	0.95678500	O	2.49308500	-3.42337900	-3.46671500
O	0.88725700	2.00172100	1.13479300	H	2.69332000	3.26337600	1.53286800	H	1.72303800	-3.83321400	-3.90209100

O	1.60838000	-4.94156500	-0.73858400	N	-3.59443500	2.16428400	-2.87128100	H	-1.94720000	4.63632500	3.56709400
H	2.57474400	-4.99566900	-0.59608100	H	-4.07231800	2.65956600	-3.61383400	H	-3.33558500	3.59104100	3.36956600
H	1.28844600	-4.40715500	0.01858000	C	-2.34353300	2.43548900	-2.42784900	C	-3.20145100	5.16422300	1.86260800
O	4.19194100	-1.30309800	0.10140300	H	-1.70604000	3.22221800	-2.80321600	H	-3.81322200	5.87819600	2.42894800
C	4.45009700	-2.48309400	-0.22205500	C	-5.50941100	0.60569900	-2.36184100	H	-2.43485100	5.72548800	1.31555800
O	3.75379600	-3.21440400	-1.02072700	H	-6.18700900	1.45965600	-2.51787700	H	-3.84391900	4.67395000	1.12120200
C	5.72533900	-3.12055400	0.33324400	H	-5.52883700	0.04329200	-3.31084300	O	3.29698700	0.88751000	3.02004000
H	6.56296800	-2.61427800	-0.17129000	C	-6.09360800	-0.25359900	-1.22364200	C	2.48607300	1.02532800	3.95222800
H	5.79658000	-2.82718200	1.38927100	H	-6.05545900	0.29646000	-0.27800100	O	1.19604300	1.14647900	3.82275900
C	5.84136700	-4.63582400	0.16403500	H	-7.15369400	-0.44267400	-1.44922500	C	2.96054400	1.06428600	5.39324500
H	5.77332200	-4.92069400	-0.89175600	C	-5.41608000	-1.60467600	-0.95784800	H	2.46237500	1.87411700	5.93773100
H	5.04177400	-5.15961800	0.70541600	O	-5.05188400	-1.93111700	0.16889300	H	4.04635800	1.18577900	5.43192500
H	6.79996400	-4.99581600	0.55972400	N	-5.27676000	-2.42983600	-2.03990400	H	2.68266000	0.12128600	5.88307500
O	0.17891600	3.25113600	-1.39491800	H	-5.66117000	-2.14063900	-2.92957900	O	-0.92269400	-0.57905100	3.28720300
C	1.26478400	3.77040600	-1.86565600	C	-4.69923700	-3.77279300	-1.92983900	C	-1.25215600	-1.71256700	2.78610900
O	2.42879700	3.43775600	-1.56763600	H	-5.22777500	-4.31798500	-1.13680100	O	-0.93896500	-2.15286400	1.63897200
C	1.02404200	4.88798900	-2.88502100	H	-4.89787800	-4.28533000	-2.87975100	C	-2.14602100	-2.57930600	3.65520500
H	0.55757100	4.42605600	-3.77199700	C	-3.19780200	-3.75864600	-1.60630700	H	-2.10406400	-3.60890300	3.28012500
H	0.26143700	5.56134300	-2.46636600	H	-3.06812100	-3.25236800	-0.64507700	H	-1.75621400	-2.55974000	4.68193300
C	2.27944700	5.66372700	-3.29224300	H	-2.85914400	-4.79660300	-1.47930700	C	-3.60095900	-2.06259100	3.64296900
H	3.02460900	4.96063200	-3.68680500	C	-2.33725900	-3.05098100	-2.67198900	H	-3.97158900	-2.04056700	2.60868300
H	2.73241800	6.10904700	-2.39565700	H	-2.89142900	-2.17914700	-3.05153500	H	-3.60678300	-1.02624600	4.00834900
C	1.98412800	6.75585300	-4.32598100	H	-2.10045500	-3.70642100	-3.51734400	C	-4.52460000	-2.92753200	4.50680200
H	1.56163500	6.33153300	-5.24821600	O	-1.21247900	-1.71513200	-1.08858700	H	-4.54979500	-3.96551200	4.14657600
H	1.26353300	7.49040200	-3.93934900	C	-1.04704500	-2.50725100	-2.07030200	H	-5.55296400	-2.54370000	4.48717900
H	2.89768500	7.29912000	-4.59936700	O	0.05635000	-2.84956700	-2.59620700	H	-4.19276100	-2.94572400	5.55457600
N	-2.03503300	1.62361600	-1.42944300	O	-1.53407600	3.16018800	0.87443100	N	0.63419100	0.36912800	-0.99871800
C	-3.13247100	0.80731600	-1.21247500	C	-1.68365900	3.09774200	2.13276800	H	-0.00463700	0.16717000	-1.78213700
H	-3.11941300	0.05933500	-0.43269400	O	-1.16260800	2.23733000	2.91766700	H	1.85001000	-0.18216200	-2.10001500
C	-4.12524200	1.12817700	-2.10727500	C	-2.56882700	4.14224600	2.80643200	H	2.28423500	-0.86769500	-3.50767100

G:

Ca	-2.75720600	0.10757300	-0.90903000	C	-3.53676100	6.13851500	-1.43691400	H	4.90169800	-1.50380500	-3.35542800
Mn	-0.07604500	-1.71155700	-0.08430900	H	-3.13620500	6.25269200	-2.45124600	C	6.50117600	-2.01513600	-1.96752300
Mn	-1.30879400	-0.70911000	2.10544300	H	-2.74760800	6.42230100	-0.72865500	H	6.81195200	-2.88837700	-1.38363600
Mn	0.17352700	1.10812200	0.65897800	H	-4.36526900	6.84794300	-1.31456700	H	7.20797800	-1.91248100	-2.80241000
Mn	-0.17992400	2.87827500	-1.80886100	O	-0.52888200	-2.76058200	-1.63290000	C	6.59282600	-0.81762800	-1.02121000
O	-1.72933300	-1.60526800	0.57337300	C	-1.70061100	-2.91077400	-2.18192700	O	6.58605400	-0.97514400	0.20747500
O	0.44154000	-0.69515700	1.39081800	O	-2.67070300	-2.15023000	-2.02053400	N	6.60344900	0.41690600	-1.58527300
O	-1.52260100	0.86060200	1.23678900	C	-1.79896800	-4.13341300	-3.08876100	H	6.58195700	0.49093700	-2.59492000
N	-0.22459200	0.02898700	-0.92889600	H	-0.99050800	-4.05503400	-3.83199200	C	6.39878300	1.63024400	-0.78301300
O	-0.12279200	2.71439200	-0.02519900	H	-1.54644500	-5.01298900	-2.47686800	H	7.06836200	1.57348000	0.08167200
O	-5.01765100	-0.70848800	-1.68598300	C	-3.15336400	-4.31382300	-3.77806300	H	6.71230200	2.48261400	-1.39846500
H	-5.33000700	-0.85607100	-0.77003400	H	-3.38792000	-3.40816400	-4.35413800	C	4.94529400	1.79268100	-0.30119800
H	-4.65790300	-1.56596500	-1.99114000	H	-3.93806500	-4.40070600	-3.01326300	H	4.68405300	0.93937200	0.33294000
O	-2.50119600	0.70615400	-3.35610900	C	-3.18415300	-5.54195900	-4.69461500	H	4.89097700	2.68454500	0.33876100
H	-3.27987800	1.23313800	-3.60326700	H	-2.42941800	-5.46577000	-5.49018400	C	3.94551200	1.91262800	-1.45314800
H	-1.72780000	1.30895500	-3.55693100	H	-2.98090200	-6.46531100	-4.13394700	H	4.11525500	1.10748900	-2.18567700
O	-0.47406700	2.48786700	-3.61302000	H	-4.16435400	-5.65363000	-5.17603800	H	4.07001500	2.85444900	-2.00437300
H	0.34756300	2.14581800	-4.00773000	N	1.92758400	-1.97145800	-0.58566700	O	2.15164600	1.30491600	0.03766800
O	0.64668500	5.05186700	-1.40611000	C	2.57726200	-2.07642200	-1.79678500	C	2.47158400	1.80236600	-1.07303100
H	-0.25925200	5.40394200	-1.52269400	H	2.02301600	-2.10281400	-2.72582700	O	1.66173700	2.18883000	-1.99462500
H	0.68440300	4.82384000	-0.45467600	C	3.93537200	-2.15844100	-1.58196400	O	0.18983600	-3.37882100	1.14682800
O	-3.29153800	2.43109100	-1.10537000	N	4.08097800	-2.13040600	-0.20066800	C	-0.27830500	-3.42396500	2.32869400
C	-2.97068400	3.60841000	-1.35161300	H	4.97539100	-2.02255100	0.28661800	O	-0.87257300	-2.48329000	2.95033200
O	-1.80371300	3.97994100	-1.76787600	C	2.85896700	-1.99690600	0.35703100	C	-0.12821200	-4.75272900	3.06526700
C	-4.01646100	4.70859300	-1.18745700	H	2.67004500	-1.88579300	1.41476700	H	0.84213800	-5.17904800	2.77919400
H	-4.84621500	4.45148000	-1.86247000	C	5.08311600	-2.23841700	-2.55780600	H	-0.88808100	-5.42544700	2.63672400
H	-4.42277400	4.59784400	-0.17228800	H	5.08819300	-3.21928600	-3.05579100	C	-0.28521400	-4.66874200	4.58444700

H	-0.18746000	-5.66529900	5.03412500	H	-5.45526300	-1.89664900	3.38719300	C	2.03604800	2.45075100	4.94068700
H	0.47965000	-4.01808400	5.02676200	H	-6.33632800	-0.60847700	2.50830600	H	2.17526100	3.14622200	4.10350800
H	-1.26313600	-4.25711100	4.85570600	O	-0.60163300	0.26899900	3.67537100	H	2.73824700	1.62035400	4.77203900
O	-4.33056000	-0.38327200	0.96440300	C	0.20796000	1.25487500	3.58801000	C	2.36449300	3.14339900	6.26762200
C	-4.20043800	-0.63887800	2.17941300	O	0.68864100	1.74612600	2.52145200	H	1.69811200	3.99941200	6.44512800
O	-3.07761500	-0.76107800	2.81390600	C	0.60016600	1.91114800	4.90539400	H	3.39665400	3.51754100	6.27465600
C	-5.42209000	-0.84993400	3.05752500	H	-0.11125700	2.73865800	5.06337700	H	2.25309000	2.45601000	7.11788900
H	-5.34647900	-0.22852900	3.95731100	H	0.42228800	1.18802600	5.71077800	H	0.54298400	0.09313500	-1.60583300

TS7:

Ca	-3.20444900	0.96359400	-0.52314400	H	-1.30181000	-3.99857100	-3.71445300	H	4.70276000	2.74623300	-0.51932100
Mn	-0.18704000	-1.30819700	-0.72887900	H	-1.77720000	-3.93117000	-2.03405400	O	2.27807000	1.13351800	0.66795500
Mn	-1.52130900	-0.89670500	1.61801800	C	-3.46157900	-3.98746300	-3.43631600	C	2.84546300	1.74471100	-0.27233300
Mn	0.21219500	1.13586700	0.95257000	H	-3.69844500	-3.57327200	-4.42555300	O	2.27775700	2.42406200	-1.20167300
Mn	0.38768800	2.87071300	-1.22431700	H	-4.18683000	-3.54146300	-2.73876700	O	-0.29599900	-3.38142400	-0.03409000
O	-1.92552800	-1.12267400	-0.16693700	C	-3.63071400	-5.51059200	-3.44715800	C	-0.85953000	-3.68069300	1.05881100
O	0.23690800	-0.85099100	1.03223700	H	-2.94065000	-5.98205700	-4.16097300	O	-1.38139000	-2.86301700	1.89116500
O	-1.55369200	0.90607500	1.32619400	H	-3.42698500	-5.94205800	-2.45702100	C	-0.95631200	-5.16364900	1.41409200
N	0.05319200	0.81199700	-0.95622900	H	-4.65144600	-5.79642300	-3.73252200	H	-0.05120300	-5.65242800	1.03102000
O	0.22634000	2.86305000	0.60233900	N	1.79302500	-1.73343900	-1.14191200	H	-1.79068100	-5.56682900	0.81754500
O	-4.72574800	-0.26652700	-1.99255400	C	2.57834500	-1.42878200	-2.23230400	C	-1.17573100	-5.46064200	2.89882400
H	-5.25516000	-0.93832400	-1.53125500	H	2.16344600	-0.91926900	-3.09128300	H	-1.25789300	-6.54262000	3.06453400
H	-4.18966900	-0.75072500	-2.66704700	C	3.86196700	-1.87370600	-2.00890900	H	-0.34161100	-5.08538200	3.50514900
O	-2.20723700	1.31578800	-2.75270900	N	3.81987500	-2.47806700	-0.75765300	H	-2.08930400	-4.97977200	3.26389500
H	-2.19544100	0.45403000	-3.24497100	H	4.64869500	-2.74819800	-0.21999000	O	-4.72443800	0.16572900	1.09527100
H	-1.43876000	1.86608300	-3.07092700	C	2.56945900	-2.35341600	-0.26440600	C	-4.45299400	-0.53177200	2.10002600
O	0.20139800	2.70784700	-3.06893200	H	2.25719400	-2.68763000	0.71380400	O	-3.29873800	-1.03176100	2.37479400
H	0.91431200	2.13466600	-3.40368800	C	5.10288900	-1.77083200	-2.86010700	C	-5.53029500	-0.83355200	3.12651700
O	1.18885600	5.04594600	-0.88885800	H	5.03768500	-2.46496300	-3.71121600	H	-5.37489600	-0.18392500	3.99864900
H	0.30396600	5.38685200	-1.13329200	H	5.12657100	-0.76433100	-3.30115100	H	-5.45246500	-1.87000100	3.47161800
H	1.13569300	4.92330700	0.07999300	C	6.45040600	-2.05137400	-2.14038900	H	-6.52246900	-0.63656400	2.71083500
O	-3.19075100	3.28352100	-0.53537100	H	6.56734900	-3.12499400	-1.95647600	O	-0.83740900	-0.56270800	3.45735600
C	-2.45839800	4.19458700	-0.98120100	H	7.26746100	-1.74374800	-2.80731000	C	0.01533900	0.34212200	3.74599000
O	-1.24421100	4.05927800	-1.37723500	C	6.56408800	-1.36918200	-0.77735200	O	0.59497400	1.11994400	2.92652100
C	-3.07113900	5.59037600	-1.11649900	O	6.36034700	-1.99960800	0.26928300	C	0.34117500	0.51200000	5.22336700
H	-3.85148400	5.50408300	-1.88768800	N	6.81697800	-0.03537100	-0.77717400	H	-0.28786600	1.34075600	5.58812100
H	-3.60581700	5.79071300	-0.17830900	H	6.93073100	0.43293800	-1.66794300	H	0.01266200	-0.39154600	5.75100000
C	-2.10755900	6.72575700	-1.45987700	C	6.60660300	0.78723700	0.42154900	C	1.81741800	0.82412500	5.50653500
H	-1.58101400	6.52920000	-2.40151100	H	7.09409500	0.28019600	1.26055000	H	2.10710700	1.71476800	4.93506800
H	-1.35862800	6.86912800	-0.66845700	H	7.12337900	1.74072000	0.25550900	H	2.43958100	-0.00181000	5.12991700
H	-2.65073700	7.67342400	-1.56674000	C	5.11564400	1.00663600	0.74025200	C	2.09034400	1.03745600	6.99920900
O	-0.65503200	-1.66539600	-2.56920700	H	4.65231500	0.03721100	0.95278400	H	1.50530200	1.88020500	7.39386300
C	-1.80505800	-2.05936200	-3.02940600	H	5.03892800	1.59537000	1.66458000	H	3.15116900	1.25431100	7.18073800
O	-2.65315300	-1.26538800	-3.49367500	C	4.36671900	1.70669000	-0.39493800	H	1.82647300	0.14724800	7.58725500
C	-2.04848900	-3.55978100	-3.03255000	H	4.56944800	1.20964500	-1.35485400	H	-0.85766100	0.89380800	-1.43440500

H:

Ca	-2.81750400	0.88980700	-0.80161600	H	-4.03399500	-0.78291000	-2.88391100	C	-3.40203600	5.54998100	-0.63172800
Mn	-0.22752100	-1.75313300	-0.64284800	O	-2.22937600	1.42471700	-3.15159500	H	-4.11993500	5.55029700	-1.46501400
Mn	-1.44298300	-0.90978200	1.64703800	H	-2.04562700	0.57462700	-3.60890800	H	-4.01142200	5.52872500	0.28206500
Mn	0.24732400	1.15588000	0.92377700	H	-1.43211900	2.00311000	-3.23112300	C	-2.52061700	6.79761800	-0.68007300
Mn	0.18295600	3.12196500	-1.02740600	O	0.01835100	3.21915600	-2.87315500	H	-1.93252100	6.83335200	-1.60546900
O	-1.90145200	-1.29599600	-0.09467900	H	0.89147800	3.05108000	-3.27155500	H	-1.82799200	6.83093300	0.17197300
O	0.28464400	-0.83803600	0.92377300	O	1.00774800	5.16967900	-0.57114800	H	-3.13665700	7.70494300	-0.63754300
O	-1.48564900	0.88107200	1.37176600	H	0.12065300	5.57413400	-0.67110800	O	-0.62507900	-1.84095500	-2.53733800
N	-0.27682600	1.32145900	-0.92017200	H	1.06965700	4.95791900	0.38350500	C	-1.76186500	-2.15188500	-3.09844200
O	0.28382500	2.93043000	0.79581200	O	-3.35266600	3.16553100	-0.55873500	O	-2.44554800	-1.32466300	-3.73010800
O	-4.49318000	-0.30866500	-2.15389300	C	-2.68246300	4.20311500	-0.69974500	C	-2.19069300	-3.60974700	-2.98000600
H	-4.94161700	-0.98325000	-1.61693800	O	-1.41150200	4.25422300	-0.92551300	H	-1.45525600	-4.20098200	-3.55017800

H	-2.05514000	-3.91663000	-1.93278600	O	6.43462200	-1.59673100	0.19598500	H	-0.81076300	-4.84881000	4.03438200
C	-3.60947500	-3.90677600	-3.47191700	N	6.72010700	0.11670900	-1.26296700	H	-2.48672800	-4.86461500	3.47941700
H	-3.71347100	-3.56072000	-4.50878700	H	6.79566900	0.39601200	-2.23334900	O	-4.43590100	0.08502000	0.80695400
H	-4.32698700	-3.31579200	-2.88241300	C	6.59315900	1.15750900	-0.23431000	C	-4.31078100	-0.49130500	1.90545400
C	-3.96599200	-5.39356200	-3.36999900	H	7.21129000	0.86085700	0.61991400	O	-3.20842600	-0.96769800	2.39013000
H	-3.28616300	-6.00748700	-3.97747300	H	7.01615000	2.07844400	-0.65421400	C	-5.51181400	-0.66989600	2.81924300
H	-3.89653300	-5.75106400	-2.33302100	C	5.14225600	1.37612100	0.23274800	H	-5.43664700	0.05088700	3.64462500
H	-4.98872800	-5.58257400	-3.72092400	H	4.77234800	0.45717300	0.69860900	H	-5.51536600	-1.67310100	3.25937600
N	1.77513800	-2.04497700	-1.07383000	H	5.14854800	2.14574900	1.01747200	H	-6.43926000	-0.48540000	2.26984900
C	2.50376200	-1.96888700	-2.24305300	C	4.20806400	1.79617300	-0.90479400	O	-0.68506200	-0.56950400	3.46150500
H	2.01223900	-1.78632300	-3.18960300	H	4.27408400	1.06760400	-1.72875400	C	0.22664600	0.28597300	3.70051300
C	3.83800900	-2.16301100	-1.96221100	H	4.49180000	2.76936100	-1.32549000	O	0.79771200	1.03583900	2.84597900
N	3.88681200	-2.38842800	-0.59176100	O	2.27106900	1.13362900	0.37080400	C	0.65680400	0.43566500	5.15288300
H	4.74969800	-2.44052000	-0.04044100	C	2.72815200	1.86487900	-0.54149400	H	0.16754800	1.34720900	5.53293200
C	2.63791700	-2.28867900	-0.09465500	O	2.05014800	2.66748500	-1.28363500	H	0.24903500	-0.40941300	5.72000800
H	2.38345500	-2.35096900	0.95356700	O	-0.37036500	-3.68940600	0.21136900	C	2.17676400	0.55592700	5.33943700
C	5.05076300	-2.11611000	-2.85923000	C	-0.88854700	-3.81862200	1.36407900	H	2.54289400	1.39096200	4.72891300
H	5.02138700	-2.95133300	-3.57408900	O	-1.29871700	-2.87016000	2.10573500	H	2.66159800	-0.35189500	4.94895200
H	4.98926800	-1.20350000	-3.46961600	C	-1.03306600	-5.23981100	1.90194400	C	2.56869300	0.75815800	6.80688700
C	6.42975700	-2.16384300	-2.15029700	H	-0.06246400	-5.73620600	1.76104500	H	2.12391500	1.67738100	7.21349100
H	6.61536300	-3.16452600	-1.74491300	H	-1.72679100	-5.75790100	1.22195300	H	3.65803100	0.83679400	6.91893100
H	7.20692600	-1.96645900	-2.90138200	C	-1.51018100	-5.34431900	3.35045800	H	2.22837000	-0.07895900	7.43231100
C	6.55320800	-1.19747400	-0.97118400	H	-1.59652000	-6.39719700	3.64895500	H	0.29627600	0.81536200	-1.60698000

K:

Ca	-3.03999600	-0.01175500	-0.80978300	C	-1.47483300	-3.88398900	-3.56220300	C	3.78327700	2.64083100	-1.07039200
Mn	0.14031300	-1.76996100	-0.30788700	H	-0.59846500	-3.82467400	-4.22526100	H	4.02685800	1.92883400	-1.87651400
Mn	-1.23602500	-1.05292900	1.90782400	H	-1.32189000	-4.79974100	-2.97048000	H	3.85197100	3.64069000	-1.51735500
Mn	0.10199000	1.09043100	0.76354800	C	-2.77069800	-3.96860800	-4.37326800	O	2.02813200	1.60060400	0.20802000
Mn	-0.42107500	3.37374300	-1.33746200	H	-2.91572000	-3.03085200	-4.92897400	C	2.31673100	2.38392300	-0.74188200
O	-1.55398600	-1.74989200	0.23689000	H	-3.62323100	-4.05486500	-3.68372600	O	1.48338900	2.94341300	-1.54477400
O	0.52162800	-0.81844300	1.24373300	C	-2.77273900	-5.15445100	-5.34446000	O	0.42160400	-3.47302700	0.65863000
O	-1.57202200	0.57196300	1.17989900	H	-1.94907500	-5.07972100	-6.06747400	C	-0.04180700	-3.69782000	1.83104100
N	0.09961000	0.09364400	-1.04062700	H	-2.66122000	-6.10785900	-4.81057600	O	-0.68866500	-2.86937000	2.54366500
O	-0.40344100	2.68861600	0.32190100	H	-3.71064600	-5.19745700	-5.91145400	C	0.18416700	-5.07891600	2.42419900
O	-4.85586300	-0.97818300	-2.13616500	N	2.16279400	-1.84090100	-0.74015200	H	-0.80188400	-5.56930600	2.42637000
H	-5.64179700	-1.37529300	-1.72539000	C	2.85485000	-1.71728100	-1.93014800	H	0.44097600	-4.93412200	3.48180600
H	-4.36545200	-1.69983200	-2.58098200	H	2.34013100	-1.72710800	-2.88193600	C	1.21771900	-5.94244900	1.70033000
O	-1.98311700	0.79141900	-2.93134000	C	4.20352500	-1.62802400	-1.66290300	H	1.29947600	-6.91863600	2.19278500
H	-2.00058900	0.22749000	-3.72161800	N	4.30423400	-1.73539800	-0.28364000	H	0.93820900	-6.10595800	0.65380200
H	-1.61315600	1.69839100	-3.18355600	H	5.16169200	-1.52324300	0.24517900	H	2.20923000	-5.47320300	1.71247900
O	-0.72068600	3.10409100	-3.16461700	C	3.06606200	-1.83837700	0.23471200	O	-4.38628200	-0.77999500	0.99011500
H	0.12193200	3.05681200	-3.65093300	H	2.84107300	-1.86348500	1.29091200	C	-4.14103000	-1.16998300	2.14789900
O	0.09511400	5.57322400	-1.01541600	C	5.38104400	-1.42827100	-2.58494400	O	-2.94919800	-1.33653200	2.64247200
H	-0.83552300	5.87392100	-0.98053700	H	5.55882200	-2.34335000	-3.16818100	C	-5.25553100	-1.49815600	3.11848000
H	0.45112000	5.72685700	-0.12153800	H	5.10784500	-0.65648200	-3.31779300	H	-5.14425300	-2.52882100	3.47652500
O	-3.38761800	2.30537000	-0.86148300	C	6.72658900	-1.04372300	-1.91027200	H	-6.22948700	-1.36811400	2.64023900
C	-3.28127000	3.54632100	-0.89830800	H	7.15412100	-1.91233100	-1.39732300	H	-5.18069700	-0.84275600	3.99512600
O	-2.17115200	4.16970200	-1.13856100	H	7.43164600	-0.75607200	-2.70147100	O	-0.63418500	-0.18592100	3.57319500
C	-4.51268400	4.41311100	-0.67303000	C	6.59893600	0.05471000	-0.85528600	C	0.08252700	0.86398600	3.61909400
H	-5.23066500	4.13296500	-1.45811300	O	6.47564500	-0.22881000	0.34610400	O	0.50090600	1.52941400	2.60859600
H	-4.96291800	4.07028700	0.26947000	N	6.53991100	1.33736900	-1.29044600	C	0.46247400	1.39027600	4.98903100
C	-4.28461400	5.92452200	-0.65914200	H	6.71599100	1.53556000	-2.26767900	H	1.21128300	2.17979600	4.85717000
H	-3.85954900	6.27200500	-1.60829800	C	6.23966600	2.44766500	-0.37649700	H	-0.44216900	1.86427300	5.40265000
H	-3.60335700	6.21732800	0.14983000	H	6.89332800	2.35752200	0.49820400	C	0.95668900	0.29803300	5.95371900
H	-5.23432100	6.44967900	-0.50153200	H	6.50016000	3.37596300	-0.89859600	H	1.84779100	-0.18507300	5.52540400
O	-0.24701600	-2.62354900	-1.97505100	C	4.77068900	2.46078000	0.08649800	H	0.18680900	-0.47943600	6.03527600
C	-1.39266800	-2.71488500	-2.59102800	H	4.55983200	1.52768300	0.61807200	C	1.29001900	0.86445300	7.33763100
O	-2.34489300	-1.92394300	-2.43589400	H	4.64928700	3.27433100	0.81529600	H	2.07519700	1.63065400	7.28041000

H	1.64502300	0.07245000	8.00849000	H	-0.57309100	0.27022000	-1.80471600					
H	0.40734400	1.32471300	7.80233600	H	1.02713400	0.24611000	-1.43926300					

TS11:

Ca	3.20784600	-0.26781200	-0.75780800	H	1.77835500	4.56716800	-2.85569400	C	-2.73495300	-2.01118500	-0.61525200	
Mn	0.09194900	1.65329500	-0.35139700	C	3.31876300	3.79940800	-4.19640200	O	-2.02066100	-2.56354300	-1.54085500	
Mn	1.34043000	0.79000300	1.90143800	H	3.49456000	2.89397800	-4.79529500	O	-0.03285400	3.43403100	0.72077700	
Mn	-0.23068600	-1.22181000	0.85064200	H	4.11934700	3.83318300	-3.44323700	C	0.44519500	3.54879500	1.89094200	
Mn	-0.10970000	-2.90721600	-1.45978700	C	3.40139000	5.03977000	-5.09310000	O	0.99026800	2.60975000	2.56810000	
O	1.77949300	1.41936100	0.25670500	H	2.63125300	5.01841700	-5.87615000	C	0.39398800	4.90746000	2.57396100	
O	-0.40594700	0.70229300	1.19329800	H	3.26069600	5.96178300	-4.51293700	H	1.43598400	5.25941600	2.62749100	
O	1.48493200	-0.91806800	1.21933700	H	4.37795700	5.10324700	-5.58831700	H	0.09134800	4.73404500	3.61522800	
N	-0.03203100	-0.68612100	-1.14439000	N	-1.89296500	1.86781000	-0.85268700	C	-0.49591300	5.94460800	1.88883900	
O	-0.08732600	-2.90041000	0.34238500	C	-2.60618400	1.77620600	-2.03461700	H	-0.45912500	6.89251700	2.43878100	
O	5.15144500	0.51204800	-2.01261400	H	-2.10533900	1.64840200	-2.98550800	H	-0.17106200	6.13027200	0.85910000	
H	5.98797100	0.78436600	-1.60041300	C	-3.95093500	1.91373100	-1.76530700	H	-1.54124400	5.61358200	1.85459800	
H	4.78442000	1.29339200	-2.47241000	N	-4.02156600	2.12568900	-0.39648300	O	4.53564300	0.31223800	1.10563100	
O	2.14308300	-0.96178000	-2.97570900	H	-4.89965000	2.11515300	0.14252400	C	4.25104600	0.64697200	2.27262400	
H	2.20698500	-0.24341800	-3.62805300	C	-2.78064000	2.07034300	0.11744000	O	3.04763900	0.85489800	2.71436900	
H	1.51900800	-1.65706700	-3.33690700	H	-2.54648600	2.14093400	1.16925200	C	5.33020800	0.84120700	3.31649100	
O	0.06727200	-2.64478800	-3.29636100	C	-5.15679700	1.83091300	-2.67054300	H	5.24165400	1.83868100	3.76312900	
H	-0.79061000	-2.50199100	-3.73389100	H	-5.16803600	2.69164400	-3.35443100	H	6.32001400	0.71123600	2.87196000	
O	-0.67038200	-5.05132800	-1.44040200	H	-5.04032700	0.94473000	-3.31008400	H	5.18883800	0.11200400	4.12420900	
H	0.22801500	-5.39447700	-1.62703900	C	-6.54409000	1.77908700	-1.97184800	O	0.62102300	0.01051000	3.60336600	
H	-0.81218100	-5.21759500	-0.48807400	H	-6.79367300	2.75925800	-1.55093500	C	-0.18878000	-0.95461500	3.66365500	
O	3.37803600	-2.58817100	-0.72141800	H	-7.29849200	1.55303300	-2.73712900	O	-0.67863800	-1.58357100	2.64908600	
C	2.84898100	-3.64617500	-1.10384100	C	-6.61416900	0.78362100	-0.81395700	C	-0.62449200	-1.46556100	5.02235200	
O	1.64397400	-3.74882500	-1.56628000	O	-6.43688000	1.15577800	0.35643200	H	-1.60727400	-1.93929700	4.90539500	
C	3.67328800	-4.93050600	-1.08796000	N	-6.77920700	-0.52597400	-1.12129200	H	0.07802600	-2.27547100	5.28092200	
H	4.49524100	-4.77425200	-1.80236400	H	-6.98323800	-0.78746500	-2.07806500	C	-0.63234900	-0.40232200	6.12953500	
H	4.14957100	-4.97749900	-0.09929200	C	-6.61169800	-1.57850800	-0.10954700	H	-1.32422200	0.40550200	5.84945900	
C	2.92478000	-6.22492400	-1.40414600	H	-7.21849200	-1.31552200	0.76363600	H	0.36337100	0.05328500	6.19692400	
H	2.47699700	-6.19424000	-2.40538800	H	-7.01543000	-2.50454600	-0.53539500	C	-1.04094400	-0.99141300	7.48380200	
H	2.13211000	-6.41773500	-0.66777900	C	-5.14228400	-1.75396700	0.32233000	H	-2.04703900	-1.43109400	7.44502700	
H	3.61008000	-7.08036600	-1.37217600	H	-4.79303700	-0.81825500	0.77000000	H	-1.04553800	-0.21692800	8.26050700	
O	0.61708000	2.33905700	-2.06913800	H	-5.10200800	-2.51520600	1.11316800	H	-0.34477700	-1.77924900	7.80281000	
C	1.80361300	2.46699600	-2.59107000	C	-4.23408600	-2.15274900	-0.84305000	H	0.74341300	-0.56830100	-1.81722500	
O	2.73849700	1.65814900	-2.40916300	H	-4.45049000	-1.52371200	-1.72114100	H	-0.90120100	-0.46999000	-1.63760400	
C	1.96688700	3.68464700	-3.48678600	H	-4.41497600	-3.18616600	-1.16846200					
H	1.13956000	3.67384400	-4.21258400	O	-2.28521500	-1.35320800	0.35624400					

L:

Ca	-3.14419000	0.33744100	-0.76746600	H	0.94818700	3.13681800	-3.40308500	C	-2.11237000	-3.26130500	-3.94894400	
Mn	-0.13883000	-1.90919800	-0.48371800	O	0.70141400	5.19484000	-0.81048400	H	-1.26869200	-3.24594500	-4.65606600	
Mn	-1.33081000	-0.94405900	1.76999100	H	-0.17952900	5.58542400	-0.98952200	H	-2.04671900	-4.24129700	-3.45203800	
Mn	0.25666500	1.14424500	0.88898400	H	0.80698700	5.22714700	0.16196800	C	-3.44510700	-3.11014800	-4.68716500	
Mn	0.21896600	3.14180100	-1.12406200	O	-3.30451200	2.65027000	-0.45860000	H	-3.49599200	-2.11350700	-5.14895200	
O	-1.80768400	-1.52367500	0.11843300	C	-2.76132400	3.73861200	-0.69632000	H	-4.26844500	-3.15765300	-3.95858100	
O	0.38732000	-0.80204500	1.00156700	O	-1.55787500	3.88558000	-1.16427300	C	-3.64501700	-4.18978800	-5.75673000	
O	-1.46195300	0.81844300	1.19396800	C	-3.56023300	5.02457600	-0.50189100	H	-2.85397600	-4.14792700	-6.51777400	
N	0.07539000	1.18877100	-1.12137400	H	-4.37601100	4.99066300	-1.23924700	H	-3.62991800	-5.19571400	-5.31608100	
O	0.17795900	2.91948800	0.65531600	H	-4.04698400	4.93716200	0.47864200	H	-4.60675900	-4.06412100	-6.26879300	
O	-5.09090100	-0.22506100	-2.12865800	C	-2.78540100	6.33660200	-0.61971600	N	1.82942100	-2.08640200	-1.03331800	
H	-5.92062200	-0.56126000	-1.75087700	H	-2.32942200	6.44524500	-1.61222800	C	2.51371300	-1.81056500	-2.20330000	
H	-4.72691700	-0.92505000	-2.70612500	H	-1.99944100	6.40630000	0.14561500	H	1.98603100	-1.59549900	-3.12327100	
O	-2.09363500	1.39683900	-2.90693800	H	-3.45544900	7.19137200	-0.46910200	C	3.86862200	-1.90496700	-1.97007600	
H	-2.09630200	0.75179200	-3.63520300	O	-0.68476600	-2.33733100	-2.29152900	N	3.97795200	-2.27422800	-0.63779100	
H	-1.50488100	2.15346800	-3.16889800	C	-1.83062100	-2.20995400	-2.88598100	H	4.86640500	-2.28009100	-0.11489200	
O	0.07550100	3.21468000	-2.97650300	O	-2.64834900	-1.29197000	-2.64690900	C	2.74566700	-2.35434700	-0.10626700	

H	2.53722800	-2.57458700	0.93029900	H	4.53156700	3.30205500	-0.82936700	H	-6.32565700	-0.88686600	2.72173200
C	5.05008300	-1.65460200	-2.87666600	O	2.33200700	1.31271400	0.40343800	H	-5.19527600	-0.42241500	4.03231200
H	5.05759700	-2.39808700	-3.68639100	C	2.80539500	2.12705400	-0.42263500	O	-0.62607000	-0.30746500	3.53223800
H	4.90685000	-0.68138600	-3.36748200	O	2.11236100	2.88488600	-1.21785200	C	0.22549600	0.61075200	3.68069200
C	6.45208400	-1.68524200	-2.20972400	O	-0.02084700	-3.68283300	0.63093800	O	0.74192300	1.29862200	2.72401600
H	6.70552000	-2.70695000	-1.90555300	C	-0.51539400	-3.75056600	1.79390200	C	0.67737700	0.97924700	5.08029100
H	7.18968500	-1.37864100	-2.96326700	O	-1.02227600	-2.76444700	2.43641400	H	1.71959200	1.31853300	5.01539400
C	6.55396100	-0.81929500	-0.95454000	C	-0.54075200	-5.08620200	2.52085400	H	0.08856900	1.86690200	5.36582300
O	6.37040700	-1.30352500	0.17295900	H	-1.59917400	-5.38542500	2.57288000	C	0.50507500	-0.13029200	6.12512700
N	6.76201800	0.50930800	-1.12657100	H	-0.24110000	-4.89813400	3.56042700	H	1.08671300	-1.01095700	5.81621500
H	6.98018200	0.85999800	-2.05105700	C	0.30356100	-6.18514800	1.87544900	H	-0.54511500	-0.44741500	6.14360200
C	6.65144700	1.45365200	-0.00660100	H	0.21216200	-7.11558400	2.44850500	C	0.94785500	0.32396500	7.52010400
H	7.24688300	1.06751400	0.82776900	H	-0.01770400	-6.38028200	0.84634700	H	2.00569500	0.62085000	7.53042300
H	7.09964900	2.39947900	-0.33291800	H	1.36474900	-5.90832300	1.84679900	H	0.82140500	-0.48306400	8.25216800
C	5.19451900	1.65154500	0.45444700	O	-4.53260200	-0.38680900	0.99361500	H	0.35741700	1.18339300	7.86658300
H	4.79511700	0.68623500	0.78123300	C	-4.25152700	-0.79094500	2.14090000	H	-0.73718800	0.98285200	-1.71908600
H	5.19459100	2.30745200	1.33556300	O	-3.05174200	-1.00673600	2.58200500	H	0.89686600	0.81021900	-1.59787400
C	4.30702600	2.24347000	-0.64364300	C	-5.33988000	-1.06811600	3.15729200				
H	4.49650400	1.72618500	-1.59829400	H	-5.26529400	-2.10523600	3.50612700				

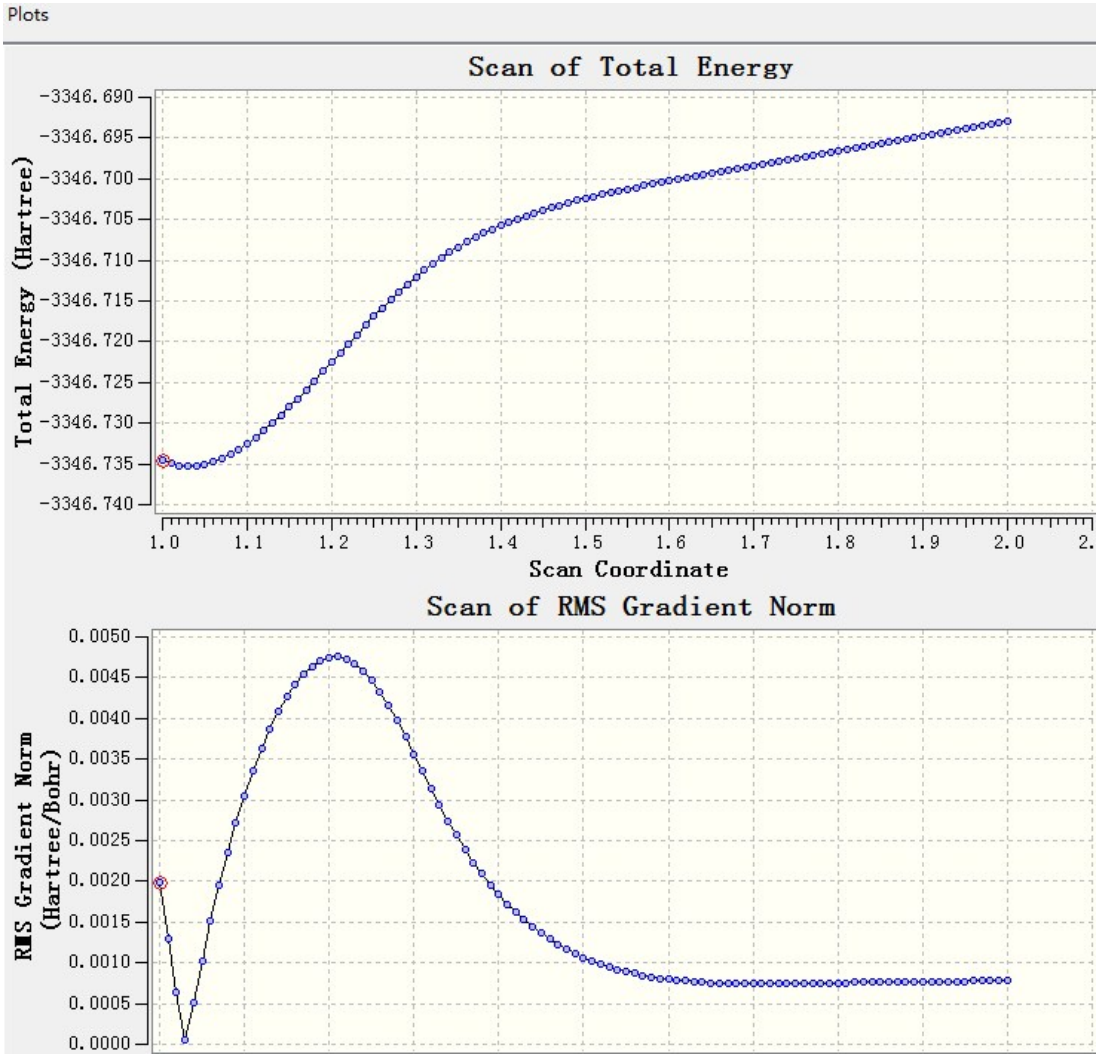
TS13:

Ca	2.75253900	-0.14541900	-1.07795400	H	0.23549700	3.27454700	-4.97957400	C	-2.20949500	-2.61103500	-0.18035900
Mn	-0.34936000	1.85374600	-0.73535900	C	1.71644800	4.42921300	-3.89573800	O	-1.41860700	-3.40127800	-0.76840900
Mn	1.19615400	1.40911400	1.45608400	H	2.65373900	4.24283400	-3.35115700	O	-0.67954300	3.75553600	0.13271000
Mn	0.02378100	-1.06746700	0.95671900	H	0.99391600	4.80504300	-3.15893800	C	-0.10713000	4.05688100	1.22366600
Mn	0.70708000	-3.26892400	-0.69219500	C	1.95070600	5.47624400	-4.98894300	O	0.60391700	3.27183000	1.92988800
O	1.41475200	1.82640900	-0.30114900	H	2.68872000	5.12855000	-5.72508700	C	-0.27586300	5.48812900	1.72528400
O	-0.50722900	0.87427600	0.86942200	H	1.02064600	5.70190400	-5.52917500	H	-1.33096600	5.75917300	1.58319600
O	1.65468500	-0.32606900	1.21066900	H	2.32427700	6.41475900	-4.55967100	H	0.28850600	6.12432700	1.02558600
O	0.48517300	-1.24402500	-0.92136400	N	-2.38518200	1.63561400	-1.03039800	C	0.18071100	5.73265600	3.16386700
O	0.55732400	-2.75367800	1.04043700	C	-3.16040900	1.27814900	-2.11288600	H	0.04543100	6.78819700	3.43345100
O	4.43977300	0.43158100	-2.90876900	H	-2.72403600	1.14657400	-3.09263200	H	-0.39399600	5.12224700	3.87131500
H	3.77660200	0.97111000	-3.38802000	C	-4.46603600	1.11792300	-1.70880500	H	1.23712500	5.47236100	3.29045500
H	4.34980100	-0.44679300	-3.33105200	N	-4.46093000	1.42059500	-0.35262900	O	4.22635200	1.05474500	0.39299700
O	2.58294100	-1.55447400	-3.26914200	H	-5.25403000	1.27380300	0.28034200	C	4.07554000	1.67000100	1.46297500
H	1.99905000	-0.96391000	-3.77643100	C	-3.19725800	1.70413400	0.01855500	O	2.94030900	1.91958600	2.04281300
H	2.03351800	-2.37445800	-3.07483100	H	-2.88446000	1.91212900	1.03122000	C	5.27821100	2.20400300	2.22285400
O	0.84429800	-3.45812400	-2.57787600	C	-5.68202300	0.65839600	-2.47401300	H	5.35274900	1.69201900	3.19095100
H	0.99945300	-4.38849400	-2.81820100	H	-5.94062600	1.39588900	-3.24790000	H	5.14653800	3.27285700	2.42988500
O	0.31466300	-5.51316600	-0.12200200	H	-5.41628900	-0.26014500	-3.01747900	H	6.19307500	2.03965900	1.64746100
H	-0.26151500	-5.34447700	0.64512000	C	-6.96021400	0.40189300	-1.63519600	O	0.68181400	0.93232500	3.35185300
H	1.22718200	-5.56302700	0.23185300	H	-7.37290400	1.34888100	-1.27014400	C	0.01595000	-0.09663700	3.65371000
O	3.69085400	-2.26517900	-0.55856600	H	-7.71481800	-0.05178000	-2.29246400	O	-0.40742400	-0.99254900	2.84014600
C	3.59661500	-3.47503700	-0.27006800	C	-6.72712300	-0.46664900	-0.39731200	C	-0.30981800	-0.34113300	5.11995100
O	2.50585500	-4.15822500	-0.35395200	O	-6.62864100	0.04174700	0.72890200	H	-1.26800700	-0.87525000	5.16553900
C	4.84846800	-4.21845700	0.19092100	N	-6.57039200	-1.79821000	-0.59885400	H	0.45064800	-1.04978700	5.48770800
H	5.56196300	-4.17422900	-0.64553200	H	-6.62174400	-2.15668400	-1.54450200	C	-0.32319000	0.91869000	5.99278000
H	5.29484700	-3.60701700	0.98724200	C	-6.10533000	-2.69237000	0.46962900	H	-1.07962100	1.61776500	5.60692800
C	4.64162200	-5.66071700	0.65350900	H	-6.69508000	-2.46931100	1.36526200	H	0.64188100	1.43147300	5.89656600
H	4.21909800	-6.27971600	-0.14728000	H	-6.34029900	-3.71731600	0.15615200	C	-0.61240300	0.60000200	7.46367100
H	3.95823700	-5.70737400	1.51082600	C	-4.60671300	-2.54083100	0.78569500	H	-1.58820800	0.10862800	7.58495500
H	5.59677400	-6.10658700	0.95995500	H	-4.41384200	-1.52334000	1.14130800	H	-0.62190000	1.51421200	8.07114500
O	-0.09220000	2.26515800	-2.64003900	H	-4.36931300	-3.21569600	1.62119300	H	0.15025800	-0.07101200	7.88359500
C	0.96470900	2.07920500	-3.35561800	C	-3.70177500	-2.85150600	-0.41047600	N	-0.89687100	-1.13597100	-2.86712400
O	1.78360000	1.14242800	-3.17597200	H	-3.97292200	-2.20309800	-1.25904100	H	-0.40955000	-1.10536000	-1.73021600
C	1.18959400	3.09385100	-4.46542600	H	-3.82228400	-3.88815100	-0.75009600	H	-0.44965500	-0.42439500	-3.45757600
H	1.90387000	2.68042900	-5.18856600	O	-1.88721500	-1.60422200	0.53465100	H	-0.62226100	-2.06657000	-3.22413200

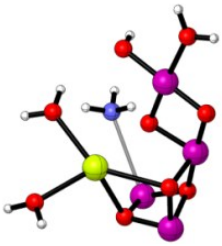
M:

Ca	-2.66857200	0.08155200	-1.27137100	H	0.13019500	-3.10564200	-5.02429300	C	2.20640900	2.54194300	-0.11589000
Mn	0.32604300	-1.90565500	-0.63231300	C	-1.09292400	-4.63533700	-4.09904900	O	1.44310100	3.25654400	-0.83897400
Mn	-1.34178300	-1.39478200	1.45430900	H	-2.05188000	-4.69810900	-3.56349900	O	0.64733100	-3.75228900	0.37144700
Mn	-0.09966300	1.03372700	0.95040700	H	-0.31452000	-4.93538800	-3.38525700	C	-0.01060100	-4.02642200	1.41956700
Mn	-0.61658000	3.29019500	-0.77672400	C	-1.10792000	-5.58785900	-5.29869500	O	-0.79769600	-3.23371000	2.03286000
O	-1.45604100	-1.88155000	-0.28327700	H	-1.89607700	-5.31784400	-6.01528300	C	0.14056500	-5.43394400	1.98936400
O	0.40676800	-0.89360000	0.96766600	H	-0.14874600	-5.56670800	-5.83509600	H	1.20692100	-5.69244400	1.93594100
O	-1.75108400	0.34393700	1.11091000	H	-1.28870200	-6.62203900	-4.97825600	H	-0.36168500	-6.10597300	1.27589900
O	-0.40407900	1.07847300	-0.98629900	N	2.36641400	-1.65903500	-0.86577700	C	-0.41799600	-5.63085500	3.39905800
O	-0.58307300	2.73868400	0.95080700	C	3.14891100	-1.23885200	-1.92071200	H	-0.28786700	-6.67272000	3.71954700
O	-4.24648800	-0.31522600	-3.24236000	H	2.71407900	-1.05215800	-2.89292600	H	0.09374900	-4.98384200	4.12222800
H	-3.65674600	-1.00094000	-3.61814900	C	4.45113800	-1.10102800	-1.49626500	H	-1.48455200	-5.38436400	3.43700600
H	-3.92006700	0.50059600	-3.67729900	N	4.43502100	-1.47738000	-0.15860000	O	-4.26763000	-1.02727400	0.14509200
O	-2.13728400	1.41720700	-3.46869400	H	5.21843900	-1.34761000	0.49010200	C	-4.21325100	-1.60948200	1.24277500
H	-1.44757700	0.83052100	-3.82684400	C	3.16833500	-1.78311000	0.18513400	O	-3.13414300	-1.84828300	1.92611100
H	-1.66620400	2.26831300	-3.22340800	H	2.84842900	-2.05534900	1.18021900	C	-5.48016300	-2.11620300	1.91154200
O	-0.69446100	3.55059900	-2.65784300	C	5.68109800	-0.62438200	-2.22867100	H	-5.60410400	-1.62247800	2.88369300
H	-1.16166500	4.37819800	-2.86641100	H	5.95256400	-1.34386000	-3.01509500	H	-5.39375400	-3.19286800	2.10314100
O	-0.23609500	5.41473800	0.36947000	H	5.42820600	0.30760600	-2.75517900	H	-6.34884700	-1.91561400	1.27896200
H	-0.07575400	4.84512300	1.14950100	C	6.94566200	-0.39066400	-1.36192300	O	-0.94987600	-0.84531200	3.36807400
H	-1.20803400	5.52882100	0.37067700	H	7.34884800	-1.34730000	-1.01160900	C	-0.28455100	0.18143000	3.67131600
O	-3.52456300	2.27424300	-0.90478600	H	7.71327400	0.07470900	-1.99548900	O	0.20641800	1.03754600	2.84918900
C	-3.48848800	3.48346500	-0.60677700	C	6.68799000	0.45096300	-0.11112900	C	-0.04144000	0.48379200	5.14229000
O	-2.40350000	4.18699200	-0.58201600	O	6.54115500	-0.08179600	0.99797300	H	0.94211300	0.96510800	5.22626500
C	-4.79082600	4.20272600	-0.26912700	N	6.56047200	1.79001000	-0.28658900	H	-0.77904600	1.25370100	5.42304300
H	-5.42774900	4.12908500	-1.16326100	H	6.66373900	2.16956600	-1.21957900	C	-0.15845100	-0.72704500	6.07422500
H	-5.29113500	3.59055400	0.49411300	C	6.04906400	2.66424700	0.77736600	H	0.57697800	-1.48724500	5.77307300
C	-4.65899800	5.65541900	0.18864100	H	6.58981700	2.41671200	1.69701500	H	-1.14452800	-1.18894800	5.94007700
H	-4.17695500	6.27405700	-0.57799300	H	6.30622000	3.69425400	0.50038700	C	0.05621900	-0.34837400	7.54366900
H	-4.06013500	5.73006500	1.10501400	C	4.53518100	2.51130200	1.00947200	H	1.05032300	0.09222800	7.70489800
H	-5.64822600	6.08238500	0.39792000	H	4.32277300	1.48473700	1.32558700	H	-0.02761900	-1.22843400	8.19428200
O	0.17515400	-2.42078300	-2.50335600	H	4.25077600	3.16314300	1.84794200	H	-0.68943800	0.38618000	7.87936000
C	-0.81556300	-2.23758800	-3.31197200	C	3.69854900	2.85545900	-0.22577200	N	1.36903800	1.62641700	-3.20770900
O	-1.70822400	-1.37191500	-3.16051200	H	4.05723400	2.27140400	-1.08906300	H	0.38546100	1.00984800	-1.57377800
C	-0.84198100	-3.17140000	-4.51384000	H	3.79425000	3.91360100	-0.50091100	H	2.28155100	1.85427400	-3.63274800
H	-1.61769100	-2.82859700	-5.20956200	O	1.85592600	1.57229400	0.62420400	H	0.80901700	2.49804900	-3.29177100

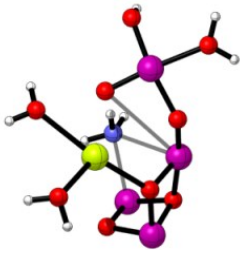
Relaxed PES scan plots for step12:



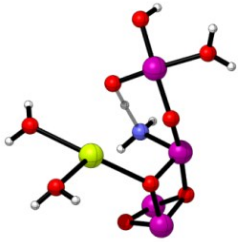
3D image for TSs:



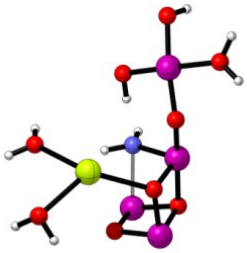
TS1



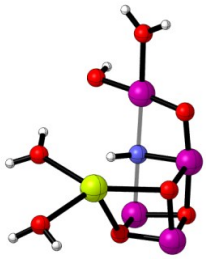
TS2



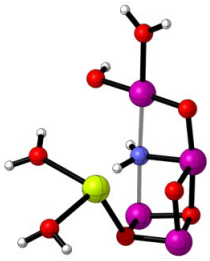
TS3:



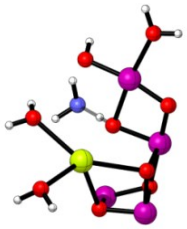
TS4



TS7

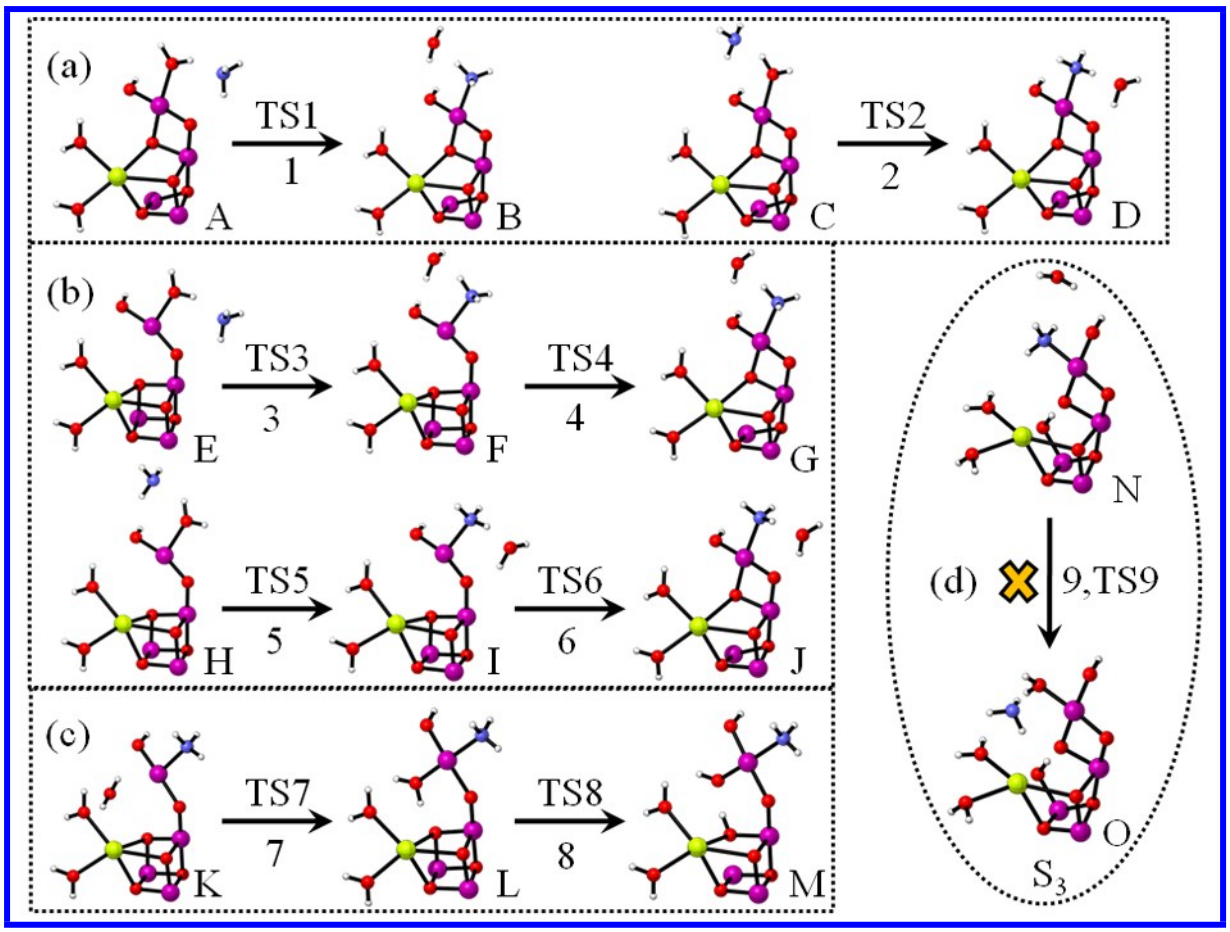


TS11



TS13

III. W1 substitution scheme



Scheme S3. Graphical expressions for the W1 substitution mechanism both on the (a) open and (b) closed-cubane structures from O4 and W2 sides in the S_2 state. Image (c) stands for the external water Wx binding to Mn4 and then deprotonation to O5. Image (d) represents the verification of infeasibility for NH_3 departure in the S_3 state.

IVa. Open-cubane structure as reactant

Table SIVa. Gibbs free energies and Mulliken spin populations for the W1 substitution scheme with the open-cubane structure as reactant:

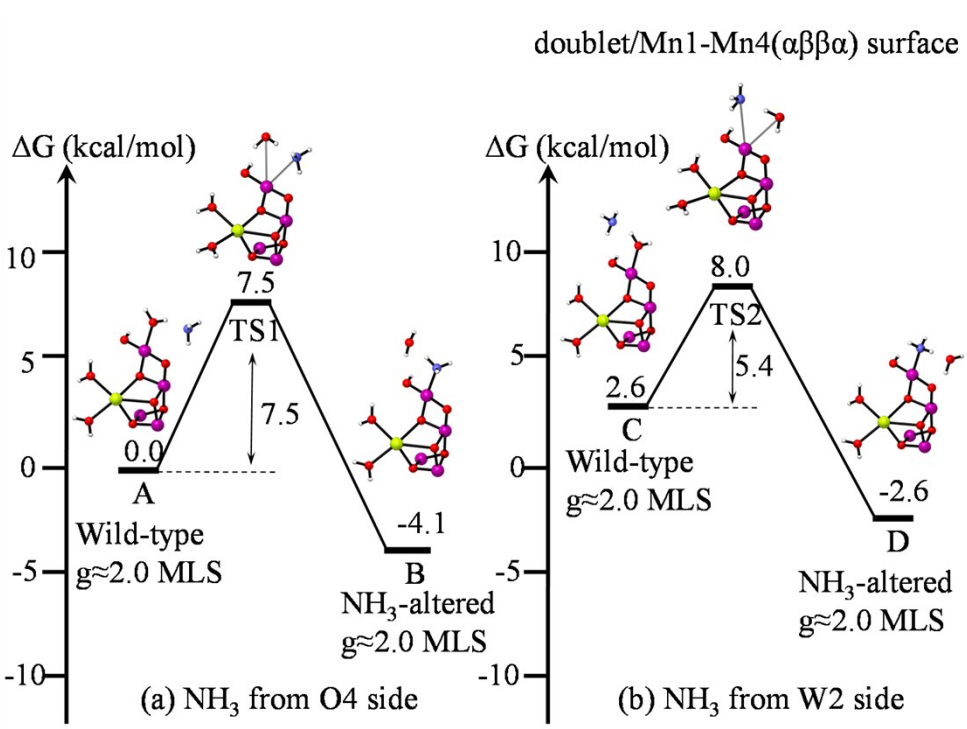
Spin states	Spin topology (Mn1-Mn4)	Gibbs Free energy (a.u.)		
		A	TS1	B
doublet	ααββ	-3347.6415	-3347.6298	-3347.6479
	αβαβ	-3347.6439	-3347.6313	-3347.6503
	αββα	-3347.6441	-3347.6322	-3347.6507
sextet	βααα	-3347.6446	-3347.6324	-3347.6512
octet	αααβ	-3347.6440	-3347.6319	-3347.6504
	ααβα	-3347.6437	-3347.6323	-3347.6499
	αβαα	-3347.6447	-3347.6322	-3347.6510
14-et	αααα	-3347.6441	-3347.6326	-3347.6503
		C	TS2	D
doublet	ααββ	-3347.6399	-3347.6283	-3347.6508
	αβαβ	-3347.6423	-3347.6304	-3347.6503
	αββα	-3347.6399	-3347.6313	-3347.6483
sextet	βααα	-3347.6430	-3347.6318	-3347.6510
octet	αααβ	-3347.6424	-3347.6304	-3347.6509
	ααβα	-3347.6423	-3347.6306	-3347.6545
	αβαα	-3347.6427	-3347.6315	-3347.6508
14-et	αααα	-3347.6422	-3347.6310	-3347.6502

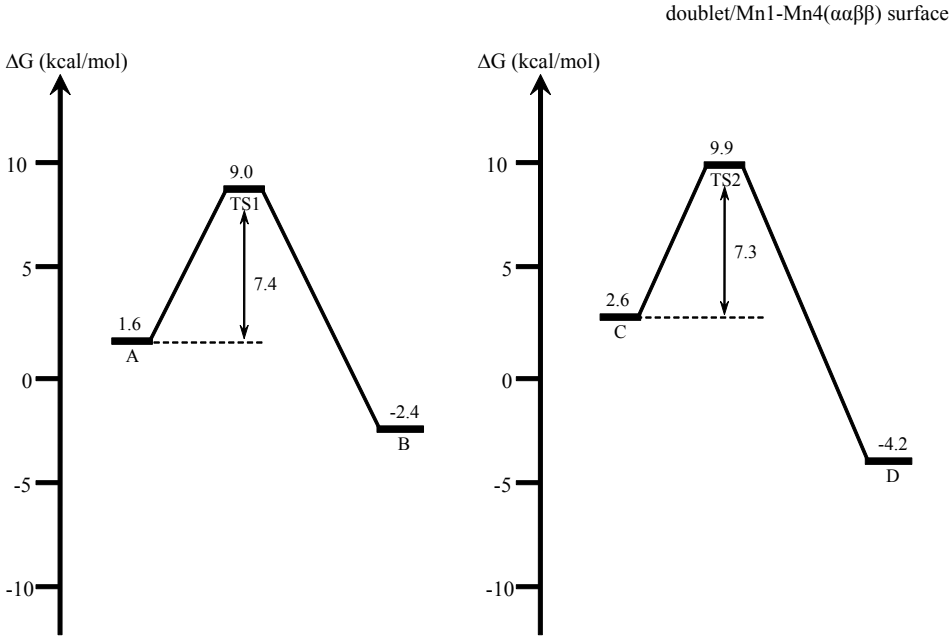
Spin states	Spin topology (Mn1-Mn4)	Mulliken spin density		
		A	TS1	B
doublet	α Mn1	3.87	3.87	3.87

	α	Mn2	2.97	2.97	2.97
	β	Mn3	-2.90	-2.88	-2.90
	β	Mn4	-2.91	-2.88	-2.90
	α	Mn1	3.87	3.87	3.87
	β	Mn2	-2.90	-2.91	-2.90
	α	Mn3	2.89	2.87	2.90
	β	Mn4	-2.86	-2.86	-2.86
	α	Mn1	3.86	3.87	3.87
	β	Mn2	-2.92	-2.92	-2.92
	β	Mn3	-2.90	-2.89	-2.91
	α	Mn4	2.87	2.88	2.87
sextet	β	Mn1	-3.86	-3.87	-3.87
	α	Mn2	2.92	2.92	2.92
	α	Mn3	2.92	2.91	2.92
	α	Mn4	2.91	2.89	2.91
octet	α	Mn1	3.88	3.88	3.88
	α	Mn2	2.98	2.98	2.98
	α	Mn3	2.91	2.90	2.92
	β	Mn4	-2.86	-2.86	-2.86
	α	Mn1	3.87	3.87	3.87
	α	Mn2	2.97	2.97	2.97
	β	Mn3	-2.88	-2.86	-2.89
	α	Mn4	2.87	2.88	2.87
	α	Mn1	3.87	3.88	3.88
	β	Mn2	-2.90	-2.90	-2.90

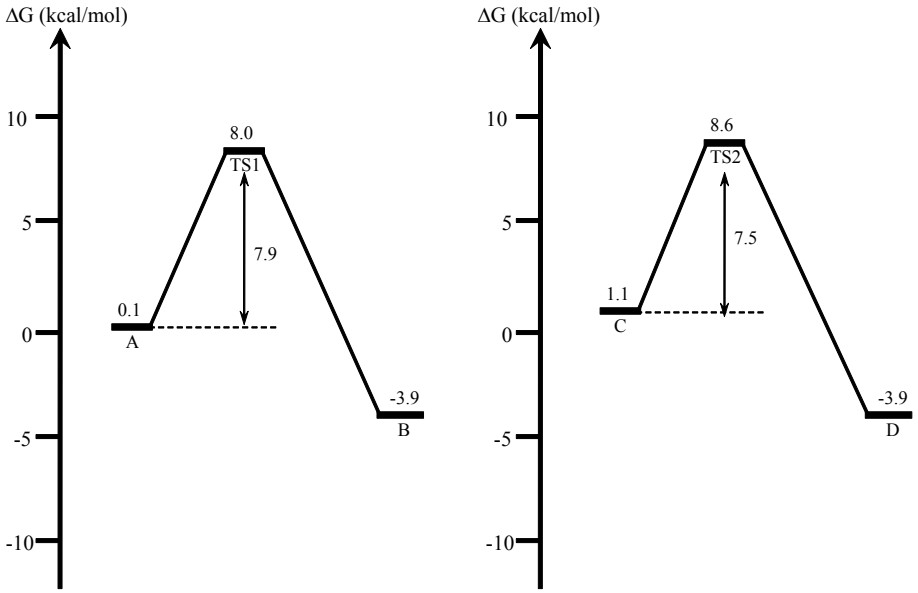
	α	Mn3	2.90	2.89	2.91
	α	Mn4	2.92	2.90	2.92
14-et	α	Mn1	3.88	3.88	3.88
	α	Mn2	2.98	2.98	2.98
	α	Mn3	2.93	2.93	2.93
	α	Mn4	2.92	2.91	2.92
			C	TS2	D
doublet	α	Mn1	3.87	3.88	3.87
	α	Mn2	2.97	2.97	2.97
	β	Mn3	-2.90	-2.89	-2.90
	β	Mn4	-2.90	-2.86	-2.91
	α	Mn1	3.87	3.88	3.87
	β	Mn2	-2.90	-2.90	-2.90
	α	Mn3	2.89	2.87	2.90
	β	Mn4	-2.85	-2.85	-2.87
	α	Mn1	3.87	3.87	3.87
	β	Mn2	2.97	-2.92	2.97
	β	Mn3	-2.90	-2.88	-2.90
	α	Mn4	-2.90	2.88	-2.91
sextet	β	Mn1	-3.87	-3.87	-3.87
	α	Mn2	2.92	2.92	2.92
	α	Mn3	2.92	2.91	2.92
	α	Mn4	2.90	2.87	2.91
octet	α	Mn1	3.88	3.89	3.88

	α	Mn2	2.98	2.98	2.98
	α	Mn3	2.92	2.90	2.92
	β	Mn4	-2.85	-2.85	-2.87
	α	Mn1	3.87	3.88	3.87
	α	Mn2	2.97	2.97	2.97
	β	Mn3	-2.88	-2.86	-2.90
	α	Mn4	2.86	2.88	2.89
	α	Mn1	3.88	3.88	3.88
	β	Mn2	-2.90	-2.91	-2.90
	α	Mn3	2.90	2.90	2.90
	α	Mn4	2.91	2.90	2.92
14-et	α	Mn1	3.88	3.89	3.88
	α	Mn2	2.98	2.98	2.98
	α	Mn3	2.93	2.93	2.93
	α	Mn4	2.91	2.91	2.92

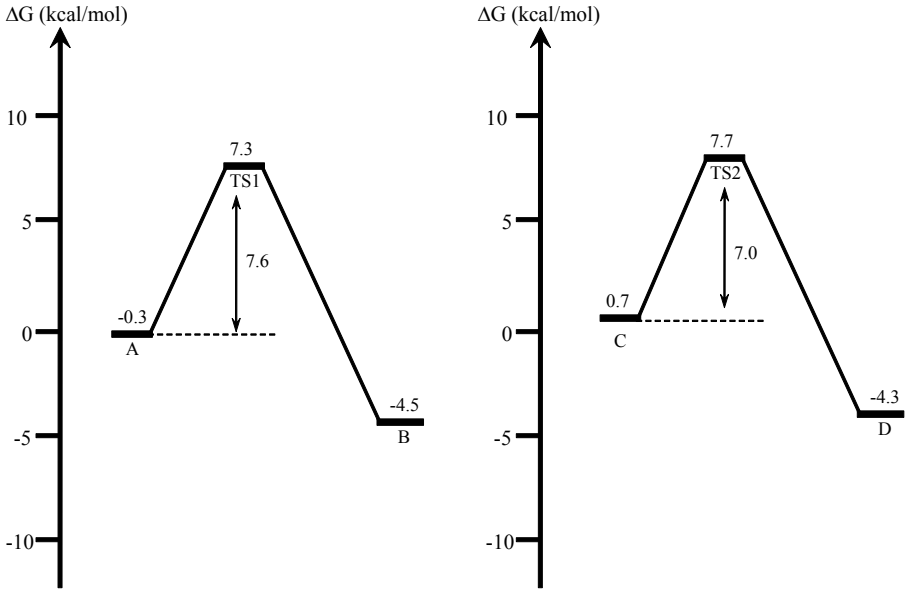

doublet/Mn1-Mn4(αββα) surface
ΔG (kcal/mol)
10
5
0
-5
-10
7.5
TS1
7.5
0.0
A
Wild-type
g≈2.0 MLS
-4.1
B
NH3-altered
g≈2.0 MLS
(a) NH3 from O4 side
ΔG (kcal/mol)
8.0
TS2
5.4
2.6
C
Wild-type
g≈2.0 MLS
-2.6
D
NH3-altered
g≈2.0 MLS
(b) NH3 from W2 side


doublet/Mn1-Mn4(ααββ) surface
ΔG (kcal/mol)
10
5
0
-5
-10
9.0
TS1
7.4
1.6
A
-2.4
B
ΔG (kcal/mol)
9.9
TS2
7.3
2.6
C
-4.2
D

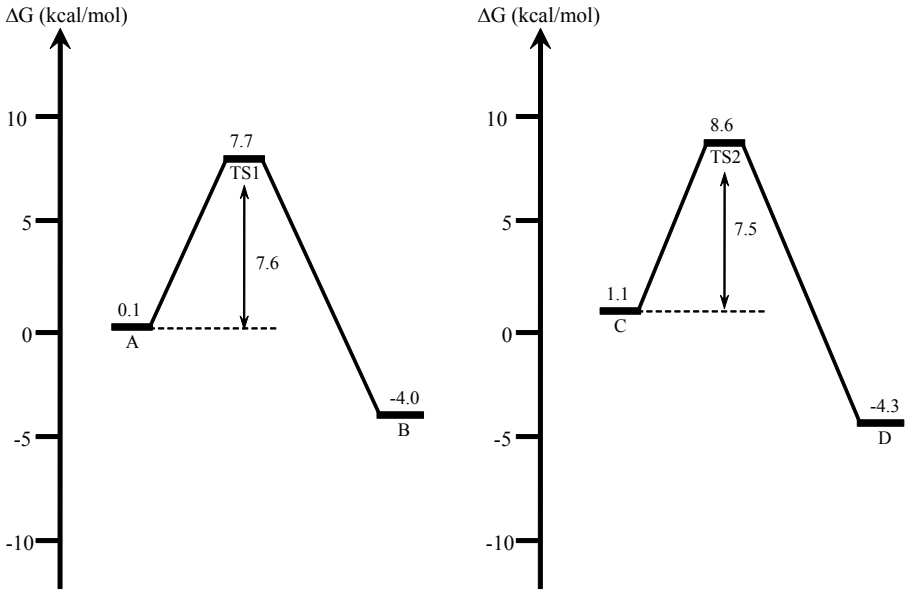
doublet/Mn1-Mn4(αβαβ) surface



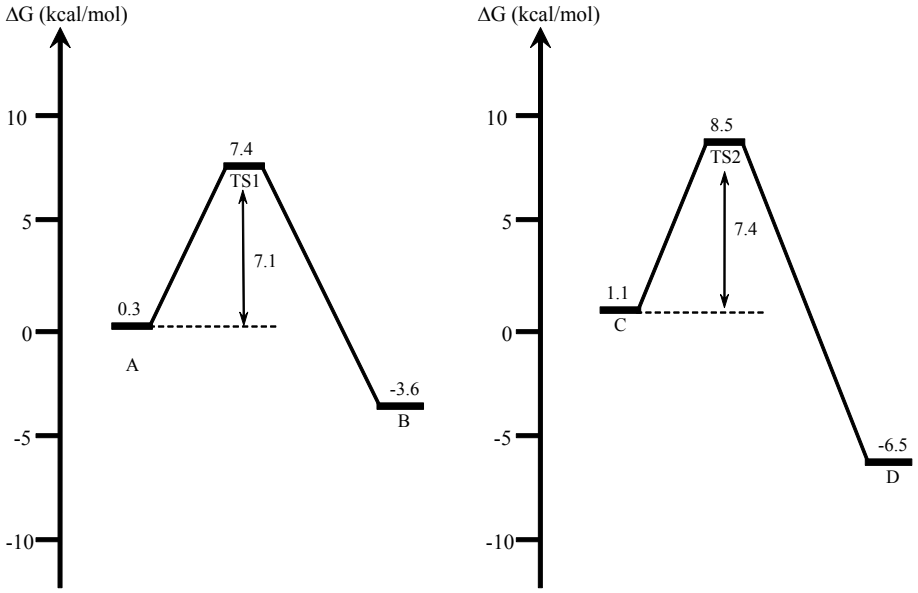
sextet/Mn1-Mn4(βααα) surface



octet/Mn1-Mn4(αααβ) surface



octet/Mn1-Mn4(ααβα) surface



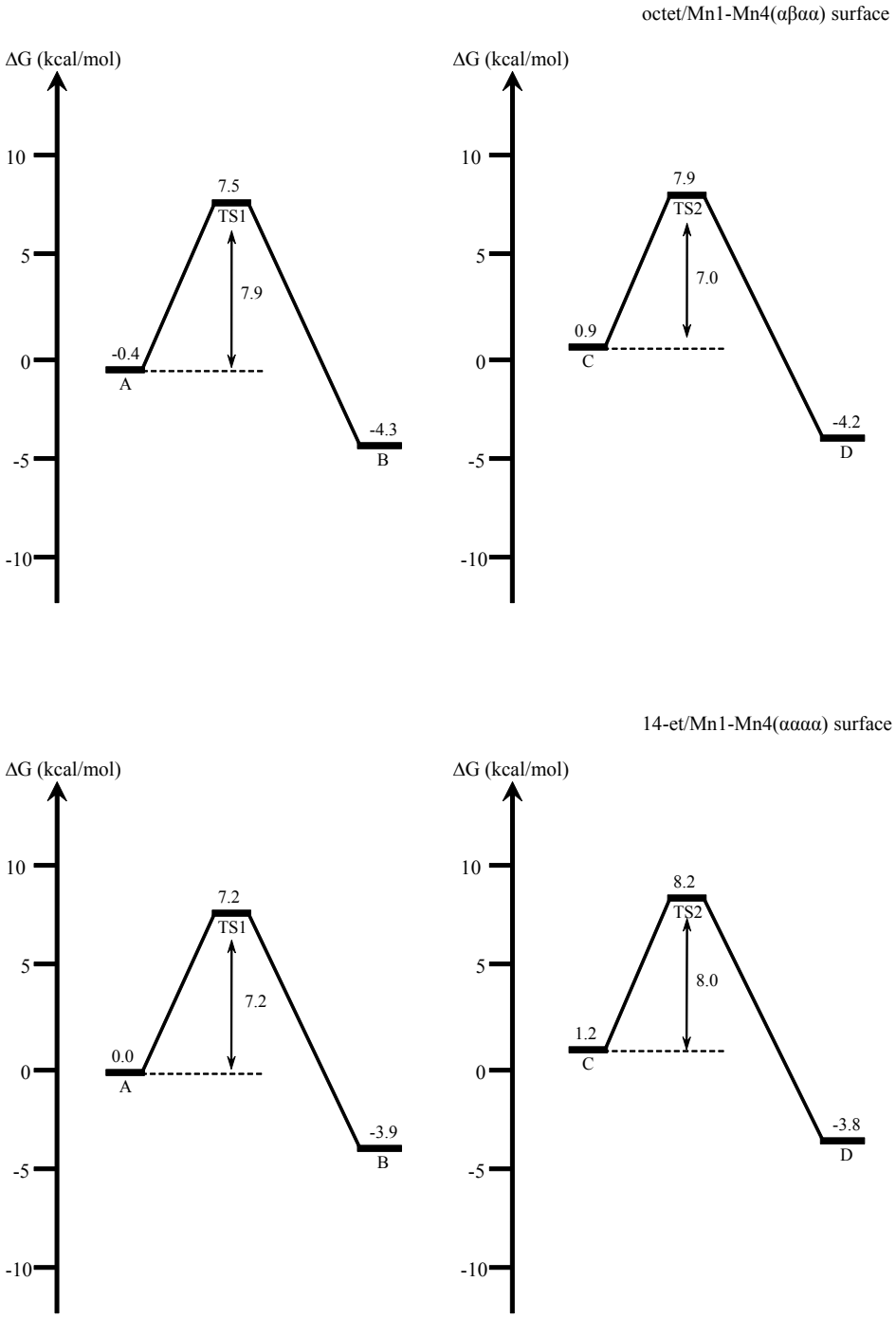


Figure SIVa. Free energy profiles for the W1 substitution scheme with the open-

cubane structure as reactant for all spin states.

The Cartesian coordinates for A to D and TS1, TS2:

A:

Ca	-2.74544900	-0.00526200	-1.00008400	H	-1.06353100	-4.27829100	-3.97633000	C	2.21646000	2.32581600	-0.50869000
Mn	0.33274700	-1.91535000	-0.62802900	C	-2.32879900	-3.07681800	-5.28304200	O	1.37501100	3.06803000	-1.13051200
Mn	-1.14823600	-1.39954700	1.61074900	H	-2.35949100	-2.04260600	-5.65485600	O	0.72408600	-3.76971700	0.31441800
Mn	-0.02606300	1.04717200	0.95943100	H	-3.23784200	-3.21331000	-4.68009600	C	0.17623100	-4.04071200	1.42457000
Mn	-0.53957100	3.08862300	-0.77142100	C	-2.34308900	-4.05425200	-6.46369400	O	-0.53169200	-3.24116100	2.11863400
O	-1.40996800	-1.88464000	-0.12805500	H	-1.46048800	-3.91939400	-7.10479000	C	0.37343600	-5.45169700	1.97167100
O	0.52229600	-0.86401100	0.92591000	H	-2.34450800	-5.09726600	-6.11780400	H	1.43573800	-5.70181200	1.84420000
O	-1.63402300	0.33000100	1.33904200	H	-3.23403500	-3.90885400	-7.08779200	H	-0.17041200	-6.12213100	1.28816300
O	-0.57575000	1.28508500	-0.80335600	N	2.35495000	-1.68504100	-1.00469100	C	-0.08526800	-5.66272700	3.41475000
O	-0.33139100	2.79933200	1.02116600	C	3.09513200	-1.53319200	-2.15782600	H	0.07414100	-6.70585100	3.71768100
O	-4.47413000	-0.44574000	-2.83163200	H	2.61939600	-1.55679800	-3.12902000	H	0.46973700	-5.01635000	4.10564700
H	-3.92408300	-1.12050400	-3.27786400	C	4.42315900	-1.37355000	-1.83173000	H	-1.14859200	-5.42509800	3.52805100
H	-4.20131400	0.38139200	-3.28275500	N	4.46377800	-1.46305700	-0.44479000	O	-4.18323400	-1.15657600	0.55478700
O	-2.39589200	1.28160000	-3.24731500	H	5.28753200	-1.26425100	0.13015000	C	-4.01634100	-1.71121900	1.65443500
H	-1.79984100	0.61900300	-3.63967000	C	3.20617600	-1.62853400	0.01203300	O	-2.87534100	-1.89679900	2.24901600
H	-1.83083500	2.10205100	-3.09325800	H	2.92510300	-1.66386200	1.05462700	C	-5.20297600	-2.24683100	2.43840500
O	-0.81214100	3.32748000	-2.61173300	C	5.62658900	-1.11122100	-2.70287700	H	-6.12837600	-2.09050500	1.87786700
H	0.07015600	3.28567600	-3.02333800	H	5.83955200	-1.99125100	-3.32732000	H	-5.26272200	-1.73562500	3.40757000
O	-0.21079300	5.15907700	-0.53335700	H	5.36963700	-0.30597300	-3.40639800	H	-5.06168500	-3.31528900	2.64300400
H	-1.13322800	5.44330200	-0.68495100	C	6.93723200	-0.74365800	-1.96021600	O	-0.55641500	-0.88318700	3.46355100
H	-0.02319100	5.34645700	0.45995900	H	7.35261700	-1.62552100	-1.46050500	C	0.12762400	0.15291100	3.71546900
O	-3.85487600	2.04345800	-0.58458500	H	7.67372200	-0.41380100	-2.70587400	O	0.52286700	1.02084000	2.86674500
C	-3.55319200	3.23839100	-0.46219700	C	6.75712900	0.31385400	-0.86958900	C	0.49555700	0.41785700	5.16957400
O	-2.35778500	3.73464000	-0.54078700	O	6.73366400	-0.00249400	0.32799000	H	1.41930000	1.01102600	5.17996800
C	-4.62823700	4.29196900	-0.19411500	N	6.55219800	1.59149500	-1.27638200	H	-0.29553500	1.07176900	5.57316300
H	-4.38583100	4.76065400	0.77157200	H	6.55253700	1.79441000	-2.26842700	C	0.62393500	-0.83961700	6.03752800
H	-4.50886000	5.08375300	-0.94771100	C	6.14091200	2.64549000	-0.34074200	H	1.41010800	-1.48692000	5.62127800
C	-6.05198500	3.73692100	-0.19144800	H	6.82534400	2.62028500	0.51460100	H	-0.30869600	-1.41351900	5.97361900
H	-6.16842100	2.95769100	0.57000700	H	6.28089200	3.60319600	-0.85714600	C	0.94596100	-0.50705100	7.49840800
H	-6.77438800	4.53728200	0.01513800	C	4.69205100	2.49963600	0.15909400	H	1.89121500	0.04728000	7.58655600
H	-6.30206000	3.28799500	-1.15980800	H	4.60115300	1.58122900	0.74785600	H	1.03795600	-1.42005700	8.10088700
O	-1.90381700	-1.45634100	-2.98822800	H	4.49086300	3.33642200	0.84389700	H	0.15672800	0.11114100	7.94939700
C	-1.00579300	-2.30115100	-3.20524500	C	3.66026100	2.49410100	-0.97504000	N	0.22750000	5.33115100	2.11463000
O	0.06113200	-2.43545300	-2.49054100	H	3.71617700	3.41285900	-1.57189400	H	0.09691000	4.31024700	2.15712400
C	-1.09986300	-3.25841200	-4.38906200	H	3.86111200	1.64916700	-1.65181200	H	-0.45760700	5.76568600	2.73353700
H	-0.17197800	-3.15191200	-4.97196700	O	1.95551000	1.48871500	0.39131700	H	1.15564000	5.55278900	2.47559500

TS1:

Ca	2.78404400	0.54316200	0.74027600	O	4.58615800	1.09417800	2.44999600	H	-0.48715100	5.81413100	-1.28603000
Mn	-0.15439800	-1.50918400	1.35324500	H	4.15238500	0.62075100	3.18751000	O	3.60728200	2.31108300	-0.63371300
Mn	1.26033500	-1.93589100	-0.95120100	H	4.25553400	2.01079500	2.55647000	C	3.12036000	3.37605800	-1.03771800
Mn	-0.07460000	0.44542500	-1.34117300	O	2.33268700	2.63626600	2.28418800	O	1.88987900	3.74998600	-0.84325600
Mn	0.23154200	2.97128700	-0.41125400	H	1.87985500	2.10172400	2.96220100	C	3.95209300	4.39005000	-1.81307500
O	1.57349700	-1.61273100	0.80910800	H	1.64005900	3.27210400	1.93938800	H	3.54086300	4.41912200	-2.83423200
O	-0.45477300	-1.28731800	-0.50529100	O	0.31252500	4.01666500	1.14655700	H	3.75200900	5.38169100	-1.38470200
O	1.59433200	-0.20793400	-1.43151000	H	-0.55658700	3.95951300	1.58462000	C	5.44719800	4.07424800	-1.83734600
O	0.38191300	1.34399900	0.27086400	O	-0.62642800	6.30345800	-0.44357100	H	5.63361700	3.08811000	-2.27657200
O	0.14048200	2.09475500	-1.99509400	H	-0.12550000	5.77434100	0.20534800	H	5.98631300	4.82698100	-2.42646900

H	5.86575200	4.06782100	-0.82376600	H	-7.12359000	-1.13335500	2.43281300	H	-0.16697700	-6.33752700	-1.62744400
O	2.13227400	0.01400900	3.18130200	H	-7.50719700	0.55278900	2.79801500	H	1.48503400	-6.38123200	-1.00281400
C	1.29516300	-0.70557400	3.77401500	C	-6.73608800	0.15572600	0.79970400	O	4.28343000	-1.05839700	-0.23702900
O	0.22039000	-1.17499600	3.23402200	O	-6.66790800	-0.78273700	-0.00716300	C	4.14543700	-2.03543100	-0.99277900
C	1.48080600	-1.07605700	5.24109200	N	-6.70031300	1.44999000	0.39593900	O	3.01187100	-2.52939800	-1.39631500
H	0.56342500	-0.78037500	5.77293700	H	-6.73851800	2.18056200	1.09618500	C	5.35706900	-2.76798500	-1.54182900
H	1.49843800	-2.17562600	5.29060900	C	-6.37606600	1.81661700	-0.98904900	H	6.27430300	-2.35559400	-1.11351500
C	2.71915800	-0.48083900	5.91556600	H	-7.00894100	1.21586500	-1.65092900	H	5.37951100	-2.66554100	-2.63435000
H	2.69167800	0.61475000	5.82669200	H	-6.65487800	2.86962900	-1.11770500	H	5.28068400	-3.83868700	-1.31719800
H	3.61828300	-0.81084300	5.37584900	C	-4.89494300	1.58620600	-1.34167700	O	0.63226700	-2.26281900	-2.84138500
C	2.82926000	-0.87912500	7.39161800	H	-4.66800800	0.51857800	-1.25571600	C	-0.10235800	-1.45953500	-3.48387600
H	1.95734500	-0.53380800	7.96471000	H	-4.74780200	1.85403600	-2.39747000	O	-0.55691200	-0.34245900	-3.05098300
H	2.89023900	-1.97019600	7.50667400	C	-3.94194300	2.39480100	-0.45859500	C	-0.47649100	-1.81230400	-4.91538200
H	3.72507700	-0.44465000	7.85310800	H	-4.05702100	3.47541800	-0.61385300	H	-1.48888700	-1.42810500	-5.09892100
N	-2.17089000	-1.24890500	1.71909600	H	-4.16651600	2.21005800	0.60401700	H	0.19224800	-1.21938400	-5.56113400
C	-2.87318000	-0.47726800	2.62104400	O	-2.10553400	0.94246000	-1.04935700	C	-0.36635400	-3.30051500	-5.26378400
H	-2.36058800	0.08702100	3.38845400	C	-2.46272200	2.06528900	-0.62075800	H	-1.03174500	-3.87644800	-4.60422500
C	-4.22106500	-0.58049600	2.35942800	O	-1.68076200	3.01357000	-0.23692700	H	0.65163800	-3.64612100	-5.04468000
N	-4.31109600	-1.46027900	1.28787100	O	-0.44644000	-3.61011900	1.27590100	C	-0.71828100	-3.57852800	-6.72928400
H	-5.17094700	-1.64661900	0.76049200	C	0.11363800	-4.30190200	0.37426300	H	-1.74511200	-3.26374100	-6.96346300
C	-3.06527800	-1.82101500	0.92192500	O	0.77673800	-3.84083300	-0.61261600	H	-0.63757600	-4.64894200	-6.95828900
H	-2.82970000	-2.45582300	0.08034000	C	-0.00294100	-5.81889300	0.48400500	H	-0.04391400	-3.04050700	-7.41043300
C	-5.40531500	0.09420900	3.00762800	H	-1.04396000	-6.04410100	0.75339300	N	-0.23379700	4.82319000	-2.97065900
H	-5.51511100	-0.25720200	4.04394400	H	0.59665200	-6.10659300	1.36171900	H	-0.19014000	3.80172100	-3.04141700
H	-5.18865200	1.16976100	3.08174700	C	0.44118100	-6.59996800	-0.75308900	H	0.64585800	5.18448200	-3.34070900
C	-6.77508600	-0.10241600	2.30639800	H	0.34244000	-7.67911500	-0.57827800	H	-0.97964900	5.14862700	-3.58712300

B:

Ca	-2.74794300	0.24505500	-0.79122100	O	-1.85766200	0.26550800	-3.23575000	C	5.95192700	2.76249600	1.36956300
Mn	0.47953400	-1.26922100	-1.50947600	C	-0.90631800	-0.23530200	-3.87911800	H	6.65462900	2.30900700	2.07743700
Mn	-0.95350700	-2.20953500	0.62108900	O	0.18525300	-0.67336600	-3.34922300	H	6.01603800	3.85203100	1.48186900
Mn	-0.05434300	0.27842600	1.44005600	C	-0.96461800	-0.35015200	-5.39917900	C	4.52785400	2.26246300	1.67282300
Mn	-0.78354700	2.87265600	1.14371400	H	-0.06215400	0.13662500	-5.80006000	H	4.51173700	1.16846300	1.63926400
O	-1.23837900	-1.67443200	-1.10252700	H	-0.84610900	-1.41736500	-5.64163700	H	4.28622100	2.54965400	2.70656900
O	0.64256300	-1.24163000	0.36956400	C	-2.22635200	0.21884500	-6.05244400	C	3.47228200	2.82512700	0.71316700
O	-1.58498900	-0.66297000	1.33865900	H	-2.33995100	1.27482600	-5.76806900	H	3.45669800	3.92237100	0.73464900
O	-0.66634200	1.39848700	0.08725000	H	-3.10747500	-0.30304200	-5.65269200	H	3.71278300	2.52185900	-0.31762600
O	-0.49868400	1.68702300	2.45400400	C	-2.20291500	0.09172500	-7.57982200	O	1.87366300	1.11366300	1.24574400
O	-4.51034800	0.71985600	-2.58273700	H	-1.34915100	0.63197000	-8.01274400	C	2.05349700	2.32627900	0.97939900
H	-3.91358500	0.48361000	-3.32105000	H	-2.12189600	-0.95895100	-7.89121400	O	1.14442200	3.22795500	0.87110900
H	-4.36218700	1.68421000	-2.48887300	H	-3.11801800	0.50183400	-8.02567800	O	1.04604000	-3.29408600	-1.75230400
O	-2.63069000	2.59863800	-1.93168500	N	2.46979500	-0.71300700	-1.66350800	C	0.56409500	-4.17978700	-0.98438100
H	-2.01648800	2.30242400	-2.62782400	C	3.16843800	0.10899500	-2.52176000	O	-0.17204500	-3.96150800	0.03174200
H	-2.10745300	3.23957500	-1.36056400	H	2.67096500	0.59848400	-3.34827000	C	0.88605700	-5.63502100	-1.31226800
O	-1.07620300	4.10134800	-0.34441800	C	4.49091600	0.15132800	-2.14072500	H	1.95858600	-5.68369100	-1.54607600
H	-0.20513900	4.16378900	-0.77667300	N	4.57280700	-0.69536600	-1.04096400	H	0.36864900	-5.85529200	-2.25895100
O	-1.65006600	6.44790200	0.85154300	H	5.39531600	-0.79563900	-0.43952600	C	0.49809500	-6.64842500	-0.23527800
H	-1.55886100	5.63675600	0.27487900	C	3.34116500	-1.17534400	-0.77564200	H	0.74548300	-7.66684900	-0.56218500
H	-1.02347100	7.08653300	0.47258200	H	3.09013400	-1.80727200	0.06396600	H	1.02879900	-6.45134400	0.70420700
O	-3.98928800	1.58376100	0.71202100	C	5.65218700	0.93754600	-2.69684800	H	-0.57497600	-6.60200900	-0.02009900
C	-3.76800000	2.56714600	1.43032300	H	5.91173600	0.56948000	-3.70031400	O	-4.03523000	-1.69570500	-0.17086600
O	-2.62141700	3.15609900	1.58940200	H	5.32309600	1.97703000	-2.84036200	C	-3.78330700	-2.74513700	0.44509200
C	-4.88888600	3.22026600	2.23692600	C	6.95104600	0.92365000	-1.84973100	O	-2.60883600	-3.12512100	0.85355500
H	-4.62599200	3.10113800	3.29907000	H	7.44065300	-0.05381300	-1.91856100	C	-4.89327300	-3.72138500	0.79697300
H	-4.85094800	4.30095100	2.04111500	H	7.64372100	1.66579500	-2.27006600	H	-5.83957600	-3.39104400	0.36059800
C	-6.27494500	2.64523100	1.94818900	C	6.72230800	1.17658900	-0.35849900	H	-4.99046100	-3.78269200	1.88856400
H	-6.30628000	1.57017600	2.15726500	O	6.75255700	0.24607500	0.45835900	H	-4.63819200	-4.72514100	0.43627100
H	-7.03166400	3.14362900	2.56783500	N	6.41353100	2.44457400	0.01270600	O	-0.34587900	-2.74759700	2.45646000
H	-6.54813100	2.78274600	0.89516600	H	6.37683400	3.16622600	-0.69655500	C	0.25814800	-1.96350000	3.24894200

O	0.55690500	-0.74444100	3.01969200	H	1.64976400	-4.30802700	3.98512800	H	0.38317000	-4.26157000	6.80276400
C	0.64471100	-2.50323000	4.61895900	H	-0.06158000	-4.51799800	4.31652800	N	-0.58906100	4.43493400	2.54969400
H	1.54075200	-1.96245400	4.95069600	C	1.18747000	-4.50481200	6.09406300	H	-1.17108200	4.17121700	3.34464100
H	-0.16432600	-2.20264600	5.30530800	H	2.10971500	-4.03767800	6.46789700	H	-0.93862000	5.31775400	2.12854100
C	0.84658400	-4.02156300	4.68019600	H	1.33237900	-5.59275800	6.11612300	H	0.38013400	4.53208800	2.85078700

C:

Ca	2.74173700	-0.00009900	0.95770700	H	0.62792200	-2.50247100	5.33656200	C	-1.93179300	2.50124000	-0.52334800
Mn	-0.53777500	-1.53930900	1.27248300	C	2.03845300	-1.02191700	6.09124800	O	-0.99930700	3.31263300	-0.18636600
Mn	0.94941300	-2.09285900	-0.96105100	H	2.19060100	0.06448500	6.01757800	O	-1.15417500	-3.55155500	1.10043400
Mn	0.10814900	0.52216100	-1.32010000	H	2.91784000	-1.48741600	5.62372000	C	-0.66617500	-4.28789400	0.19156000
Mn	0.88867500	2.97538500	-0.50121900	C	1.95977500	-1.43693600	7.56474700	O	0.11967000	-3.90112900	-0.73258400
O	1.18521300	-1.90754200	0.85515300	H	1.10721300	-0.96057600	8.06914000	C	-1.04460400	-5.76597000	0.21372600
O	-0.64342900	-1.14565000	-0.58096400	H	1.83900100	-2.52435000	7.66672600	H	-2.12888800	-5.81838700	0.38403300
O	1.61956100	-0.45241700	-1.34572100	H	2.87034000	-1.15054800	8.10631500	H	-0.58408100	-6.18488400	1.12186100
O	0.71898800	1.35034600	0.25156800	N	-2.51682400	-0.96778400	1.47350300	C	-0.63017600	-6.56506000	-1.02203100
O	0.62184700	2.08668600	-2.04566400	C	-3.21789800	-0.28895800	2.44733700	H	-0.92415100	-7.61713100	-0.91275000
O	4.44002600	0.10111600	2.86930200	H	-2.73542600	0.01773800	3.36562600	H	-1.10453200	-6.16846600	-1.92795300
H	3.81242600	-0.26343400	3.52529000	C	-4.52121800	-0.11732500	2.03767500	H	0.45369900	-6.51989800	-1.17443000
H	4.29353600	1.06725200	2.94990800	N	-4.59066600	-0.74049200	0.79692800	O	4.00657200	-1.83625900	0.03645700
O	2.61562900	2.10762500	2.51052500	H	-5.39238700	-0.69047100	0.16130500	C	3.75845500	-2.73122100	-0.78806600
H	1.95854800	1.70699600	3.10809600	C	-3.36873700	-1.21763000	0.48666800	O	2.59541800	-2.97891900	-1.31644200
H	2.13480400	2.85758100	2.03891500	H	-3.10777100	-1.69091300	-0.44876600	C	4.85530000	-3.66291900	-1.27523200
O	1.22805600	3.93221000	1.14244500	C	-5.67196200	0.60769800	2.69084100	H	4.58097900	-4.70322800	-1.06034900
H	0.35086800	4.05202600	1.54923200	H	-5.97469700	0.08422900	3.60957100	H	5.80344400	-3.41673300	-0.79007400
O	0.74930300	4.76523700	-1.61561600	H	-5.31250800	1.59413300	3.01845300	H	4.95726500	-3.57203800	-2.36392000
H	1.17272300	4.48207800	-2.44719100	C	-6.94355900	0.79000500	1.82242800	O	0.37967100	-2.26370000	-2.88015800
H	1.38854000	5.44140500	-1.16980300	H	-7.46271900	-0.16688900	1.70076200	C	-0.18615100	-1.32956000	-3.52544400
O	4.08653000	1.52018600	-0.25468700	H	-7.62711500	1.46725700	2.35287200	O	-0.47028800	-0.16830800	-3.08178600
C	3.88011800	2.57702600	-0.87025100	C	-6.66123800	1.30091000	0.40803600	C	-0.54122000	-1.59699800	-4.98166200
O	2.76660200	3.23433200	-0.90734900	O	-6.68514200	0.53274300	-0.56366600	H	-1.36850400	-0.92928600	-5.25392200
C	5.03791800	3.23301300	-1.62674200	N	-6.31429000	2.60587200	0.28114800	H	0.32870100	-1.26890100	-5.57453700
H	5.61432800	3.80600400	-0.88264300	H	-6.28186900	3.18459300	1.11141200	C	-0.86721900	-3.06091200	-5.30187200
H	5.69593900	2.42020100	-1.95636800	C	-5.78994500	3.14997600	-0.97837900	H	-1.73039300	-3.37935200	-4.69836100
C	4.63477700	4.13287200	-2.79720300	H	-6.47553800	2.85687600	-1.78118900	H	-0.02576200	-3.69073100	-4.98776300
H	4.00166900	4.96314700	-2.46250600	H	-5.82051900	4.24310500	-0.89087500	C	-1.16778900	-3.27647400	-6.78905700
H	5.52402200	4.55387500	-3.28402400	C	-4.36846900	2.66583500	-1.31698100	H	-2.02440700	-2.67147500	-7.11850700
H	4.07268100	3.56755400	-3.55163100	H	-4.38436500	1.58483900	-1.48888600	H	-1.40307600	-4.32846900	-6.99674100
O	1.76417000	-0.42179200	3.32762100	H	-4.07223500	3.13295600	-2.26707500	H	-0.30692500	-2.99811600	-7.41333100
C	0.78092600	-1.00905400	3.83515700	C	-3.34204000	3.00279900	-0.22906300	N	2.31887800	6.27635600	-0.09897300
O	-0.30128700	-1.30701500	3.19952100	H	-3.28351400	4.08434800	-0.05448600	H	2.09347000	5.58469700	0.63414000
C	0.78432100	-1.41331200	5.30612500	H	-3.64116900	2.53217500	0.72050800	H	2.06037700	7.20847300	0.22437000
H	-0.11724500	-0.98127300	5.76725300	O	-1.77778700	1.35904500	-1.02604000	H	3.32704300	6.25890200	-0.24996000

TS2:

Ca	2.66422900	1.24036100	0.55957700	H	1.64047200	2.32293600	2.98349200	H	0.07462500	5.11544000	-2.94492900
Mn	0.43225300	-1.50784800	1.29323500	H	0.90723400	3.42899100	2.13951200	H	1.29290700	5.88267700	-3.99097100
Mn	1.70435200	-1.50408200	-1.13232300	O	-0.70658900	3.75684300	1.59500300	H	1.24168800	4.11437900	-3.82583900
Mn	-0.24126000	0.43610300	-1.25845500	H	-1.45824200	3.38333700	2.08970900	O	2.49048000	0.43813700	3.00757900
Mn	-0.59017600	2.82304900	-0.03868600	O	-2.59739800	4.18787000	-2.16794000	C	1.92673700	-0.50574300	3.61056000
O	2.07928800	-1.17376900	0.61080800	H	-1.85273800	3.60082600	-2.39375500	O	0.92938800	-1.18033700	3.14632100
O	-0.07834900	-1.36149000	-0.53139800	H	-2.22944400	4.86468100	-1.54279700	C	2.38374900	-0.92624200	5.00265600
O	1.52615800	0.27356000	-1.51497300	O	2.72977100	3.16670600	-0.88757300	H	1.49754800	-0.92098400	5.65546400
O	0.09070600	1.25721100	0.43601000	C	1.87464700	4.03785400	-1.09644800	H	2.68051800	-1.98406300	4.93159200
O	-0.52736100	2.14772200	-1.71336500	O	0.72947600	4.10030000	-0.46869900	C	3.51200400	-0.08431300	5.60345100
O	4.40769800	2.25356100	2.10634600	C	2.09825200	5.15300200	-2.10444900	H	3.20179600	0.97014300	5.63684500
H	4.25683400	1.62446000	2.83943300	H	1.96602800	6.11414700	-1.58667000	H	4.38681000	-0.12633900	4.93914100
H	3.82467800	3.00595000	2.34163700	H	3.13607200	5.09225000	-2.44940900	C	3.90746500	-0.55358500	7.00802800
O	1.80278400	3.02746700	2.32833400	C	1.11486700	5.06086000	-3.28602400	H	3.05867800	-0.49254300	7.70356400

H	4.25218000	-1.59687500	6.99730100	H	-7.20346500	0.93493900	-0.86895400	O	3.50534600	-1.59364900	-1.73779000
H	4.71906200	0.06137600	7.41730700	C	-5.15467600	0.18122200	-1.09034100	C	5.81028500	-1.20110700	-2.06926300
N	-1.54028700	-1.73439700	1.86789100	H	-4.62601600	-0.74974700	-0.85934100	H	6.03182000	-2.26213700	-1.90258400
C	-2.33139000	-1.01546600	2.73938500	H	-5.11398600	0.29470300	-2.18175800	H	6.62307000	-0.57907000	-1.68546700
H	-1.90680600	-0.25453900	3.38027500	C	-4.45744900	1.36643500	-0.41492200	H	5.71264000	-1.05533900	-3.15270500
C	-3.63771400	-1.43440300	2.62422400	H	-4.68514900	2.31817900	-0.91728300	O	1.02938400	-1.89128400	-2.99495300
N	-3.60672000	-2.44621200	1.67341700	H	-4.78808700	1.48566500	0.62747300	C	0.07665200	-1.26252300	-3.53813300
H	-4.44280600	-2.86774500	1.25228700	O	-2.31989900	0.35547300	-0.91727300	O	-0.61061600	-0.32318500	-3.00113800
C	-2.34002500	-2.58241200	1.23216800	C	-2.93992600	1.29796700	-0.37404500	C	-0.29672000	-1.61305200	-4.96989700
H	-2.02775100	-3.26713100	0.45727300	O	-2.39817500	2.28737300	0.25411800	H	-1.37949100	-1.46545000	-5.07710300
C	-4.89077800	-0.94446000	3.30853600	O	0.63301900	-3.62167500	1.10309700	H	0.17661300	-0.84670400	-5.60584500
H	-4.82701800	-1.14551700	4.38785200	C	1.27473700	-4.12164200	0.13147100	C	0.13027200	-3.01372600	-5.42219300
H	-4.92910700	0.15042000	3.21206900	O	1.74609900	-3.47678400	-0.86311600	H	-0.34173300	-3.76343500	-4.77048500
C	-6.23031200	-1.54324700	2.80563600	C	1.51992700	-5.62733500	0.15840600	H	1.21237100	-3.12336800	-5.27782600
H	-6.29947300	-2.60338600	3.07382300	H	0.57763500	-6.10191400	0.46513900	C	-0.24146000	-3.28707700	-6.88367700
H	-7.04984100	-1.02142400	3.31858700	H	2.22229100	-5.80630700	0.98741100	H	-1.32595600	-3.20849500	-7.04460300
C	-6.39678400	-1.46461300	1.28803900	C	2.05488500	-6.22663100	-1.14246400	H	0.06843500	-4.29522800	-7.18773100
O	-6.13633600	-2.43800800	0.56582500	H	2.21807300	-7.30587900	-1.02616400	H	0.24592700	-2.57056400	-7.55985000
N	-6.76340000	-0.26550200	0.77061000	H	1.35013600	-6.07352300	-1.96888900	N	-1.60473100	6.04520800	-0.20023500
H	-6.93752900	0.50284100	1.40674100	H	3.00309700	-5.75973600	-1.43019200	H	-1.31157200	5.49120100	0.61280600
C	-6.62538400	0.02572400	-0.66385500	O	4.44554900	0.12240200	-0.59841300	H	-2.30417100	6.72093900	0.10968300
H	-7.08611000	-0.80010100	-1.21570900	C	4.50154800	-0.83210300	-1.39314100	H	-0.78442200	6.56969200	-0.50388100

D:

Ca	-2.72838400	-0.38474300	-1.09437100	H	0.04495000	-4.47494200	-3.86431600	H	3.94350600	1.14831600	-1.91587400
Mn	0.32506400	-2.03498600	-0.03690300	H	-0.88525600	-5.29275500	-2.63112400	O	1.89810400	1.53775500	-0.03041000
Mn	-1.24968000	-0.86912600	1.87948000	C	-2.09397400	-4.54150400	-4.28217700	C	2.22260000	2.07753300	-1.11602700
Mn	-0.09260200	1.25332100	0.53152700	H	-2.11488700	-3.65713700	-4.93507600	O	1.42149700	2.57499800	-1.98751200
Mn	-0.53499000	2.63925700	-1.77195500	H	-3.03103800	-4.52115900	-3.70766400	O	0.68129400	-3.49137000	1.45083400
O	-1.43403400	-1.89490600	0.36175800	C	-2.04049400	-5.81490600	-5.13374400	C	0.09112600	-3.41338500	2.56985400
O	0.45569400	-0.53914500	1.12918200	H	-1.12783600	-5.84859100	-5.74536600	O	-0.65060900	-2.45090500	2.95027500
O	-1.71525000	0.67182300	1.04343300	H	-2.05072100	-6.71587300	-4.50475300	C	0.27802400	-4.57684200	3.53921800
O	-0.54393000	0.89708100	-1.24111800	H	-2.90001000	-5.87330200	-5.81360100	H	1.34968600	-4.81970100	3.54821900
O	-0.42643400	2.95057300	0.03285200	N	2.36588300	-1.92029500	-0.36798700	H	-0.21544100	-5.44384200	3.07336500
O	-4.39829400	-1.38736200	-2.75351800	C	3.16054700	-2.07904100	-1.48322100	C	-0.25729900	-4.34270900	4.95198300
H	-3.82231400	-2.14768900	-2.96984900	H	2.73231600	-2.37500100	-2.43146600	H	-0.09817800	-5.23380700	5.57310500
H	-4.13927000	-0.72425100	-3.42770500	C	4.47125200	-1.81620600	-1.15286200	H	0.24734400	-3.49529100	5.43176900
O	-2.34374400	0.19732000	-3.61187700	N	4.44499300	-1.52137400	0.20539800	H	-1.32913900	-4.11708900	4.93411700
H	-1.74492300	-0.55614900	-3.76388400	H	5.23955900	-1.15795600	0.74001200	O	-4.23220300	-1.06039300	0.66946500
H	-1.77023000	1.02078500	-3.70442000	C	3.16722900	-1.57418200	0.63187100	C	-4.11286700	-1.22157800	1.89483200
O	-0.66635200	2.27847100	-3.62103700	H	2.83767800	-1.32540800	1.63018400	O	-2.99920500	-1.16269400	2.56603600
H	0.20545500	1.93035800	-3.88295200	C	5.71582100	-1.78603700	-2.00525800	C	-5.32549200	-1.52041500	2.76009000
O	-0.39510800	5.58098400	0.52642700	H	5.95798300	-2.80020600	-2.35533700	H	-5.19128000	-2.48648900	3.26284900
H	-1.27845900	5.78948400	0.87374500	H	5.49443200	-1.20591700	-2.91296900	H	-6.23081300	-1.54038400	2.14777700
H	-0.34288300	4.59048200	0.59288600	C	6.98974000	-1.21398500	-1.33075300	H	-5.41758100	-0.75711900	3.54266200
O	-3.87316800	1.68708200	-1.23155900	H	7.37692400	-1.91926900	-0.58735700	O	-0.73616400	0.20676200	3.49577100
C	-3.53514600	2.85322800	-1.47434100	H	7.76302800	-1.09569200	-2.10229000	C	-0.07125400	1.28613400	3.43477100
O	-2.35328200	3.24936300	-1.83846800	C	6.75887500	0.10204100	-0.58568300	O	0.35930300	1.84932700	2.37552800
C	-4.53779400	3.99606600	-1.34325500	O	6.66396600	0.12800700	0.64915400	C	0.22181300	1.99980300	4.74754900
H	-4.47975200	4.62085400	-2.24455400	N	6.58976100	1.21678400	-1.34007400	H	1.07148900	2.67417700	4.58342800
H	-5.54204700	3.56298900	-1.28262100	H	6.65157200	1.13795700	-2.34766900	H	-0.65196800	2.64019700	4.95319900
C	-4.23786200	4.85004100	-0.09884500	C	6.12573600	2.48244700	-0.75787000	C	0.46575900	1.06224600	5.93746400
H	-3.21768000	5.25147000	-0.14746900	H	6.74693300	2.69564300	0.11900600	H	1.33355700	0.42137100	5.72008600
H	-4.93969900	5.69020400	-0.02530800	H	6.31402100	3.26529300	-1.50309900	H	-0.39433800	0.38944800	6.04208500
H	-4.32459700	4.25017900	0.81606600	C	4.64347100	2.46392700	-0.34254600	C	0.70409100	1.82966300	7.24225000
O	-1.79908400	-2.32467500	-2.53068600	H	4.50108900	1.73710500	0.46360200	H	1.57667900	2.49364200	7.16509500
C	-0.88461100	-3.17705400	-2.45299900	H	4.39881800	3.45090300	0.07584100	H	0.88145900	1.14167600	8.07914100
O	0.14279100	-3.08037700	-1.67827200	C	3.69713700	2.13960300	-1.50443200	H	-0.16371800	2.45262700	7.50124400
C	-0.91011400	-4.43310000	-3.31820900	H	3.80215000	2.86470100	-2.32157700	N	-0.22783000	4.68383800	-2.19630700

H	-0.95216400	4.93981900	-2.86647200	H	0.69408300	4.83497800	-2.60484400	H	-0.32944700	5.22844000	-1.31937400

IVb. Closed-cubane structure as reactant

Table SIVb. Gibbs free energies and Mulliken spin populations for the W1 substitution scheme with the closed-cubane structure as reactant:

Spin states	Spin topology (Mn1-Mn4)	Gibbs Free energy (a.u.)		
		E	TS3	F
doublet	αββα	-3347.6523	-3347.6343	-3347.6503
	βαβα	-3347.6518	-3347.6352	-3347.6497
	ββαα	-3347.6528	-3347.6347	-3347.6504
sextet	αααβ	-3347.6555	-3347.6381	-3347.6523
octet	ααβα	-3347.6550	-3347.6376	-3347.6519
	αβαα	-3347.6533	-3347.6354	-3347.6516
	βααα	-3347.6542	-3347.6361	-3347.6520
14-et	αααα	-3347.6560	-3347.6379	-3347.6542
		TS4	G	H
doublet	αββα	-3347.6362	-3347.6522	-3347.6498
	βαβα	\	\	-3347.6500
	ββαα	\	\	-3347.6490
sextet	αααβ	\	\	-3347.6523
octet	ααβα	-3347.6362	-3347.6517	-3347.6516
	αβαα	-3347.6368	-3347.6524	-3347.6538
	βααα	\	\	-3347.6500

14-et	αααα	-3347.6380	-3347.6524	-3347.6523
		TS5	I	TS6
doublet	αββα	-3347.6426	-3347.6535	-3347.6399
	βαβα	-3347.6436	-3347.6541	\
	ββαα	-3347.6410	-3347.6532	\
sextet	αααβ	-3347.6443	-3347.6560	\
octet	ααβα	-3347.6441	-3347.6553	-3347.6404
	αβαα	-3347.6411	-3347.6565	-3347.6411
	βααα	-3347.6437	-3347.6559	\
14-et	αααα	-3347.6460	-3347.6567	-3347.6423

	J	
doublet	αββα	-3347.6564
	βαβα	\
	ββαα	\
sextet	αααβ	\
octet	ααβα	-3347.6559
	αβαα	-3347.6565
	βααα	\
14-et	αααα	-3347.6563

Spin states	Spin topology (Mn1-Mn4)		Mulliken spin density		
			E	TS3	F
doublet	α	Mn1	2.93	2.93	2.93
	β	Mn2	-2.93	-2.93	-2.93

	β	Mn3	-2.81	-2.79	2.79
	α	Mn4	3.82	3.83	3.79
	β	Mn1	-2.92	-2.92	-2.92
	α	Mn2	2.94	2.94	2.94
	β	Mn3	-2.79	-2.77	-2.77
	α	Mn4	3.82	3.82	3.79
	β	Mn1	-2.93	-2.93	-2.93
	β	Mn2	-2.94	-2.94	-2.94
	α	Mn3	2.85	2.85	2.87
	α	Mn4	3.88	3.90	3.86
sextet	α	Mn1	2.92	2.92	2.92
	α	Mn2	2.93	2.93	2.93
	α	Mn3	2.82	2.80	2.80
	β	Mn4	-3.82	-3.83	-3.79
octet	α	Mn1	2.94	2.94	2.94
	α	Mn2	2.94	2.94	2.94
	β	Mn3	-2.77	-2.75	-2.75
	α	Mn4	3.82	3.82	3.79
	α	Mn1	2.94	2.93	2.94
	β	Mn2	-2.94	-2.94	-2.93
	α	Mn3	2.87	2.87	2.88
	α	Mn4	3.88	3.90	3.86
	β	Mn1	-2.92	-2.92	-2.92
	α	Mn2	2.93	2.93	2.93
	α	Mn3	2.89	2.89	2.91

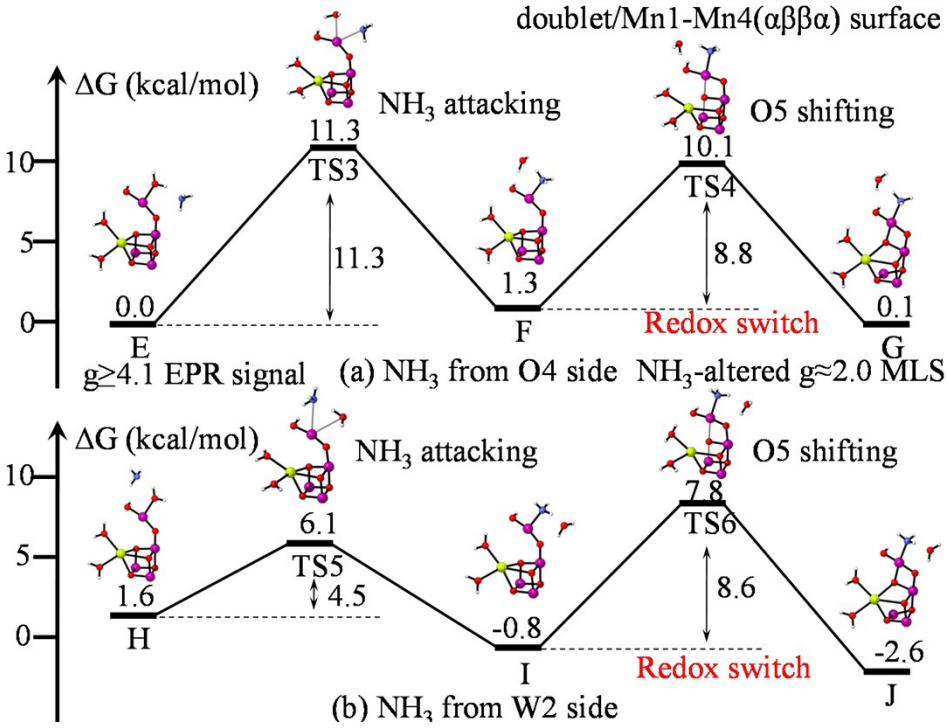
	α	Mn4	3.88	3.90	3.86
14-et	α	Mn1	2.94	2.93	2.94
	α	Mn2	2.93	2.93	2.93
	α	Mn3	2.90	2.90	2.91
	α	Mn4	3.88	3.90	3.86
			TS4	G	H
doublet	α	Mn1	3.44	3.88	2.93
	β	Mn2	-2.92	-2.92	-2.93
	β	Mn3	-2.86	-2.90	-2.80
	α	Mn4	3.56	2.86	3.82
	β	Mn1	\	\	-2.92
	α	Mn2	\	\	2.94
	β	Mn3	\	\	-2.78
	α	Mn4	\	\	3.82
	β	Mn1	\	\	-2.93
	β	Mn2	\	\	-2.94
	α	Mn3	\	\	2.86
	α	Mn4	\	\	3.89
sextet	α	Mn1	\	\	2.92
	α	Mn2	\	\	2.93
	α	Mn3	\	\	2.80
	β	Mn4	\	\	-3.82
octet	α	Mn1	3.49	3.88	2.94
	α	Mn2	2.95	2.97	2.94

	β	Mn3	-2.83	-2.88	-2.76
	α	Mn4	3.52	2.86	3.81
	α	Mn1	3.44	3.89	2.94
	β	Mn2	-2.91	-2.90	-2.93
	α	Mn3	2.87	2.90	2.88
	α	Mn4	3.58	2.90	3.89
	β	Mn1	\	\	-2.92
	α	Mn2	\	\	2.93
	α	Mn3	\	\	2.90
	α	Mn4	\	\	3.88
14-et	α	Mn1	3.51	3.89	2.94
	α	Mn2	2.95	2.97	2.93
	α	Mn3	2.90	2.93	2.90
	α	Mn4	3.53	2.90	3.88
			TS5	I	TS6
doublet	α	Mn1	2.94	2.93	3.44
	β	Mn2	-2.93	-2.93	-2.92
	β	Mn3	-2.82	-2.81	-2.87
	α	Mn4	3.86	3.80	3.60
	β	Mn1	-2.92	-2.92	\
	α	Mn2	2.94	2.94	\
	β	Mn3	-2.80	-2.80	\
	α	Mn4	3.86	3.80	\
	β	Mn1	-2.92	-2.92	\

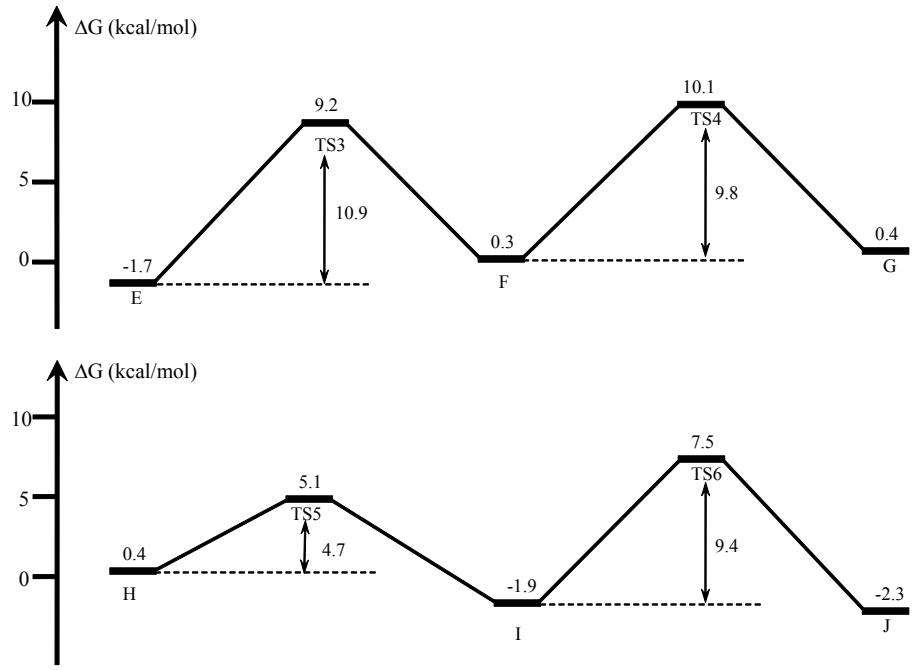
	β	Mn2	-2.94	-2.94	\
	α	Mn3	2.85	2.87	\
	α	Mn4	3.92	3.86	\
sextet	α	Mn1	2.92	2.93	\
	α	Mn2	2.93	2.93	\
	α	Mn3	2.82	2.82	\
	β	Mn4	-3.86	-3.80	\
octet	α	Mn1	2.95	2.94	3.48
	α	Mn2	2.94	2.95	2.95
	β	Mn3	-2.78	-2.78	-2.84
	α	Mn4	3.86	3.80	3.57
	α	Mn1	2.96	2.94	3.42
	β	Mn2	-2.93	-2.94	-2.92
	α	Mn3	2.85	2.88	2.88
	α	Mn4	3.91	3.86	3.62
	β	Mn1	-2.92	-2.92	\
	α	Mn2	2.93	2.93	\
	α	Mn3	2.89	2.90	\
	α	Mn4	3.92	3.86	\
14-et	α	Mn1	2.96	2.94	3.49
	α	Mn2	2.93	2.93	2.95
	α	Mn3	2.89	2.91	2.91
	α	Mn4	3.91	3.86	3.57
			J		

doublet	α	Mn1	3.87
	β	Mn2	-2.92
	β	Mn3	-2.91
	α	Mn4	2.89
	β	Mn1	\
	α	Mn2	\
	β	Mn3	\
	α	Mn4	\
	β	Mn1	\
	β	Mn2	\
	α	Mn3	\
	α	Mn4	\
sextet	α	Mn1	\
	α	Mn2	\
	α	Mn3	\
	β	Mn4	\
octet	α	Mn1	3.87
	α	Mn2	2.97
	β	Mn3	-2.89
	α	Mn4	2.89
	α	Mn1	3.87
	β	Mn2	-2.90
	α	Mn3	2.90
	α	Mn4	2.93

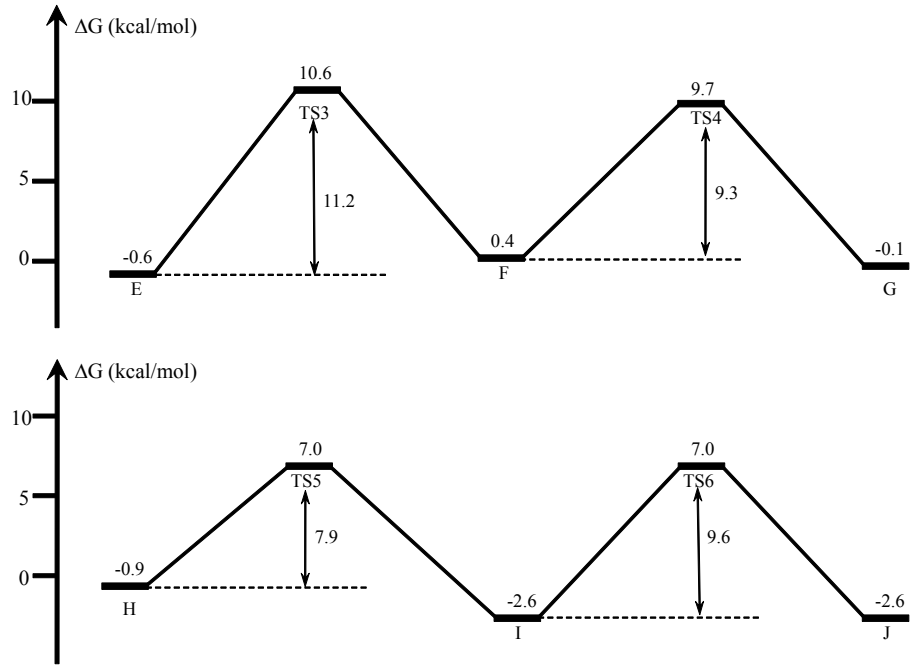
	β	Mn1	\
	α	Mn2	\
	α	Mn3	\
	α	Mn4	\
14-et	α	Mn1	3.88
	α	Mn2	2.98
	α	Mn3	2.93
	α	Mn4	2.93



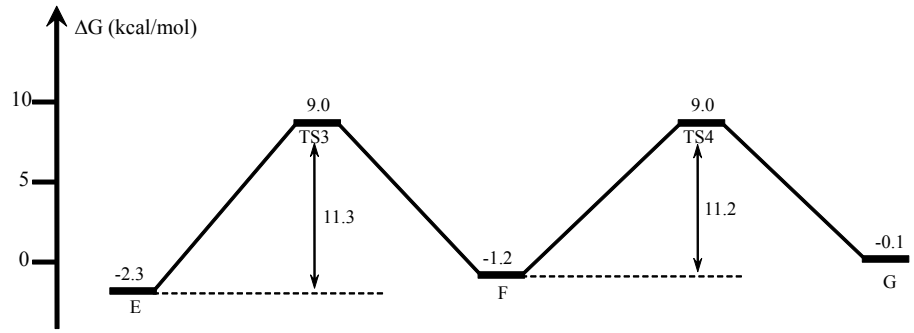
octet/Mn1-Mn4(ααβα) surface

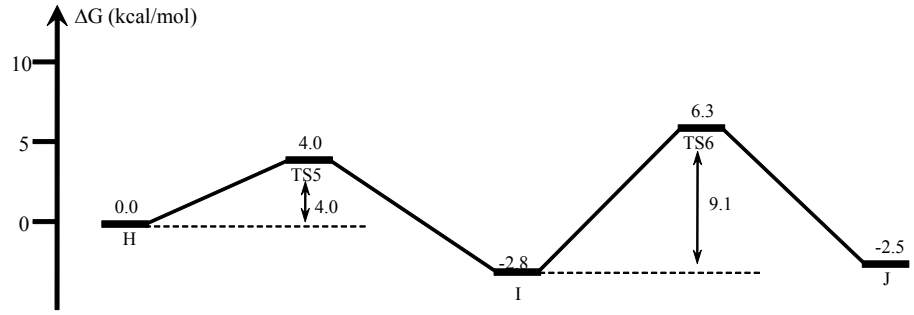


octet/Mn1-Mn4(αβαα) surface

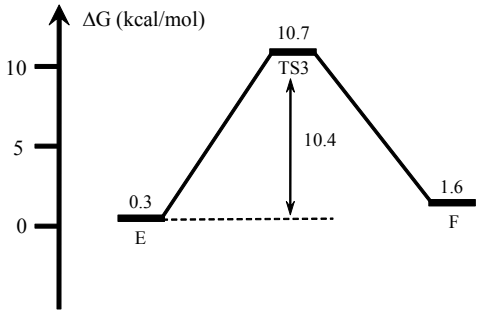


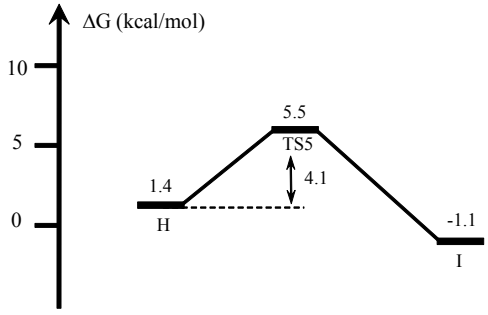
14-et/Mn1-Mn4(αααα) surface



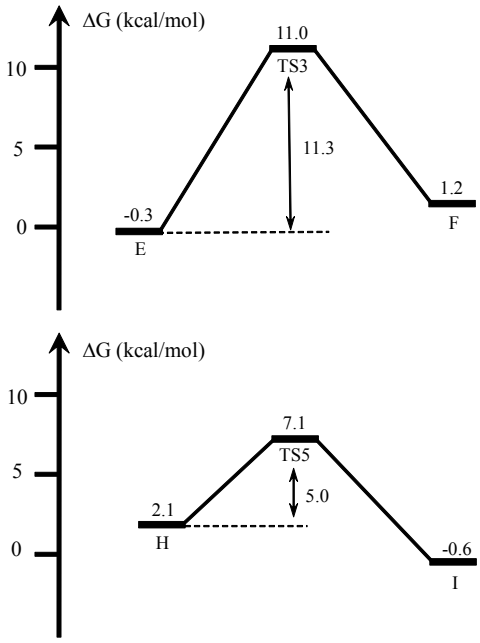


doublet/Mn1-Mn4(βαβα) surface

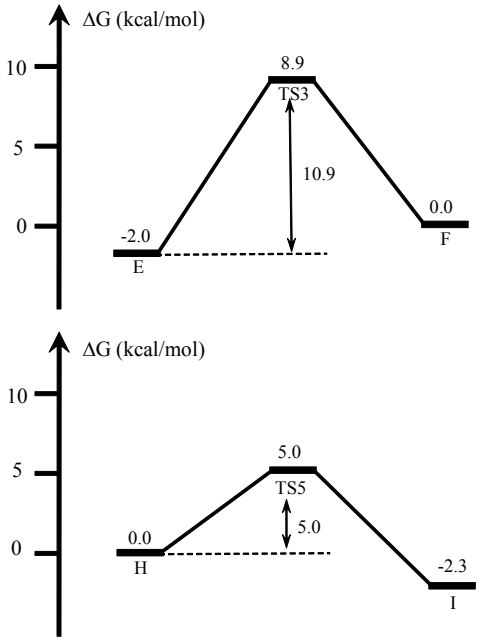




doublet/Mn1-Mn4(ββαα) surface



sextet/Mn1-Mn4(αααβ) surface



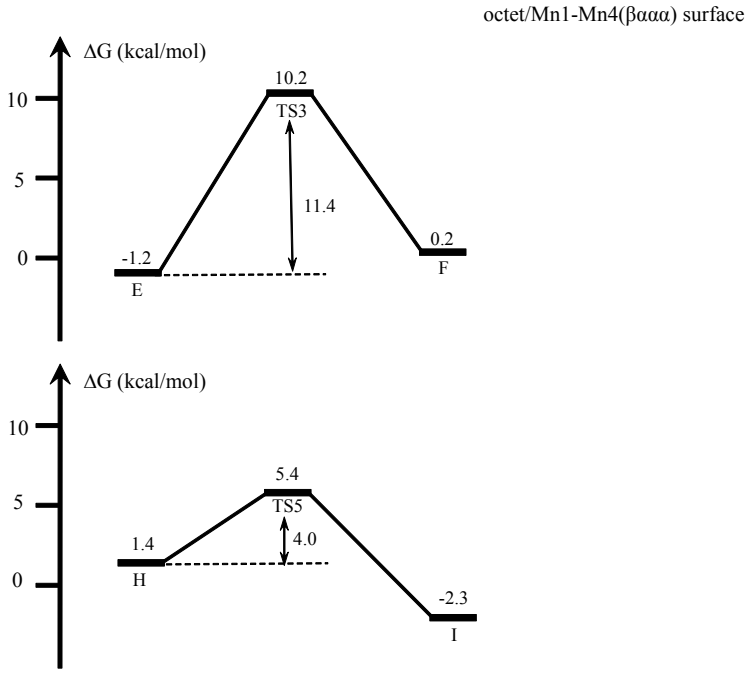


Figure SIVb. Free energy profiles for the W1 substitution scheme with the closed-cubane structure as reactant for all spin states.

The Cartesian coordinates for E to J and TS3 to TS6:

E:

Ca	-2.60171000	-0.37507700	-1.11903100	O	0.28237700	4.89043600	-2.03420800	H	-0.66750000	-5.38630400	-2.15561000
Mn	0.22942600	-1.77231900	0.04621900	H	-0.54648700	5.22162000	-2.42778500	C	-2.02060900	-4.93931400	-3.80722100
Mn	-1.37983200	-0.91615800	2.03338300	H	0.22240800	5.14539600	-1.05068300	H	-2.18143200	-4.12144400	-4.52346100
Mn	-0.03355700	1.00979400	0.59666400	O	-3.37434800	1.81917700	-1.53817300	H	-2.93067100	-4.98637800	-3.19265700
Mn	-0.27912600	2.70617400	-2.04079900	C	-3.19680800	2.95989200	-2.00051500	C	-1.83364000	-6.26281400	-4.55734000
O	-1.50208800	-1.92945700	0.52365500	O	-2.04964500	3.46342000	-2.32144100	H	-0.94777100	-6.23211200	-5.20736000
O	0.42425100	-0.67014800	1.51485300	C	-4.41209100	3.85391300	-2.23964000	H	-1.70278300	-7.10249200	-3.86034200
O	-1.73530400	0.55734700	1.07162000	H	-5.03897600	3.32528200	-2.97291400	H	-2.70259100	-6.48657300	-5.18945200
O	-0.06058800	-0.19824900	-0.83616500	H	-4.99059700	3.85123200	-1.30510900	N	2.29249200	-1.79513100	-0.21738700
O	-0.52008200	2.45826500	-0.25999600	C	-4.11839600	5.27967900	-2.70651000	C	3.06135300	-1.83118700	-1.35849100
O	-4.58091000	-1.65232800	-2.01449500	H	-3.55877100	5.27916000	-3.64924700	H	2.60261100	-1.89092000	-2.33604000
H	-4.93913700	-1.84683600	-1.12516100	H	-3.52340200	5.82722200	-1.96420600	C	4.39388000	-1.78925500	-1.01333000
H	-4.06572400	-2.43699300	-2.28590600	H	-5.05344300	5.83321800	-2.86313100	N	4.40311900	-1.75023100	0.37620600
O	-1.91657400	0.02706300	-3.48114300	O	0.11344500	-2.98070700	-1.46171200	H	5.22805300	-1.53696000	0.94314700
H	-1.43737700	-0.77661600	-3.74125400	C	-0.93580100	-3.27788400	-2.16049300	C	3.12437100	-1.73356600	0.81112100
H	-1.32889600	0.79757400	-3.73053600	O	-1.95882100	-2.56840400	-2.25550800	H	2.82549300	-1.64740700	1.84549700
O	-0.25732800	2.15311300	-3.82414500	C	-0.82615000	-4.60183800	-2.91159300	C	5.63414800	-1.77725300	-1.87109800
H	0.65549300	1.88308900	-4.03177400	H	0.10665600	-4.57329800	-3.49555900	H	5.80600500	-2.77342200	-2.30553400

H	5.44716100	-1.11125600	-2.72542200	C	2.33348700	1.92248300	-0.89904600	H	-6.36918200	-1.55992600	1.98039000
C	6.94822300	-1.35189100	-1.16178200	O	1.61638900	2.21686000	-1.91658900	O	-0.95568900	0.27278600	3.58897900
H	7.31072100	-2.15892900	-0.51580100	O	0.57912600	-3.33766500	1.33922500	C	-0.32581200	1.37298200	3.47045600
H	7.71502700	-1.17915200	-1.92941900	C	0.01338600	-3.42661500	2.47872700	O	0.15670000	1.87061400	2.39899300
C	6.78497200	-0.12725800	-0.26156500	O	-0.76303900	-2.57285300	3.01288700	C	-0.13772500	2.19784000	4.73507900
O	6.68734700	-0.24780200	0.96711900	C	0.29122200	-4.70632300	3.26239400	H	-0.49788800	1.61294000	5.58906600
N	6.67455300	1.07708900	-0.87833400	H	1.33943200	-4.98033600	3.08510900	H	0.94063800	2.37158000	4.86613300
H	6.71478200	1.10669100	-1.88985000	H	-0.30858900	-5.49462900	2.78041900	C	-0.86724900	3.55227000	4.65529100
C	6.19889500	2.26802400	-0.16348400	C	-0.02986900	-4.62731700	4.75569700	H	-1.94095600	3.37259400	4.49657500
H	6.76173400	2.33842800	0.77317600	H	0.17436700	-5.59036400	5.24101500	H	-0.50634300	4.09600100	3.77167900
H	6.45577100	3.13907200	-0.77920600	H	0.57670200	-3.85930600	5.25175800	C	-0.66516800	4.39766800	5.91689000
C	4.68928200	2.22774200	0.13881200	H	-1.08203100	-4.37036700	4.91794700	H	-1.04147800	3.87883300	6.80923100
H	4.47986500	1.38869100	0.81045300	O	-4.27350300	-1.06392600	0.63209100	H	-1.19528700	5.35613000	5.84071500
H	4.42667800	3.14230700	0.68965700	C	-4.23318300	-1.25540700	1.86372900	H	0.39923100	4.61548000	6.08381900
C	3.83263000	2.11257500	-1.12391500	O	-3.16892200	-1.20267800	2.60325300	N	-0.01493100	5.18330000	0.66057500
H	4.14990300	1.23885700	-1.71422700	C	-5.49628400	-1.58992000	2.63813600	H	-0.26898900	4.18858300	0.73355200
H	3.95425800	2.98775000	-1.77601300	H	-5.62355200	-0.87748100	3.46202700	H	-0.78535700	5.73233000	1.04358600
O	1.93558400	1.47317600	0.20961000	H	-5.39936600	-2.58776800	3.08474200	H	0.79699500	5.33862900	1.25899400

TS3:

Ca	-2.71533600	0.10097500	-0.90412600	H	-1.45421500	-4.82859200	-2.93049300	C	2.49646400	1.86169300	-0.59400800
Mn	-0.00528600	-1.77436900	-0.22895900	C	-2.83656600	-3.95652300	-4.37455400	O	1.79389400	2.47264500	-1.47644000
Mn	-1.38458700	-1.12976700	1.99860400	H	-2.94021400	-3.01318700	-4.92898600	O	0.24131100	-3.57446300	0.74479900
Mn	0.08294500	0.87469100	0.81416700	H	-3.70969900	-4.01345300	-3.70947600	C	-0.26634900	-3.80973200	1.89095700
Mn	-0.04533900	3.08845500	-1.44394700	C	-2.84947700	-5.13976400	-5.34874500	O	-0.90863000	-2.99183000	2.62253700
O	-1.71114100	-1.83494200	0.34836100	H	-2.00402600	-5.08998200	-6.04944700	C	-0.09487900	-5.23185800	2.41737400
O	0.40073400	-0.98090500	1.38893600	H	-2.77961700	-6.09787500	-4.81477100	H	0.89587500	-5.58373100	2.10162500
O	-1.62499300	0.52173200	1.33240100	H	-3.77290000	-5.15528200	-5.94187300	H	-0.82106900	-5.84989400	1.86573600
O	-0.15583400	-0.04696000	-0.80181500	N	2.02167700	-1.95856600	-0.66250400	C	-0.29850100	-5.38650800	3.92544700
O	-0.28331600	2.48658800	0.24421200	C	2.71365600	-1.79222600	-1.84067100	H	-0.18298000	-6.43747000	4.22010900
O	-4.88856300	-0.78367900	-1.83339600	H	2.19489000	-1.57078700	-2.76349200	H	0.43264000	-4.79193000	4.48747600
H	-5.20743400	-1.08821000	-0.95994300	C	4.06041400	-1.96199800	-1.60813200	H	-1.29625400	-5.04740400	4.22342200
H	-4.48488900	-1.55980000	-2.26884700	N	4.15545800	-2.25846000	-0.25345100	O	-4.35347800	-0.69665200	0.83235300
O	-2.22020800	0.81933100	-3.22532600	H	5.03118200	-2.26451400	0.27640400	C	-4.26371400	-1.11939300	2.00261600
H	-1.92325900	0.01526900	-3.68201900	C	2.91425000	-2.22509700	0.27854200	O	-3.15929300	-1.32814600	2.64852900
H	-1.49851000	1.50405700	-3.35244000	H	2.68912100	-2.36407900	1.32562900	C	-5.51042600	-1.44355900	2.80738200
O	-0.23019100	2.63058300	-3.30168300	C	5.24207500	-1.86697700	-2.54044100	H	-5.50877200	-0.86149000	3.73697600
H	0.60115700	2.19225400	-3.55896700	H	5.26949100	-2.74010000	-3.20941100	H	-5.50166700	-2.50403400	3.08926200
O	0.68572000	5.08407300	-2.65327100	H	5.08715900	-0.99804000	-3.19570800	H	-6.41055500	-1.21810200	2.22909300
H	0.20338200	4.60755300	-3.36379800	C	6.63620100	-1.76190300	-1.86484200	O	-0.74248000	-0.29798500	3.69414600
H	0.00506200	5.57670400	-2.15934400	H	6.93319500	-2.73209100	-1.45180200	C	0.01438300	0.72808300	3.72131900
O	-3.18297300	2.42587800	-0.90386500	H	7.37358000	-1.49537600	-2.63447500	O	0.47893800	1.36255100	2.71978500
C	-2.90977500	3.59258400	-1.22800500	C	6.67354100	-0.77255100	-0.70045300	C	0.42468400	1.22267600	5.10238900
O	-1.72949600	4.02459200	-1.54680000	O	6.61964000	-1.16572600	0.47261100	H	-0.28816700	0.81592400	5.82990200
C	-4.03308900	4.62693600	-1.27465300	N	6.68874900	0.54767100	-1.01764300	H	1.40127800	0.76174500	5.32515400
H	-4.79390200	4.22188700	-1.95725400	H	6.68624400	0.80858000	-1.99621800	C	0.53596100	2.74900400	5.21843200
H	-4.50057400	4.61890500	-0.27931900	C	6.39179400	1.58186600	-0.01882600	H	-0.43656700	3.20077600	4.97258500
C	-3.63277600	6.04492900	-1.68169800	H	6.98644600	1.35968300	0.87322400	H	1.24477200	3.11234600	4.46355200
H	-3.19592000	6.06096400	-2.68751200	H	6.73969000	2.53845300	-0.42848200	C	0.97524300	3.19456000	6.61729200
H	-2.89165000	6.46358100	-0.98950600	C	4.89869500	1.64585100	0.35334100	H	0.26472800	2.86062900	7.38627100
H	-4.50909600	6.70612600	-1.68092100	H	4.60270000	0.69714900	0.81331300	H	1.04503900	4.28836200	6.68105700
O	-0.35531100	-2.67317700	-1.90807100	H	4.76860400	2.41990900	1.12311700	H	1.96069300	2.78153700	6.87582100
C	-1.47446900	-2.73665600	-2.55635800	C	4.00027000	1.94514700	-0.84856500	N	0.37909900	5.20799300	0.35094800
O	-2.41705200	-1.92534300	-2.44308000	H	4.19662600	1.22002800	-1.65385000	H	0.15551400	4.38918100	0.92356000
C	-1.56209600	-3.91029100	-3.52824800	H	4.20511000	2.93758900	-1.27172300	H	-0.27233000	5.94900100	0.61342600
H	-0.66659800	-3.87725200	-4.16759300	O	2.07833600	1.19915400	0.38889000	H	1.31724300	5.52096200	0.60355700

F:

Ca	-2.61599900	-0.22839300	-0.97671000	Mn	0.39619300	-1.63022800	-0.52169700	Mn	-1.14606600	-1.76006700	1.68915500

Mn	-0.07347300	0.69878300	1.05898100	H	-2.06370500	-2.27126500	-5.59952400	O	1.33733200	2.90395600	-0.86218700
Mn	-0.61042200	3.18796800	-0.75290900	H	-2.65057400	-3.66002400	-4.70105600	O	0.96067400	-3.52563500	0.06726100
O	-1.27840400	-2.13940500	-0.09266300	C	-1.52791500	-4.18054000	-6.47968700	C	0.48030000	-4.09448800	1.10213700
O	0.58871800	-1.14628600	1.24896000	H	-0.68904900	-3.80569500	-7.08302800	O	-0.32620100	-3.58774800	1.94512700
O	-1.69094400	-0.07775700	1.36892200	H	-1.28076200	-5.20622100	-6.17175700	C	0.91106300	-5.54072900	1.32969100
O	-0.08800000	0.11757000	-0.73283700	H	-2.40979300	-4.23139600	-7.13112100	H	1.96048300	-5.62517600	1.01872000
O	-0.72497100	2.30511200	0.79432500	N	2.44017400	-1.35264300	-0.81643100	H	0.33676200	-6.14581600	0.61019900
O	-4.52302600	-1.27444600	-2.24655200	C	3.16013900	-0.91894900	-1.90652500	C	0.69740300	-6.05781000	2.75327300
H	-4.80754300	-1.82609000	-1.49014300	H	2.66587800	-0.66821600	-2.83530800	H	1.00807900	-7.10784300	2.82813700
H	-3.96429100	-1.84155200	-2.81265500	C	4.50018700	-0.89257900	-1.58886700	H	1.28089200	-5.47654100	3.47823900
O	-2.18249700	1.12333700	-3.03063300	N	4.56603600	-1.34885300	-0.27741800	H	-0.35580500	-5.98326500	3.04399000
H	-1.72067000	0.49206400	-3.60751000	H	5.39714100	-1.28818100	0.31621400	O	-4.10416900	-1.69964700	0.41257800
H	-1.62861100	1.95334000	-3.01562600	C	3.30930700	-1.59227000	0.15353000	C	-3.96411100	-2.32276100	1.48405700
O	-0.60895500	3.32412200	-2.66465200	H	3.04949600	-1.90334000	1.15476800	O	-2.86133100	-2.42919700	2.15768100
H	0.30592900	3.16816200	-2.96036800	C	5.69871300	-0.47258500	-2.40200700	C	-5.13804000	-3.04730000	2.11914300
O	-1.57367300	5.90113000	-2.69491100	H	5.93126100	-1.23499900	-3.16047700	H	-5.29425200	-2.66995100	3.13709200
H	-1.18643200	5.01365600	-2.91048800	H	5.42375500	0.42985200	-2.96627600	H	-4.91014400	-4.11746700	2.20176600
H	-2.40026100	5.63425400	-2.25312800	C	7.00348400	-0.20617900	-1.60287700	H	-6.04517100	-2.90262800	1.52616400
O	-3.61465900	1.84331000	-0.43742600	H	7.46226300	-1.15265200	-1.29696900	O	-0.72944100	-1.20869900	3.56032500
C	-3.54908200	3.08098800	-0.49680100	H	7.71712700	0.30283100	-2.26524600	C	-0.20147800	-0.08491000	3.85009100
O	-2.47655200	3.76142700	-0.76077700	C	6.78052100	0.59099200	-0.31758200	O	0.16796300	0.82167200	3.03335000
C	-4.80744700	3.90171400	-0.21874000	O	6.75957000	0.02890000	0.78542600	C	-0.00455900	0.22263900	5.32596000
H	-5.65720600	3.32011700	-0.59652500	N	6.53057500	1.91867800	-0.45359700	H	-0.24501100	-0.67663000	5.90463900
H	-4.91838900	3.92142000	0.87706700	H	6.51633500	2.31465300	-1.38556900	H	1.05801800	0.46069600	5.48136600
C	-4.81622500	5.32679100	-0.77475900	C	5.99799800	2.71986900	0.65530800	C	-0.86664100	1.41527700	5.78304300
H	-4.73770200	5.32741800	-1.87042700	H	6.60460400	2.50409600	1.54104200	H	-1.92607700	1.18369800	5.59862000
H	-3.98412400	5.91611300	-0.37141400	H	6.14693900	3.77475800	0.39233300	H	-0.62219300	2.28549900	5.15989700
H	-5.75114900	5.83797900	-0.51175200	C	4.51627900	2.42781900	0.95782100	C	-0.65962300	1.74745600	7.26418300
O	0.29620300	-2.18678300	-2.37591600	H	4.41428600	1.38991600	1.29112600	H	-0.92060500	0.89451100	7.90598300
C	-0.75773700	-2.28857500	-3.11923700	H	4.20876200	3.05878800	1.80395700	H	-1.28395600	2.59754800	7.56878800
O	-1.84297300	-1.70433900	-2.91164700	C	3.60333100	2.67947200	-0.24449500	H	0.38757500	2.01045700	7.47027400
C	-0.57577700	-3.19426700	-4.33427000	H	3.94500700	2.08255500	-1.10433700	N	-0.20354500	5.35733100	-0.22590500
H	0.31320400	-2.84034400	-4.87885700	H	3.63890500	3.72995900	-0.56395000	H	0.77645200	5.62306000	-0.13217600
H	-0.30104200	-4.18974200	-3.95288500	O	1.83257400	1.44777300	0.81375100	H	-0.69999600	5.63832400	0.62002000
C	-1.78707900	-3.28122000	-5.26589500	C	2.13331200	2.30618800	-0.05478500	H	-0.61897900	5.84299300	-1.04272000

TS4:

Ca	2.79812100	-0.03961500	-1.05579200	C	2.84858800	-2.94580300	-1.45577500	N	-2.09009200	1.79553700	-0.25495300
Mn	-0.04029800	1.54223800	0.02579700	O	1.90567500	-2.28143800	-2.08918800	C	-2.87445900	1.90158700	-1.38242400
Mn	1.42880500	0.52116700	2.07513500	C	2.77163500	-4.45837700	-1.41483200	H	-2.43666200	1.86843100	-2.37093200
Mn	-0.12065200	-1.28633400	0.73001000	H	3.52698200	-4.81171300	-0.70492300	C	-4.19221200	2.05450800	-1.01162700
Mn	-0.02978400	-2.09580400	-1.89967900	H	1.78457600	-4.73338700	-1.02047100	N	-4.17302900	2.06485900	0.37814600
O	1.68705900	1.46121300	0.53837300	C	3.00748200	-5.08549700	-2.80092100	H	-5.00574700	2.00228900	0.97024900
O	-0.36917500	0.47357700	1.51849300	H	4.01328200	-4.84443700	-3.16822600	C	-2.90015900	1.88596900	0.79004400
O	1.61873600	-1.03079700	1.15925900	H	2.28260000	-4.71803800	-3.53717400	H	-2.59221000	1.79784500	1.82140500
O	0.10380800	-0.28314200	-0.86436200	H	2.92224800	-6.17853200	-2.74997600	C	-5.44463000	2.17190400	-1.84453400
O	0.03389900	-2.77117100	-0.22682000	O	0.24285300	2.69506700	-1.49982300	H	-5.48354000	3.15564600	-2.33551900
O	4.89560900	1.17478100	-1.76545600	C	1.37060100	3.08598900	-2.00948400	H	-5.37741700	1.43794000	-2.66024800
H	5.23298800	1.23539300	-0.84851400	O	2.41276100	2.40111300	-2.03048800	C	-6.78874700	1.98161800	-1.08975800
H	4.46113800	2.02991000	-1.95139600	C	1.32850800	4.48009600	-2.62587500	H	-7.01539800	2.86741900	-0.48651300
O	2.35498900	0.06801000	-3.52164800	H	0.45764100	4.52045900	-3.29773300	H	-7.59025100	1.88009300	-1.83434600
H	2.23837700	1.01779800	-3.69187500	H	1.09347600	5.17962500	-1.80832700	C	-6.78346100	0.79821500	-0.12175400
H	1.46975400	-0.36304400	-3.67469800	C	2.60562100	4.90405300	-3.35539900	O	-6.63909600	0.97233900	1.09582500
O	-0.01015000	-1.28089000	-3.64116700	H	2.83378900	4.17431100	-4.14544400	N	-6.86051200	-0.44351100	-0.66588700
H	-0.84840600	-0.80177200	-3.76183700	H	3.45076000	4.86464800	-2.65443700	H	-6.93403000	-0.52506900	-1.67263900
O	0.62080700	-3.31703100	-5.31507700	C	2.49541000	6.30818900	-3.95979300	C	-6.52084900	-1.64359700	0.11057500
H	0.37196400	-2.47687700	-4.84028200	H	1.67628500	6.36618100	-4.69045000	H	-7.06461300	-1.58970600	1.05937800
H	1.59281200	-3.30098900	-5.29956300	H	2.30051700	7.06242000	-3.18447600	H	-6.90001500	-2.50870400	-0.44774700
O	3.80768100	-2.33061600	-0.96460200	H	3.42196000	6.59185600	-4.47526100	C	-5.00999000	-1.77076800	0.38331800

H	-4.68568700	-0.91606500	0.98593100	C	0.44504500	4.31275400	4.81713100	C	-0.18362300	-2.35713800	4.85391900
H	-4.84010700	-2.66488200	0.99877500	H	0.38555000	5.28551100	5.32208300	H	0.23669200	-1.79909100	5.69838500
C	-4.18107900	-1.84794500	-0.89986900	H	-0.32689700	3.65984700	5.24405700	H	-1.27560500	-2.40307900	4.97887200
H	-4.47528000	-1.04815700	-1.59539000	H	1.41771600	3.86155600	5.03922700	C	0.38461400	-3.78871600	4.80423700
H	-4.36082000	-2.79140000	-1.43592200	O	4.39987700	0.47818600	0.80178300	H	1.47255500	-3.73779300	4.64977000
O	-2.18819500	-1.40962600	0.38634300	C	4.31659200	0.59338500	2.04008000	H	-0.03368300	-4.30361500	3.92948900
C	-2.66759000	-1.70570600	-0.73685700	O	3.21436100	0.59531500	2.72131800	C	0.07964400	-4.57812800	6.08123800
O	-2.01273300	-1.89305000	-1.82457400	C	5.56397900	0.74026700	2.89318400	H	0.50957800	-4.08910300	6.96638300
O	-0.21494400	3.18487000	1.36535100	H	6.45713500	0.78124100	2.26390800	H	0.49482800	-5.59283900	6.02587100
C	0.35469600	3.19121600	2.50056000	H	5.63574500	-0.11415800	3.57789900	H	-1.00368700	-4.66811400	6.24410800
O	1.02020600	2.23842800	3.02599800	H	5.49120100	1.64487500	3.50903300	N	-0.48572300	-4.06817700	-2.78947500
C	0.25252900	4.48320100	3.30870000	O	0.85171400	-0.56290500	3.66680300	H	-1.50200900	-4.13833300	-2.84802600
H	-0.71320500	4.94683800	3.07072200	C	0.10558500	-1.58686900	3.57680700	H	-0.13906800	-4.84891600	-2.23286900
H	1.02138000	5.15855600	2.90018300	O	-0.42521700	-2.05181400	2.50957400	H	-0.08447300	-4.09298500	-3.74370300

G:

Ca	2.68782300	0.02406700	-1.08345400	H	1.14499500	5.17248700	-2.59530500	C	-2.51442100	-1.96633900	-0.76908300
Mn	-0.18315800	1.98727600	-0.05171300	C	2.50304700	4.44576800	-4.14001300	O	-1.77420800	-2.47504700	-1.69314900
Mn	1.32910000	0.85358900	1.92625600	H	2.59916300	3.55927100	-4.78240900	O	-0.40577500	3.56603700	1.37620200
Mn	-0.06808700	-1.19728400	0.74176200	H	3.38982300	4.44619800	-3.49028800	C	0.20675900	3.51796000	2.48268200
Mn	0.18112400	-2.52439800	-1.58577700	C	2.49246900	5.71499300	-4.99920800	O	0.90068300	2.53647400	2.91102700
O	1.56345600	1.73456300	0.35566600	H	1.63338400	5.72616600	-5.68485000	C	0.12600800	4.74871100	3.38228800
O	-0.42293300	0.65385000	1.28058800	H	2.43005300	6.61857100	-4.37670600	H	-0.90452900	5.12430700	3.32609900
O	1.62828200	-0.77064100	1.15675500	H	3.40383200	5.79046600	-5.60606900	H	0.74839200	5.51930000	2.90048800
O	0.23081800	-0.78581500	-1.03679100	N	-2.22947000	2.02943300	-0.36996500	C	0.56880200	4.52844700	4.82938700
O	0.16424400	-2.89077400	0.16696300	C	-3.01251700	2.10637200	-1.50185200	H	0.49885600	5.46515300	5.39760900
O	4.69110100	1.24454900	-2.00990300	H	-2.56446700	2.21779000	-2.48020700	H	-0.05973600	3.77903900	5.32635800
H	5.02574800	1.47070600	-1.11788800	C	-4.34053400	2.02860800	-1.14614500	H	1.60249800	4.16910900	4.87366300
H	4.19300700	2.02357800	-2.32530900	N	-4.33397900	1.92942900	0.24036700	O	4.29596600	0.85785000	0.63692700
O	2.27173300	-0.36584100	-3.49716900	H	-5.15681100	1.72138400	0.81385700	C	4.21707800	1.05613400	1.86655700
H	1.99026300	0.51475200	-3.79975700	C	-3.05377200	1.91301200	0.66341800	O	3.12849800	1.02958400	2.56398600
H	1.48718700	-0.97392800	-3.60037600	H	-2.74372300	1.78559900	1.69041000	C	5.46311700	1.35794900	2.68194600
O	0.20790700	-2.12125600	-3.48020500	C	-5.58905600	2.01326600	-1.99325300	H	6.35179200	1.34417200	2.04503600
H	-0.67846600	-1.80164900	-3.72319200	H	-5.72933800	2.99201100	-2.47508400	H	5.56672700	0.61288200	3.48020000
O	1.31691000	-4.36036800	-4.49616800	H	-5.43607800	1.29918200	-2.81549600	H	5.36119100	2.33826000	3.16422100
H	0.88916800	-3.47538400	-4.32870600	C	-6.90956200	1.66908300	-1.25586800	O	0.80274400	-0.11209800	3.61500700
H	2.24414800	-4.18923200	-4.25552900	H	-7.21388600	2.50063100	-0.61089800	C	0.05849500	-1.13802600	3.62702000
O	3.86858400	-2.13154200	-0.59994500	H	-7.69813500	1.53456200	-2.00902500	O	-0.45292600	-1.71236200	2.60615300
C	3.02726100	-2.99147300	-0.88685300	C	-6.80726900	0.44218100	-0.34858800	C	-0.26312500	-1.75741200	4.97792900
O	2.07475000	-2.71417600	-1.76022500	O	-6.68667900	0.56304800	0.87825600	H	0.21885700	-1.15583500	5.75707800
C	3.10282600	-4.39856600	-0.32843000	N	-6.77868400	-0.77173600	-0.95460600	H	-1.35251000	-1.69162700	5.12225000
H	3.83771700	-4.39570000	0.48345300	H	-6.85470100	-0.81432500	-1.96342700	C	0.17339000	-3.23108400	5.06798800
H	2.12307400	-4.63568500	0.10750800	C	-6.42021000	-1.99240000	-0.22150400	H	1.25891100	-3.29491200	4.90077800
C	3.49560900	-5.43139700	-1.40047300	H	-7.02156300	-2.02130900	0.69358500	H	-0.30303100	-3.79007700	4.25217200
H	4.49465200	-5.21595700	-1.80069400	H	-6.71771100	-2.84254600	-0.84802800	C	-0.17884200	-3.85977600	6.41996200
H	2.79025100	-5.43204900	-2.24051500	C	-4.92616500	-2.06921200	0.14294000	H	0.30701400	-3.32600800	7.24856600
H	3.51754400	-6.44131200	-0.97186600	H	-4.67878800	-1.25044100	0.82611300	H	0.14355800	-4.90830300	6.46416600
O	0.09310700	2.94811200	-1.71616600	H	-4.75905000	-3.00287700	0.69881200	H	-1.26308100	-3.83531900	6.59956700
C	1.17683500	3.05429800	-2.41806200	C	-4.00821700	-2.01672000	-1.08129500	N	-0.05518200	-4.56048300	-2.03590200
O	2.09909200	2.21213700	-2.43646000	H	-4.21684500	-1.10503300	-1.66333400	H	-1.05005400	-4.74011200	-2.17657300
C	1.24619800	4.31380700	-3.27661600	H	-4.18371900	-2.86570600	-1.75511300	H	0.27824000	-5.13655600	-1.26298200
H	0.33916600	4.33494000	-3.90071900	O	-2.12146600	-1.42581400	0.29073800	H	0.47098200	-4.75891500	-2.91097000

H:

Ca	-2.80042500	0.16446000	-0.59192700	O	-1.59767600	-1.96314900	-0.07355800	O	-4.97587500	-0.54495300	-1.65165900
Mn	0.05302300	-1.59705700	-0.69643800	O	0.54041500	-1.31636300	1.06047800	H	-5.21348900	-1.13292700	-0.90637300
Mn	-1.18156200	-1.77704100	1.69579300	O	-1.55658600	-0.02360500	1.59812900	H	-4.56162100	-1.10979100	-2.33290100
Mn	0.08977600	0.59987900	1.12257700	O	-0.24033600	0.20537700	-0.68900700	O	-2.48765400	1.64432000	-2.58127200
Mn	-0.37574900	3.27948200	-0.39774300	O	-0.38822900	2.28518600	1.08715300	H	-2.16701100	1.02282900	-3.25614100

H	-1.84471000	2.40943500	-2.56940300	H	2.05112000	-0.55053400	-3.19719000	C	0.34902800	-5.70193300	0.72733300
O	-0.63915700	3.61711000	-2.25882600	C	4.01372200	-1.10161900	-2.29571100	H	1.33469500	-5.86229900	0.27126700
H	0.19717600	3.37141300	-2.69462600	N	4.22220500	-1.74034400	-1.07884500	H	-0.37623100	-6.16903500	0.04221400
O	0.40456900	5.28050800	0.29856500	H	5.13311300	-1.82808100	-0.62039800	C	0.25681600	-6.33521400	2.11651700
H	-0.00869200	5.88961600	-0.41358300	C	3.02275300	-1.93699900	-0.48928000	H	0.45123200	-7.41388200	2.05766900
H	-0.12982900	5.43425200	1.09814500	H	2.88110500	-2.36280000	0.49320000	H	0.98932400	-5.89304600	2.80338500
O	-3.44509700	2.28606000	0.22596600	C	5.11719300	-0.67401900	-3.23061900	H	-0.73609300	-6.18218500	2.55249600
C	-3.22169100	3.50578400	0.29264400	H	5.14478700	-1.33146800	-4.11248500	O	-4.25579100	-1.26392900	0.87478100
O	-2.11088300	4.08355500	-0.03827300	H	4.86558000	0.32471500	-3.61503500	C	-4.04937700	-2.00599500	1.85635900
C	-4.31561600	4.43049000	0.82461100	C	6.54877200	-0.65003800	-2.62987000	O	-2.88785500	-2.30140300	2.34969300
H	-5.27629100	4.00325800	0.51211400	H	6.93225400	-1.67013200	-2.51873800	C	-5.20728300	-2.65908100	2.59098100
H	-4.28576700	4.33746800	1.92185200	H	7.21039300	-0.12760700	-3.33450700	H	-6.16136400	-2.35701500	2.15054100
C	-4.19928400	5.90055600	0.41685000	C	6.61436800	-0.01668600	-1.24006600	H	-5.17802300	-2.37210700	3.64919900
H	-4.25565000	6.01222800	-0.67435800	O	6.68113500	-0.71953800	-0.22266300	H	-5.10276200	-3.75053400	2.54832500
H	-3.24773000	6.32888900	0.75277500	N	6.51669600	1.33600800	-1.17692000	O	-0.45319100	-1.46910400	3.52378700
H	-5.01481200	6.48954400	0.85607800	H	6.41381900	1.85201700	-2.04225100	C	0.23679800	-0.44078600	3.83056300
O	-0.36808000	-1.95754900	-2.55635300	C	6.23045900	2.02847700	0.08645300	O	0.59873200	0.49758500	3.04985900
C	-1.52028400	-1.87935100	-3.13823500	H	6.91462300	1.63066700	0.84306300	C	0.64814400	-0.31476900	5.29079600
O	-2.48769000	-1.20098200	-2.72988600	H	6.47070800	3.08857500	-0.06324500	H	-0.07938800	0.36653900	5.76166800
C	-1.62216400	-2.69022200	-4.42755000	C	4.77461900	1.84706700	0.55389400	H	0.52025900	-1.29517200	5.76518300
H	-0.77450200	-2.40044300	-5.06738400	H	4.59088100	0.78462100	0.74503700	C	2.06921800	0.22886700	5.49718000
H	-1.43316600	-3.74120700	-4.15963300	H	4.65414700	2.36200000	1.51723600	H	2.15773000	1.19423100	4.98348500
C	-2.94756100	-2.54847000	-5.17978700	C	3.75496400	2.38057200	-0.45428200	H	2.78869600	-0.44811100	5.01212100
H	-3.13125600	-1.48701400	-5.39779400	H	3.94354200	1.95006200	-1.45004700	C	2.42269500	0.38089900	6.98043100
H	-3.77035700	-2.86905700	-4.52536800	H	3.83455300	3.47005700	-0.57039600	H	1.73825000	1.07925900	7.48250300
C	-2.97302400	-3.36132800	-6.47901200	O	2.01645200	1.17011400	0.68538700	H	3.44318100	0.76559300	7.10678700
H	-2.17992400	-3.03837200	-7.16820000	C	2.29091500	2.07061400	-0.14978500	H	2.36072100	-0.58075700	7.50892400
H	-2.82412400	-4.43253800	-6.28334300	O	1.46063500	2.76635100	-0.83404500	N	-0.85963700	6.48380800	-1.74651300
H	-3.93279500	-3.24781800	-6.99932700	O	0.46629200	-3.58799500	-0.35568100	H	-0.90481600	5.56657100	-2.21712700
N	2.05145800	-1.49337100	-1.27245200	C	0.06316000	-4.20322300	0.68617700	H	-0.49155400	7.17675400	-2.39813900
C	2.64650500	-0.97217500	-2.39882400	O	-0.56028700	-3.70187100	1.67436400	H	-1.81749000	6.74555900	-1.51248200

TS5:

Ca	-2.73919800	0.88202200	-0.59161900	H	-2.94629400	5.44946800	1.31135100	C	4.56689500	-1.80403400	-3.28991500
Mn	-0.45609100	-1.57323800	-0.57134700	C	-1.97182600	6.85111300	-0.03947600	H	4.38448000	-2.36215400	-4.22041800
Mn	-1.60123300	-1.20962100	1.84815600	H	-1.77330000	6.97268500	-1.11194000	H	4.56949400	-0.74278700	-3.57633700
Mn	0.24578000	0.66157300	1.04906400	H	-1.01118800	6.87146600	0.48976600	C	5.97920500	-2.20346100	-2.78391700
Mn	0.47262800	2.98235500	-0.89022700	H	-2.56023400	7.71562600	0.29415300	H	6.07704400	-3.29413200	-2.74854700
O	-2.11774300	-1.42995800	0.11097300	O	-1.05832400	-1.96923700	-2.37091900	H	6.72053700	-1.83193700	-3.50467500
O	0.15585500	-1.28915900	1.14802200	C	-2.18907600	-1.66980600	-2.92247100	C	6.27659000	-1.69599300	-1.37365100
O	-1.49319500	0.56635000	1.59105700	O	-2.93247100	-0.72806600	-2.56993100	O	6.15481200	-2.43996300	-0.39057100
O	-0.25685500	0.24592200	-0.72213000	C	-2.56374500	-2.56571700	-4.09939300	N	6.59679400	-0.38238300	-1.25044900
O	0.27551900	2.40228100	0.79666700	H	-1.70801500	-2.57609500	-4.79167000	H	6.63093600	0.18211700	-2.09055100
O	-5.07413100	0.72481300	-1.51872600	H	-2.62914700	-3.59319000	-3.70922200	C	6.52599800	0.30531500	0.04676600
H	-5.43654200	0.30568400	-0.71221900	C	-3.85213500	-2.17536100	-4.82772000	H	7.06422900	-0.30946600	0.77530300
H	-4.88244500	0.00104000	-2.14641100	H	-3.77502200	-1.13465000	-5.17286400	H	7.06336800	1.25596100	-0.05763100
O	-2.15603600	1.97356800	-2.77340900	H	-4.68983400	-2.19683400	-4.11652400	C	5.07570000	0.52309900	0.51429000
H	-2.14128800	1.20695100	-3.37133900	C	-4.15559700	-3.09784900	-6.01356400	H	4.59128800	-0.45508500	0.60667400
H	-1.29371500	2.45714900	-2.90780000	H	-3.34779600	-3.07019400	-6.75841600	H	5.09069400	0.95470100	1.52389300
O	0.29943400	3.16660500	-2.76111200	H	-4.26969800	-4.14159800	-5.68884400	C	4.27207000	1.42556600	-0.42716200
H	0.97654200	2.59087100	-3.16043500	H	-5.08428800	-2.80235500	-6.51842000	H	4.50792000	1.21955100	-1.48123200
O	2.62213100	4.27526200	0.71975800	N	1.46457000	-2.00676500	-1.23201100	H	4.49945700	2.48850200	-0.26021700
H	2.25724100	4.82311500	-0.02113600	C	2.13418000	-1.55033900	-2.34506800	O	2.25059900	0.63873100	0.60972900
H	1.85343200	3.98211700	1.24246600	H	1.64103900	-0.91799200	-3.07015600	C	2.76018900	1.33417700	-0.30506700
O	-2.62775100	3.18220100	-0.04390100	C	3.42775200	-2.02048300	-2.32514700	O	2.11513300	2.00699400	-1.19225000
C	-2.02507200	4.26032600	-0.17158500	N	3.51158900	-2.79299400	-1.17283500	O	-0.54745900	-3.55479100	-0.05239800
O	-0.82181200	4.38685400	-0.64119200	H	4.39265800	-3.12302900	-0.76703300	C	-1.06021000	-3.95364200	1.04757200
C	-2.72727200	5.55156000	0.23815900	C	2.32072700	-2.74084800	-0.53702600	O	-1.50838100	-3.22636300	1.98767500
H	-3.70547200	5.54661200	-0.26243900	H	2.11029400	-3.20910000	0.41302400	C	-1.15555900	-5.46608800	1.22472000

H	-0.25532700	-5.90806000	0.77801700	H	-6.52373800	-0.35312800	2.45479700	H	2.55091600	0.96541700	4.79669400
H	-1.99455500	-5.79441900	0.59081200	H	-5.51350000	-0.51019000	3.92682800	H	2.66006600	-0.77988300	4.99730600
C	-1.36035600	-5.93120500	2.66730600	H	-5.86904700	-1.94550800	2.96206700	C	2.63556100	0.31468600	6.86743500
H	-1.44179900	-7.02497800	2.70669200	O	-0.75187400	-0.95583200	3.63079800	H	2.21227400	1.23430500	7.29548600
H	-0.52056800	-5.62782600	3.30484200	C	0.18989100	-0.12100700	3.83728000	H	3.72844500	0.38340300	6.94496300
H	-2.27072800	-5.49737200	3.09431400	O	0.75797200	0.61688400	2.96765100	H	2.30827800	-0.52504700	7.49641400
O	-4.44997900	0.06549900	1.04712700	C	0.67033700	0.02243600	5.27346100	N	1.57596600	5.64624500	-1.60169800
C	-4.41247100	-0.62639300	2.08497900	H	0.20055300	0.93691900	5.67082400	H	1.24427500	5.05798600	-2.37475500
O	-3.35618600	-1.19709900	2.57362200	H	0.27260700	-0.82065500	5.85076200	H	2.30393300	6.26588600	-1.95966300
C	-5.66927400	-0.86833700	2.90184600	C	2.19669200	0.12846200	5.41125000	H	0.77674500	6.21521300	-1.32208600

I:

Ca	-2.73004800	-0.14451500	-0.97264800	H	-1.29791800	-5.31054000	-2.06355000	C	2.36667400	1.70769600	-1.11663300
Mn	0.03664000	-1.78000400	0.04684300	C	-2.71165700	-4.75216400	-3.62848700	O	1.61170600	2.09893100	-2.07130300
Mn	-1.36623500	-0.76267100	2.11606100	H	-2.84701200	-3.92508700	-4.33928900	O	0.32614900	-3.35448400	1.34045100
Mn	0.04078800	1.01869500	0.55906500	H	-3.58009400	-4.71787500	-2.95553800	C	-0.17032100	-3.37970600	2.51496800
Mn	-0.25135100	2.78303900	-2.05749000	C	-2.69054200	-6.08906700	-4.37783400	O	-0.83080500	-2.45330900	3.08285000
O	-1.66668000	-1.77883300	0.63012000	H	-1.84996900	-6.13792000	-5.08445800	C	0.04288100	-4.67045600	3.30053900
O	0.41752800	-0.67771800	1.47862000	H	-2.58803600	-6.93506200	-3.68374600	H	1.05239900	-5.03429600	3.06848000
O	-1.65579700	0.72086400	1.14914400	H	-3.61531100	-6.23752000	-4.95004900	H	-0.64769800	-5.40966300	2.86452900
O	-0.17122600	-0.19510500	-0.84505200	N	2.07592000	-1.98837800	-0.32436100	C	-0.18405200	-4.54962600	4.80821500
O	-0.40150200	2.50170700	-0.26812400	C	2.77998200	-2.17107400	-1.49282700	H	-0.03407500	-5.52174100	5.29521500
O	-4.85746700	-1.25705200	-1.73214800	H	2.26880600	-2.25453800	-2.44228300	H	0.51247000	-3.83103800	5.25795300
H	-5.17806100	-1.41414500	-0.82132800	C	4.12675000	-2.23158400	-1.21068400	H	-1.19976900	-4.20275500	5.02593200
H	-4.42894500	-2.08503000	-2.02441500	N	4.20909300	-2.10406600	0.17117100	O	-4.33996100	-0.68078100	0.88647600
O	-2.12904400	0.21393400	-3.36788200	H	5.07644700	-1.93756500	0.68743100	C	-4.24260300	-0.85643900	2.11698300
H	-1.68224000	-0.60060700	-3.65051000	C	2.96060200	-1.93943800	0.65981100	O	-3.13441200	-0.89068200	2.79132800
H	-1.54204800	0.96850200	-3.66113700	H	2.72212800	-1.75831500	1.69774500	C	-5.48073200	-1.05677300	2.97324000
O	-0.38017900	2.25937200	-3.84916200	C	5.31870800	-2.38789400	-2.12079600	H	-6.38463200	-0.99588600	2.36114400
H	0.48013300	1.87317500	-4.09511700	H	5.38624500	-3.42332900	-2.48675300	H	-5.51060200	-0.29166400	3.75859800
O	0.51902900	4.75405900	1.01474500	H	5.14426600	-1.77064100	-3.01351200	H	-5.43030000	-2.03233300	3.47295400
H	-0.02791400	3.98192600	0.72884300	C	6.69677600	-2.02734400	-1.50286100	O	-0.75271400	0.41251500	3.61187000
H	1.22600000	4.31079600	1.51389600	H	7.02842000	-2.81992800	-0.82338100	C	-0.05647000	1.46529300	3.43532900
O	-3.35198100	2.09910200	-1.35983800	H	7.43450300	-1.96430300	-2.31458100	O	0.42325000	1.88625900	2.33168400
C	-3.11769700	3.24294200	-1.78797200	C	6.67801100	-0.74168000	-0.67591700	C	0.20560400	2.29770000	4.68411500
O	-1.96346000	3.66582700	-2.19165600	O	6.64935000	-0.77959900	0.56130300	H	-0.78161400	2.62211000	5.04839900
C	-4.26611400	4.24510400	-1.88048300	N	6.61580100	0.42857500	-1.36161800	H	0.59152100	1.61377900	5.45413500
H	-4.98440800	3.82086500	-2.59798300	H	6.59767600	0.39614700	-2.37362300	C	1.13183300	3.50282400	4.49766200
H	-4.77613400	4.22351200	-0.90740700	C	6.29689400	1.69696800	-0.69559800	H	0.72416600	4.15253600	3.71184000
C	-3.88343100	5.67174500	-2.27428300	H	6.93440900	1.77534900	0.19139600	H	2.11103800	3.15363500	4.13810100
H	-3.39031000	5.69214700	-3.25323300	H	6.57716800	2.50293600	-1.38546800	C	1.31000000	4.29974300	5.79500900
H	-3.19539700	6.11337600	-1.54245000	C	4.81791400	1.81355000	-0.28177100	H	0.34823600	4.68682200	6.15940300
H	-4.77657900	6.30813500	-2.32582100	H	4.59118500	1.04825300	0.46771500	H	1.97744700	5.15802800	5.64393900
O	-0.26918500	-2.98520400	-1.43573700	H	4.68048700	2.78670900	0.21170300	H	1.74049500	3.67767600	6.59246100
C	-1.38000500	-3.18638200	-2.07212500	C	3.85506300	1.68389600	-1.46501100	N	0.60090200	4.88512800	-1.93029500
O	-2.33601900	-2.38529400	-2.11633800	H	4.01878700	0.72066800	-1.97297100	H	1.45575200	5.07497500	-2.45283900
C	-1.43631700	-4.51819200	-2.81519500	H	4.03182200	2.46657500	-2.21487500	H	0.76268000	5.05917100	-0.92448600
H	-0.54487800	-4.57434500	-3.45891200	O	2.01038200	1.31635200	0.02825100	H	-0.13001400	5.51857000	-2.25655000

TS6:

Ca	-2.95973500	0.59099900	-0.50471000	O	0.18641400	2.73494900	0.31077400	O	2.00537200	4.71432600	0.70659200
Mn	-0.31450700	-1.49380600	-0.35636300	O	-5.31588700	-0.06339600	-1.14267300	H	1.60290700	5.37135800	1.29886500
Mn	-1.31754500	-0.84521100	2.09302000	H	-5.54833500	-0.32272600	-0.22806300	H	1.38116100	3.94214000	0.74815500
Mn	0.24388300	1.07157300	0.92148700	H	-5.06944900	-0.88647200	-1.60773400	O	-3.22526700	2.92599300	-0.27978000
Mn	0.06544600	2.48298800	-1.51424900	O	-2.78297700	1.21332900	-2.92526900	C	-2.66830700	3.75898700	-1.01834600
O	-1.91919100	-1.37906300	0.45591900	H	-2.90550400	0.34279800	-3.34148700	O	-1.56349100	3.57407300	-1.66121400
O	0.36278600	-0.83960000	1.25588200	H	-1.87366700	1.52701300	-3.19705000	C	-3.35716800	5.10570100	-1.24372700
O	-1.43864100	0.88510400	1.57711700	O	-0.21314100	2.00848300	-3.29945300	H	-4.28191300	4.88228300	-1.79654800
O	-0.33807400	0.51856000	-0.79328600	H	0.40180500	1.27846500	-3.49334800	H	-3.68166100	5.45910600	-0.25569800

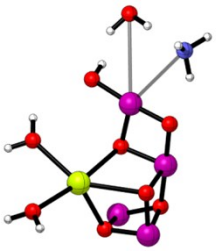
C	-2.54015100	6.17054100	-1.97483000	H	4.57751800	-0.99648900	-3.74069700	H	-0.50752700	-6.33201700	3.98548200
H	-2.23381700	5.81918400	-2.96738500	C	6.06814900	-2.24059600	-2.74701800	H	0.36747400	-4.79840500	4.18512600
H	-1.63525400	6.43406000	-1.41080800	H	6.21847100	-3.30702800	-2.54649800	H	-1.40027700	-4.80250300	4.17601500
H	-3.12970700	7.08759900	-2.10434500	H	6.77345000	-1.95473100	-3.53941900	O	-4.39447700	-0.10096300	1.40932000
O	-0.99684600	-2.19992100	-2.02546900	C	6.37907900	-1.51067500	-1.44040100	C	-4.16267100	-0.56610300	2.54460100
C	-2.22372000	-2.26156300	-2.43836400	O	6.33881300	-2.10528500	-0.35458700	O	-2.99685600	-0.90084200	2.99474400
O	-3.11865000	-1.44624400	-2.13147700	N	6.61381600	-0.17561800	-1.52244900	C	-5.29066400	-0.78319200	3.53767500
C	-2.50882100	-3.42655000	-3.38009800	H	6.58260200	0.25972000	-2.43638700	H	-6.25130800	-0.50366000	3.09671400
H	-1.74523900	-3.40630900	-4.17251400	C	6.52640300	0.69053000	-0.33791900	H	-5.10570600	-0.17882900	4.43443700
H	-2.30914100	-4.34881600	-2.81235400	H	7.12062800	0.22601900	0.45538300	H	-5.31088000	-1.83356600	3.85328700
C	-3.91830800	-3.44772300	-3.97656100	H	6.99707100	1.64683400	-0.59799700	O	-0.39035000	-0.23088800	3.75716700
H	-4.10239400	-2.50451000	-4.51036100	C	5.07557600	0.88807000	0.14060300	C	0.44225100	0.73031200	3.77473900
H	-4.65439100	-3.48273300	-3.16142600	H	4.66513500	-0.08746500	0.42329000	O	0.86110400	1.39106300	2.76580500
C	-4.13464600	-4.63326000	-4.92356800	H	5.08219700	1.49552500	1.05515100	C	0.99361000	1.14481600	5.12973000
H	-3.43138800	-4.60430400	-5.76778300	C	4.18895000	1.54473800	-0.92046800	H	0.53931500	2.11795400	5.37528300
H	-3.98839000	-5.59091400	-4.40447200	H	4.36018300	1.09910300	-1.90991500	H	0.64640700	0.42149600	5.87658500
H	-5.15137300	-4.63011700	-5.33701000	H	4.42827600	2.61407400	-1.02446800	C	2.52561600	1.27701000	5.14881300
N	1.60824900	-1.87805900	-1.07152600	O	2.25159200	1.02856400	0.41472200	H	2.82965200	1.98206700	4.36481500
C	2.21961600	-1.62329300	-2.27994500	C	2.68320600	1.46707000	-0.68293600	H	2.97389100	0.30642300	4.88762200
H	1.68151300	-1.15004300	-3.08961800	O	1.97507500	1.88309100	-1.66365800	C	3.05116700	1.73795100	6.51218500
C	3.52562700	-2.05773800	-2.23536400	O	-0.15461700	-3.41150700	0.54990600	H	2.64264700	2.72166300	6.78341700
N	3.67578900	-2.60720700	-0.96786700	C	-0.55622700	-3.63228800	1.73601900	H	4.14580600	1.82141300	6.50622200
H	4.57686800	-2.85979400	-0.55166100	O	-1.00877900	-2.77338700	2.56132300	H	2.77434000	1.03293500	7.30841500
C	2.51356600	-2.46020600	-0.29739900	C	-0.51119300	-5.08395500	2.20911000	N	1.01825900	4.42100400	-1.99900800
H	2.35316800	-2.75979800	0.72717900	H	0.36393800	-5.55613000	1.74433900	H	1.70758200	4.29741100	-2.73906800
C	4.62550600	-1.98650700	-3.26548000	H	-1.39026400	-5.57595300	1.76290500	H	1.46692000	4.79241500	-1.14623200
H	4.43760000	-2.71100200	-4.07185400	C	-0.51444600	-5.26497900	3.72824800	H	0.27572800	5.04174900	-2.31877300

J

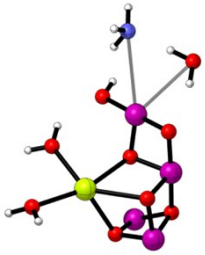
Ca	-2.91953300	0.20361700	-0.65855600	H	-4.27229600	6.84609600	-1.13136400	N	6.48386100	0.36187500	-1.91796000
Mn	-0.09757300	-2.00713600	-0.27419800	O	-0.67681600	-2.72513500	-1.98905800	H	6.41208900	0.47404900	-2.92181300
Mn	-1.18917200	-0.93742700	1.99571400	C	-1.82965500	-2.62791300	-2.56959900	C	6.30813500	1.54390400	-1.06360200
Mn	0.11458600	1.16141600	0.76579000	O	-2.66858500	-1.72871200	-2.34813800	H	7.03246500	1.47476600	-0.24485500
Mn	-0.31921400	2.81785300	-1.36340000	C	-2.10163700	-3.71287100	-3.60832100	H	6.56818300	2.41956300	-1.67126200
O	-1.73551300	-1.67741800	0.41850700	H	-1.29583200	-3.65534300	-4.35720200	C	4.88783100	1.67708500	-0.48454300
O	0.42577200	-0.77034200	1.06659500	H	-1.95957000	-4.68283900	-3.10841400	H	4.69035800	0.83682800	0.18888500
O	-1.50733400	0.76044800	1.43951000	C	-3.47290200	-3.63906700	-4.28411100	H	4.85511700	2.58778400	0.12990100
O	-0.56218800	1.05828400	-0.95309400	H	-3.60173500	-2.64769600	-4.74000000	C	3.80558000	1.73965500	-1.56681800
O	0.00514100	2.92231900	0.44090500	H	-4.25840100	-3.72457400	-3.51940500	H	3.84727200	0.83187000	-2.18916300
O	-5.13170900	-0.79806800	-1.34985700	C	-3.66387900	-4.73109100	-5.34253800	H	3.95859300	2.59394300	-2.23884000
H	-5.33526300	-1.08780500	-0.43688300	H	-2.91235400	-4.64934500	-6.14054400	O	2.08021200	1.22783900	0.03040800
H	-4.75767900	-1.57002800	-1.81543200	H	-3.57155000	-5.73429100	-4.90334700	C	2.37554800	1.81413500	-1.03887600
O	-2.88150500	1.04543800	-3.00926700	H	-4.65453700	-4.66146200	-5.80976000	O	1.57212000	2.47074500	-1.79565800
H	-2.72070900	0.22726100	-3.50989300	N	1.87514300	-2.15590500	-0.88958600	O	0.20686400	-3.71642500	0.95413500
H	-2.09850400	1.64317300	-3.18666100	C	2.49008200	-2.21269300	-2.12220200	C	-0.21352200	-3.72349400	2.14956300
O	-0.67417600	2.61217200	-3.19754500	H	1.90648800	-2.22866600	-3.03294700	O	-0.73151600	-2.73426800	2.76306700
H	0.06529300	2.08166900	-3.54686000	C	3.85610300	-2.25046000	-1.95126900	C	-0.10192500	-5.03668200	2.91974500
O	1.71812500	4.95331100	0.86090600	N	4.04413800	-2.24288300	-0.57407200	H	0.88060000	-5.46792300	2.68445900
H	1.31830200	5.51444600	1.54665600	H	4.95053900	-2.13235700	-0.10949600	H	-0.83906200	-5.71874600	2.46758900
H	1.18904900	4.11192700	0.90678800	C	2.83824000	-2.16528200	0.02347900	C	-0.32333400	-4.92794100	4.42883000
O	-3.61098700	2.43305000	-0.27005700	H	2.68139500	-2.08300400	1.08910300	H	-0.24541700	-5.91688500	4.89908200
C	-3.19039300	3.50667500	-0.72119800	C	4.97721700	-2.25988700	-2.96111000	H	0.42126700	-4.26880700	4.89207300
O	-2.02231600	3.71348900	-1.24622000	H	4.97856000	-3.21058500	-3.51426600	H	-1.31155800	-4.51168900	4.65226400
C	-4.11822800	4.72312700	-0.70454400	H	4.76804800	-1.48298800	-3.71079600	O	-4.32019800	-0.62180100	1.22652800
H	-4.98786700	4.44698700	-1.31842200	C	6.40668200	-2.05318700	-2.39512000	C	-4.06126900	-0.95505000	2.40296400
H	-4.49680400	4.80379400	0.32385800	H	6.73551600	-2.94731400	-1.85435500	O	-2.87881900	-1.08197500	2.90577700
C	-3.52031600	6.04756100	-1.17749500	H	7.09348400	-1.91222700	-3.24107600	C	-5.18417300	-1.25243300	3.38295000
H	-3.16665900	5.97480700	-2.21327800	C	6.51693700	-0.89299400	-1.40404300	H	-6.15829200	-1.09501000	2.91176800
H	-2.67350700	6.34940300	-0.54722500	O	6.56349200	-1.09953800	-0.18334600	H	-5.08572500	-0.60215900	4.26066100

H	-5.10136000	-2.28817000	3.73592500	H	0.71251900	0.56350100	5.73246800	H	4.24945200	1.92258900	6.23879200
O	-0.32690300	-0.18526300	3.64359700	C	2.59095200	1.35583100	4.93722600	H	2.87967800	1.19444700	7.09926900
C	0.47639300	0.79674800	3.62220300	H	2.89229600	2.02283000	4.11934100	N	0.33203200	4.79993300	-1.65014000
O	0.84696200	1.44525500	2.58813600	H	3.01591000	0.36663500	4.70802700	H	0.89149100	4.84857000	-2.50071900
C	1.05629700	1.25268400	4.95257300	C	3.15373200	1.86103600	6.26970600	H	0.88477000	5.10348600	-0.82755400
H	0.62662400	2.24335400	5.16930100	H	2.76938400	2.86276400	6.50846400	H	-0.51327400	5.36065000	-1.75682400

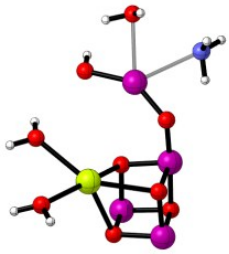
3D image for TSs:



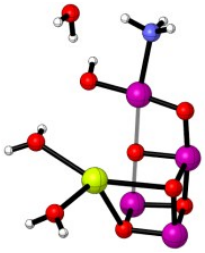
TS1



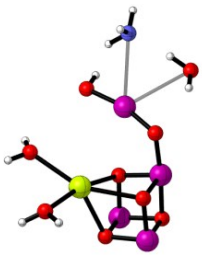
TS2



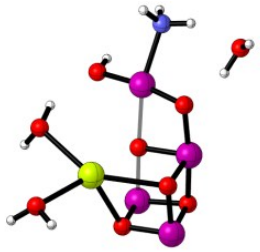
TS3



TS4



TS5



TS6

IVc. Wx binding to (or disassociating from) Mn4

After W1 is substituted for NH_3 on the closed-cubane structure, we can imagine an external water Wx binding to Mn4 (step7) and test the possibility of its deprotonation to O5 accompanied by ET from Mn4 to Mn1 (step8), instead of O5 transfer as the redox switch. We have studied the two processes in all spin states and drawn the free energy profiles (see Figure SIIc for step7 and Figure SIIIa for step8 (as step4) in the SI). It can be seen that Wx binding to Mn4 is slightly endothermic by 1~3 kcal/mol having a small barrier within 1~2 kcal/mol, except for the doublet/Mn1-Mn4(ββαα)

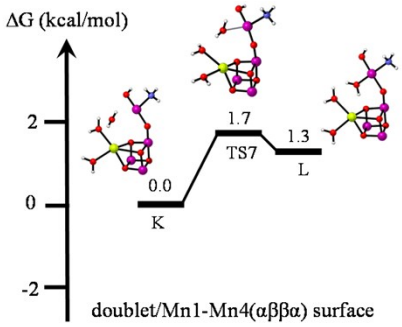
and sextet/Mn1-Mn4(αααβ) surfaces with a continuously rising trend. Bidirectional processes of step7 are facile and the ease of the reverse reaction could provide reference to the feasibility of water dissociation in Scheme S2. The evaluation of step8 and effectiveness of Scheme S3(c) are presented as the step4 in the following section owing to the equivalence of the models.

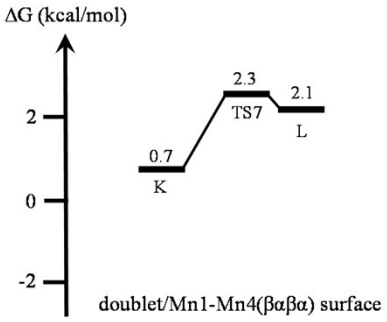
Table SIVc. Gibbs free energies and Mulliken spin populations for the Wx binding to Mn4:

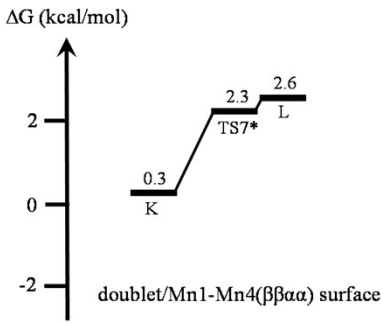
Spin states	Spin topology (Mn1-Mn4)	Gibbs Free energy (a.u.)		
		K	TS7(*)	L
doublet	αββα	-3347.6470	-3347.6443	-3347.6449
	βαβα	-3347.6459	-3347.6434	-3347.6437
	ββαα	-3347.6465	-3347.6434	-3347.6428
sextet	αααβ	-3347.6483	-3347.6460	-3347.6451
octet	ααβα	-3347.6478	-3347.6456	-3347.6460
	αβαα	-3347.6466	-3347.6440	-3347.6443
	βααα	-3347.6475	-3347.6450	-3347.6455
14-et	αααα	-3347.6495	-3347.6463	-3347.6467
Spin states	Spin topology (Mn1-Mn4)	Mulliken spin density		
		K	TS7*	L
doublet	α Mn1	2.93	2.93	2.93
	β Mn2	-2.93	-2.93	-2.93

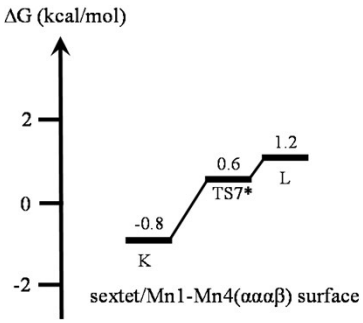
	β	Mn3	-2.76	-2.76	-3.76
	α	Mn4	3.79	3.79	2.83
	β	Mn1	-2.92	-2.93	-2.93
	α	Mn2	2.94	2.94	2.94
	β	Mn3	-2.76	-2.75	-2.76
	α	Mn4	3.79	3.80	3.82
	β	Mn1	-2.93	-2.93	-2.93
	β	Mn2	-2.94	-2.94	-2.95
	α	Mn3	2.84	2.83	2.82
	α	Mn4	3.86	3.86	3.90
sextet	α	Mn1	2.93	2.93	2.93
	α	Mn2	2.93	2.93	2.93
	α	Mn3	2.78	2.78	2.79
	β	Mn4	-3.79	-3.80	-3.82
octet	α	Mn1	2.93	2.93	2.93
	α	Mn2	2.95	2.95	2.95
	β	Mn3	-2.73	-2.72	-2.73
	α	Mn4	3.79	3.79	3.83
	α	Mn1	2.93	2.93	2.93
	β	Mn2	-2.94	-2.94	-2.94
	α	Mn3	2.86	2.86	2.85
	α	Mn4	3.86	3.86	3.90
	β	Mn1	-2.92	-2.92	-2.93
	α	Mn2	2.93	2.93	2.93
	α	Mn3	2.88	2.87	2.86

	α	Mn4	3.86	3.86	3.90
14-et	α	Mn1	2.93	2.93	2.93
	α	Mn2	2.93	2.93	2.93
	α	Mn3	2.89	2.89	2.88
	α	Mn4	3.85	3.86	3.90









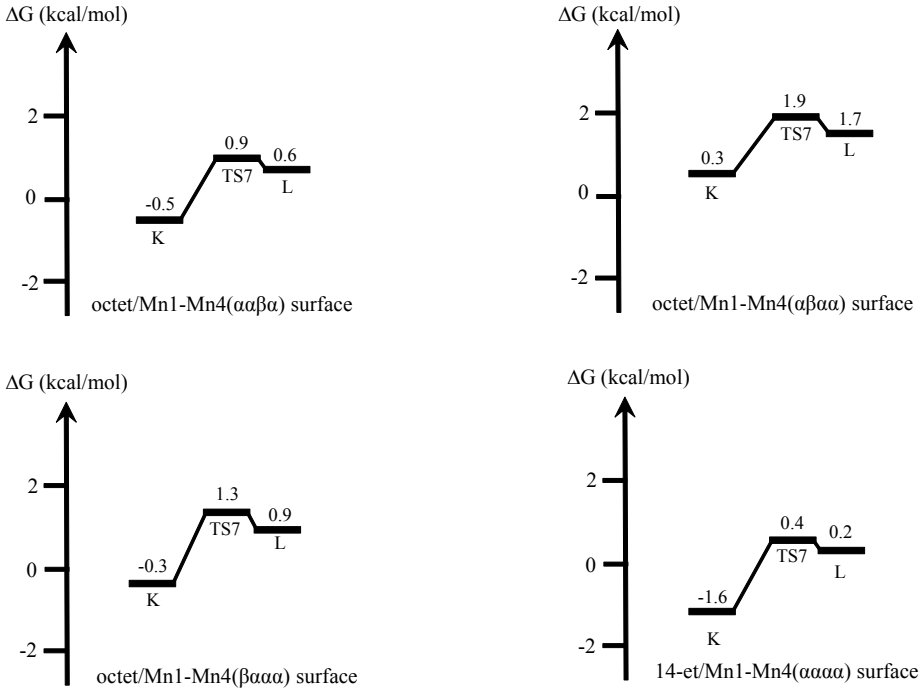


Figure SIIc. Free energy profiles for Wx binding to Mn4 for all spin states.

.

The Cartesian coordinates for K, TS7 and L:

K:

Ca	-2.35609800	0.28933000	-1.39358500	H	0.71202400	1.02192900	-3.48610600	C	-1.70104200	-4.85681100	-6.00816100
Mn	0.04676200	-1.68029200	-0.24438800	O	-2.66841700	2.58297000	-1.84929200	H	-0.66792100	-5.11675500	-6.27754800
Mn	-1.79544200	-1.09553100	1.63758300	C	-2.32005200	3.78255700	-1.87650100	H	-2.14012600	-5.72825200	-5.50245300
Mn	-0.08247000	0.93213500	0.90309400	O	-1.11837100	4.22248300	-1.75380500	H	-2.25847300	-4.69607100	-6.93999500
Mn	0.53952200	3.48003200	-1.00189600	C	-3.39976700	4.83836700	-2.12872900	N	2.07689800	-1.80956700	-0.50303600
O	-1.75520700	-1.74482500	-0.05340800	H	-3.74943000	4.68430700	-3.16124000	C	2.85054300	-1.04567400	-1.35775000
O	0.08158200	-0.94767200	1.44595600	H	-4.25345800	4.57604100	-1.48927300	H	2.41582300	-0.26098200	-1.97457600
O	-1.87242600	0.58512700	1.00363300	C	-2.97431800	6.29188200	-1.92103500	C	4.15740000	-1.46375900	-1.25778500
O	0.03488500	0.05926000	-0.76316300	H	-2.12375900	6.54911700	-2.56262500	N	4.14716700	-2.50827700	-0.33627000
O	-0.30652200	2.54154400	0.27650600	H	-2.67777600	6.47145500	-0.87886500	H	4.98139600	-2.84674800	0.14558000
O	-4.30136500	-0.43284800	-2.86424400	H	-3.80233000	6.97415500	-2.15367700	C	2.88040400	-2.66865200	0.10640800
H	-4.84517700	-0.64625500	-2.07674200	O	-0.06409200	-2.60640900	-1.97864300	H	2.56790100	-3.39243500	0.84479900
H	-3.86916900	-1.27077300	-3.12640100	C	-0.99830300	-2.61310800	-2.85504000	C	5.39646700	-0.99078900	-1.97066800
O	-1.25730400	0.74782000	-3.67156100	O	-1.89108300	-1.72959800	-2.96828100	H	5.47541100	-1.46860100	-2.95893100
H	-1.43598100	-0.16021700	-3.99491300	C	-0.97506500	-3.80744500	-3.80412500	H	5.27351500	0.08157400	-2.17149900
H	-1.74273300	1.36866100	-4.24035200	H	0.07503800	-4.06538700	-3.99553400	C	6.73944600	-1.24079100	-1.22651500
O	1.44443600	3.98923500	-2.53999000	H	-1.39079300	-4.65888100	-3.23999300	H	7.03223400	-2.29342300	-1.30933300
H	2.39602800	3.96462900	-2.32822500	C	-1.74761200	-3.61392900	-5.11257300	H	7.52509000	-0.64513000	-1.71144800
O	1.65038600	1.29358400	-3.44798500	H	-1.33222700	-2.75208700	-5.65651800	C	6.64261000	-0.93136100	0.26476300
H	1.59377200	2.26329100	-3.28410500	H	-2.79058400	-3.35696100	-4.88362000	O	6.45337700	-1.82876900	1.09408100

N	6.69334200	0.38557900	0.61069800	O	-1.45372100	-2.98306200	2.29045200	C	-0.83934300	0.68788500	3.70608600
H	6.78716800	1.06088600	-0.13857300	C	-0.48877600	-5.17347700	2.29055000	O	-0.16428300	1.36282000	2.86409300
C	6.17029400	0.86289200	1.89484000	H	0.58388500	-5.35785700	2.44673900	C	-0.78066000	1.14341800	5.15774400
H	6.46702100	0.13112400	2.65190800	H	-0.78969800	-5.85957900	1.48449800	H	-0.17443000	0.40276800	5.70319300
H	6.66720700	1.81383700	2.12806300	C	-1.28873300	-5.44063500	3.56530500	H	-0.24593800	2.09983100	5.19759800
C	4.63712900	1.01836200	1.88199700	H	-1.14062400	-6.47640500	3.89716900	C	-2.16644700	1.25118200	5.81522500
H	4.18308100	0.04444600	1.66619000	H	-0.97756600	-4.77073300	4.37551300	H	-2.67523900	0.28327800	5.72515000
H	4.29927600	1.30145000	2.88855300	H	-2.35979900	-5.27904200	3.39987700	H	-2.77529000	1.97695400	5.25536400
C	4.15832300	2.04933200	0.85747000	O	-4.40175600	-0.47444800	-0.15175000	C	-2.08173000	1.67288400	7.28575600
H	4.65217300	1.89169400	-0.11287300	C	-4.59828500	-0.98589200	0.97237100	H	-1.50454300	0.94635800	7.87505500
H	4.42568600	3.07191500	1.16269400	O	-3.68458300	-1.28284800	1.83915700	H	-3.08117800	1.74660100	7.73394300
O	1.92994900	1.18325700	1.07975600	C	-6.00772100	-1.32015700	1.42996000	H	-1.59375300	2.65162600	7.39588200
C	2.66331800	2.04855600	0.53735800	H	-6.74113400	-1.00575800	0.68235800	N	0.62805300	5.42663100	0.18209900
O	2.31720400	2.94877200	-0.30152400	H	-6.21206500	-0.82275500	2.38578000	H	1.53683300	5.88302600	0.25672200
O	0.12004600	-3.49408300	0.72267500	H	-6.09067100	-2.40063100	1.60316300	H	0.26799000	5.24904900	1.12060300
C	-0.62282200	-3.76083200	1.72778800	O	-1.55470200	-0.34079100	3.46751100	H	-0.01807400	6.04978200	-0.30334600

TS7:

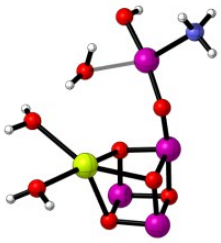
Ca	-2.36794900	0.30624800	-1.35367500	H	-1.58259500	-4.47922400	-3.52837400	C	2.64124000	2.08290000	0.61399700
Mn	0.05528500	-1.71799400	-0.30606100	C	-1.56203800	-3.29509100	-5.34807300	O	2.27812300	3.06236200	-0.11983200
Mn	-1.76261800	-1.19923400	1.61350700	H	-0.96843400	-2.47507900	-5.78075200	O	0.16188400	-3.55691000	0.60521400
Mn	-0.07572000	0.86398800	0.90543800	H	-2.58009300	-2.90369000	-5.22075900	C	-0.56242500	-3.85688400	1.61477000
Mn	0.49604700	3.55301500	-0.86063200	C	-1.57538700	-4.48313900	-6.31598500	O	-1.39399500	-3.10307000	2.20790100
O	-1.74253000	-1.79912400	-0.09676500	H	-0.56227800	-4.87486000	-6.48193800	C	-0.39756800	-5.27882800	2.14504100
O	0.11082700	-1.03016000	1.40120500	H	-2.18882600	-5.30720100	-5.92539000	H	0.67500400	-5.42529900	2.34014600
O	-1.86199600	0.49722500	1.03274600	H	-1.98599500	-4.19531700	-7.29244700	H	-0.63865700	-5.95438500	1.31094300
O	0.02247800	0.02989600	-0.77817000	N	2.08553900	-1.80853500	-0.59884300	C	-1.23294500	-5.60930000	3.38156000
O	-0.34553900	2.47522800	0.30827500	C	2.83409800	-0.96829800	-1.40177500	H	-1.05635100	-6.64674500	3.69373800
O	-4.30345600	-0.39739900	-2.84427900	H	2.37472700	-0.13867100	-1.93225800	H	-0.97937900	-4.94826100	4.21842700
H	-4.83861800	-0.65393700	-2.06366700	C	4.14767800	-1.37366600	-1.35977900	H	-2.30296900	-5.48585200	3.17936000
H	-3.85038000	-1.21302600	-3.13996300	N	4.16781900	-2.48827300	-0.52436000	O	-4.39083300	-0.54660500	-0.13104200
O	-1.32417300	0.91821900	-3.63787800	H	5.01457900	-2.84258400	-0.07753200	C	-4.57184600	-1.09625800	0.97754600
H	-1.42884400	-0.00500200	-3.95451700	C	2.91106500	-2.70110700	-0.07359100	O	-3.64821500	-1.40769700	1.82889900
H	-1.92510300	1.47750100	-4.15845200	H	2.62076900	-3.48457900	0.61124700	C	-5.97318200	-1.46639800	1.43268700
O	1.42691200	4.36335800	-2.25145600	C	5.36659800	-0.83034200	-2.05641000	H	-6.71728800	-1.12368400	0.70844500
H	2.37229200	4.32756300	-2.01532900	H	5.44426100	-1.24599800	-3.07261800	H	-6.17261900	-1.01961200	2.41407600
O	1.45923700	1.71496600	-3.10027700	H	5.21742900	0.24925500	-2.18950400	H	-6.04352200	-2.55511400	1.55230700
H	1.46218100	2.70093300	-3.09072200	C	6.72349200	-1.09417900	-1.34294700	O	-1.49903300	-0.49167500	3.45965300
H	0.53636600	1.46184800	-3.30405900	H	7.03750300	-2.13347400	-1.49104900	C	-0.79158600	0.53867400	3.71463000
O	-2.76018800	2.60745000	-1.72239600	H	7.49059800	-0.45393800	-1.79990000	O	-0.13646400	1.24428500	2.88200100
C	-2.38562100	3.79896300	-1.76331800	C	6.63382900	-0.87452200	0.16449500	C	-0.71478800	0.95439700	5.17772600
O	-1.17383400	4.21818200	-1.67003800	O	6.46051500	-1.82169300	0.93985800	H	-0.07890700	0.21403200	5.68891100
C	-3.44722600	4.87591600	-2.01012200	N	6.67257900	0.42100600	0.58506900	H	-0.20205000	1.92200000	5.23473000
H	-3.73357600	4.79208600	-3.07040500	H	6.75532500	1.13843400	-0.12533000	C	-2.08807400	1.00889500	5.86677000
H	-4.33859800	4.58341200	-1.44004700	C	6.15125300	0.82137700	1.89575900	H	-2.57524000	0.03177700	5.75889800
C	-3.02357200	6.31014000	-1.69139000	H	6.44746200	0.04460300	2.60679700	H	-2.72642000	1.73497400	5.34118100
H	-2.13313900	6.59289700	-2.26397500	H	6.64989100	1.75572000	2.18566700	C	-1.98203000	1.39017400	7.34693700
H	-2.79059400	6.42462200	-0.62367200	C	4.61847100	0.97936000	1.89285100	H	-1.37493100	0.66155900	7.90265700
H	-3.83003300	7.01532100	-1.93134100	H	4.16269400	0.02082000	1.61974600	H	-2.97307300	1.42625300	7.81782500
O	-0.06854000	-2.59475100	-2.06975100	H	4.28202800	1.20254100	2.91497000	H	-1.51551200	2.37711400	7.47555500
C	-0.98808000	-2.52790600	-2.95658200	C	4.13729300	2.06966400	0.93248000	N	0.37330000	5.35614100	0.52632100
O	-1.86089500	-1.61826200	-3.02936000	H	4.62904600	1.96876400	-0.04700900	H	1.25274300	5.82598600	0.73952300
C	-0.98866000	-3.66400700	-3.97498500	H	4.40417800	3.07283800	1.29554900	H	-0.05905400	5.04704800	1.39778600
H	0.03550900	-4.04845700	-4.05982300	O	1.92718400	1.14649500	1.05861900	H	-0.25170500	6.01659900	0.06346200

L:

Ca	-2.59403400	0.32993400	-0.92719400	Mn	0.01849600	0.60610400	0.99600000	O	0.35329500	-1.35036300	1.01473200
Mn	0.07185700	-1.62806700	-0.78504000	Mn	0.25577100	3.72249900	-0.01559600	O	-1.71736900	0.06446000	1.29465800
Mn	-1.44539100	-1.70313800	1.44009200	O	-1.67151500	-1.89276700	-0.35981900	O	-0.10029800	0.16959400	-0.82451200

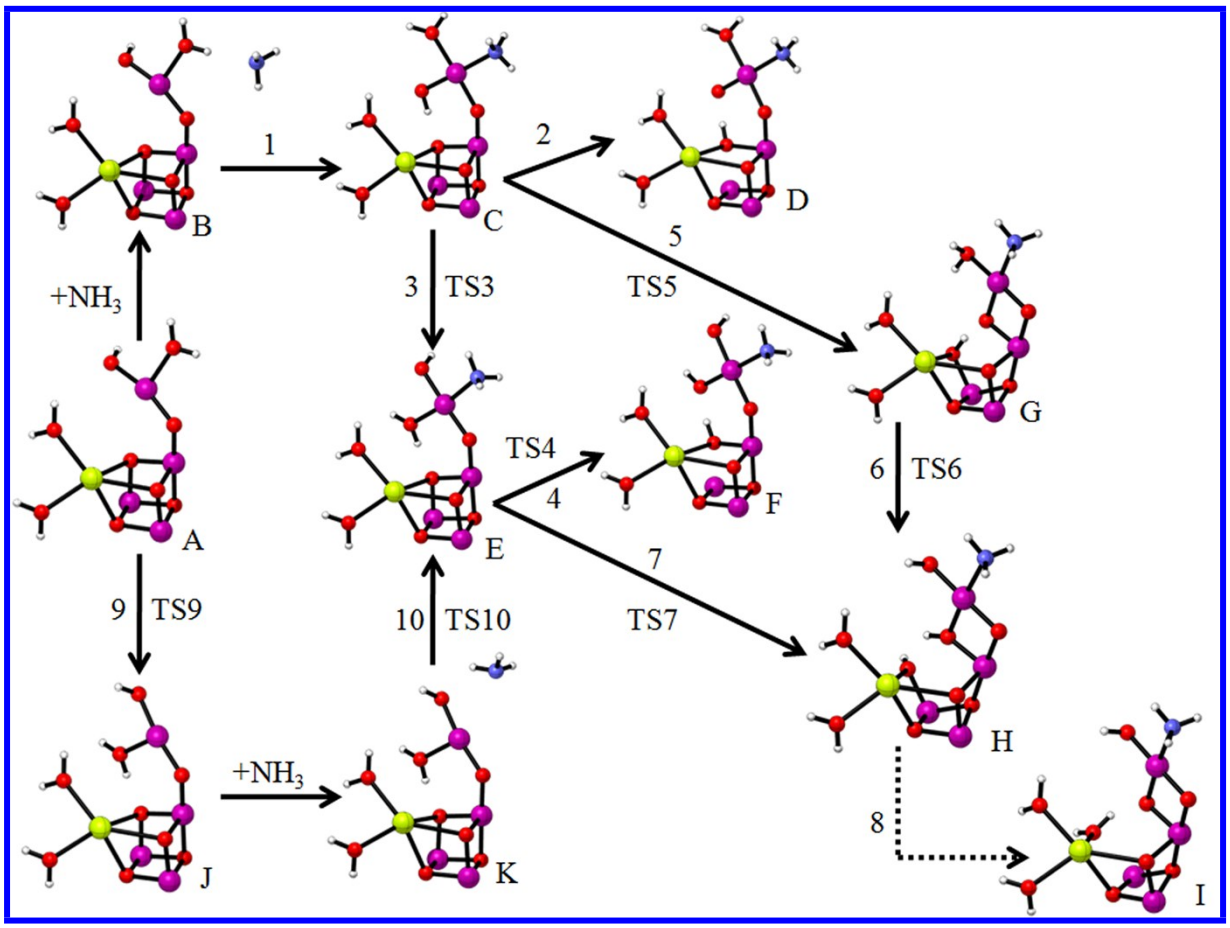
O	-0.46497900	2.25895500	0.77851400	H	-2.07759600	-3.44518200	-7.11648100	C	-0.18035500	-4.19880300	0.60968700
O	-4.67131000	-0.11877600	-2.24967300	H	-3.38559400	-2.33329400	-7.56278900	O	-0.91929100	-3.66333900	1.49153400
H	-5.06880900	-0.69600700	-1.56549300	N	2.06418300	-1.52484400	-1.30235400	C	0.09494800	-5.69490400	0.73368500
H	-4.34024500	-0.69670000	-2.96058800	C	2.71337900	-0.44910500	-1.87472700	H	1.18697500	-5.82383900	0.70705400
O	-1.19981600	2.19210600	-3.55208200	H	2.18093300	0.46961700	-2.08847300	H	-0.27760000	-6.15891400	-0.19165900
H	-1.38392800	1.23362000	-3.64275300	C	4.03977100	-0.76663900	-2.04632900	C	-0.50948300	-6.36397700	1.96779400
H	-1.87775300	2.50187600	-2.90562200	N	4.17079700	-2.07015700	-1.57459000	H	-0.26668000	-7.43439500	1.97724900
O	1.04470300	5.19825200	-0.79795500	H	5.06500500	-2.48004200	-1.30059700	H	-0.12460100	-5.91396500	2.89032900
H	1.96826700	5.21449400	-0.48574400	C	2.96531800	-2.47793600	-1.11753600	H	-1.59995900	-6.25598900	1.98077300
O	0.86970900	2.82960500	-1.95409800	H	2.76412500	-3.43867100	-0.66669400	O	-4.36700600	-0.89231500	0.32017100
H	1.08498400	3.73145500	-2.27275400	C	5.17509500	0.02752900	-2.63449000	C	-4.33174100	-1.70058300	1.27639900
H	0.12893000	2.49453800	-2.54399900	H	5.19135400	-0.07951700	-3.72994100	O	-3.26541400	-2.11687100	1.87521100
O	-2.85012700	2.63420600	-1.35229400	H	4.97074800	1.08922100	-2.44196800	C	-5.61823900	-2.29116100	1.82769900
C	-2.75453400	3.81254800	-0.87228800	C	6.59321600	-0.33897800	-2.11180200	H	-6.48912800	-1.83763100	1.34646900
O	-1.67157600	4.41076100	-0.61602000	H	6.93606800	-1.27656300	-2.56359500	H	-5.66366700	-2.13374600	2.91181400
C	-4.06799100	4.56149100	-0.63968900	H	7.29505900	0.44742100	-2.42170000	H	-5.62332400	-3.37565300	1.65799900
H	-4.51905600	4.71197600	-1.63238600	C	6.61159100	-0.54661100	-0.59977500	O	-0.93588600	-1.41108500	3.33948500
H	-4.74649400	3.87248300	-0.11671300	O	6.52246700	-1.67841100	-0.11024200	C	-0.26620000	-0.39727200	3.73303600
C	-3.94229100	5.89114600	0.10295700	N	6.64898800	0.58410300	0.15838700	O	0.20869200	0.53646100	3.01203700
H	-3.25264600	6.56710900	-0.41513700	H	6.66268000	1.47160300	-0.32976700	C	0.00193700	-0.31607600	5.23028300
H	-3.56200500	5.74095800	1.12248400	C	6.22758300	0.59084200	1.56291500	H	0.75320200	-1.08734200	5.46382300
H	-4.91927200	6.38527700	0.18232900	H	6.57813800	-0.34730000	2.00309400	H	0.45510800	0.65878100	5.44668800
O	-0.26588000	-1.97436000	-2.69334200	H	6.74615100	1.41749800	2.06640000	C	-1.25228600	-0.55098600	6.08780300
C	-1.14996500	-1.46286600	-3.46467700	C	4.69918100	0.71024200	1.71506700	H	-1.68688500	-1.52157000	5.81798200
O	-1.97807300	-0.56596400	-3.13866000	H	4.22303100	-0.14243600	1.21797300	H	-2.00780200	0.20907200	5.83757000
C	-1.13565600	-1.98641500	-4.89834300	H	4.44372400	0.63101500	2.78140600	C	-0.94838400	-0.50268800	7.58876400
H	-0.38611900	-1.38881500	-5.44411600	C	4.13984400	2.01485100	1.14094400	H	-0.21938900	-1.27517200	7.87169000
H	-0.75124800	-3.01402500	-4.88325400	H	4.54711600	2.19512200	0.13288900	H	-1.85717100	-0.66903600	8.18171300
C	-2.48578600	-1.90301600	-5.62020300	H	4.43856700	2.88387000	1.74311600	H	-0.53123400	0.47062000	7.88347300
H	-2.84150100	-0.86468500	-5.59614300	O	1.98332200	0.98651900	0.98701200	N	-0.21193200	4.86401600	1.82216500
H	-3.22800600	-2.50025200	-5.06770200	C	2.62041000	2.08332400	0.95616900	H	0.55374100	5.41839600	2.20308900
C	-2.40778100	-2.39821200	-7.06837300	O	2.15458400	3.24019000	0.74030100	H	-0.54071200	4.20006000	2.52386000
H	-1.69726200	-1.79896400	-7.65474600	O	0.36641200	-3.61807200	-0.39003200	H	-0.97675700	5.48341100	1.55254300

3D image for TS7:



V. Mn4 Addition Scheme

Va. NH_3 binding to Mn4 of the closed-cubane structure as an additional ligand



Scheme S4. Here are specific annotations for each step: 1&10: NH_3 binding to Mn4 in concomitance with W1 and W2 pivoting on Mn4; 2&4: PT from W2 to O5; 3&6&9: W1 deprotonation to W2; 5&8: Mn3 ligand exchange between W2 and O5 assisted by PT from W2 to O5; 7: PCET of PT from W2 to $O5H^-$ and ET from Mn4 to Mn1.

Proton transfer between W1 and W2 and NH_3 binding to Mn4

Computation on the protonation states and magnetic interactions of the S_2 state substantiates different protonation states of W1 (H_2O) and W2 (OH^-),[1] reaching optimal experimental consensus on several important spectroscopic measurements,

which brings diversification for the reaction pathways and elaboration on the mechanism. We have testified the potentiality for smooth proton transfer from W1 to W2 (step9) with small free energy barriers of 5.7~7.3 kcal/mol for all spin states (separately listed for the different model size in the section Va of the SI). This undoubtedly yields two kinds of local environments around Mn4 for NH_3 binding and the ensuing transitions. For the TS searching of NH_3 binding process, we append an approximation in our model that NH_3 binding to Mn4 is posterior to the carousel rearrangement of W1 and W2 which is acknowledged to be very facile. Otherwise, NH_3 binding will be mixed with ligands pivoting course which would confuse stationary point locations. This approximate treatment brings convenience to TS optimizations and is considered to be advisable for its non-interference to the NH_3-Mn4 interaction and the potential ambiguity about the motion sequence. Practically, we only sought out the TS10 but none for step1 (ΔG in -3.7~ -5.0 kcal/mol and $\Delta G^{\neq}$ in 0.9~4.5 kcal/mol for step10, Figure 7 for doublet/Mn1-Mn4($\alpha\beta\beta\alpha$) surface and others in Figure SIIIa of the SI, the same below), and the latter is assumed to be also achievable temporarily because of the stability of C and analogy to step10. Starting with C, there are several alternative routes and we first exclude the feasibility of step2 judged by the ceaselessly increasing tendency and non-vanishing gradient on the scan plots for W2 deprotonation to O5 (see PES scan for step2 in the section SVa of the SI). For step3 of PT from W1 to W2 after NH_3 binding, we obtained 8.6~10.1 kcal/mol barriers and 4.6~6.1 kcal/mol energetically lower E (Figure 7) which shows the easiness to exchange their protonation forms and a minor preference for hydroxyl trans to O4.

Attempt to realize Brudvig et al.'s proposal with our model

For step4, we have located the TS4* on the electronic PES whose barrier is

removed after thermal corrections, and the deprotonation presents an ascending process in free energy within 8.3~9.3 kcal/mol (Figure 7), showing a slight disinclination for proton transfer. Especially, what matters is the non-PCET character observed for the deprotonation judged from spin density distributions along the reaction coordinate (see Figure SVa in the SI), so valence rearrangement cannot be triggered by NH_3 binding to Mn4 and the subsequent Wx deprotonation to O5 by our QM-only model. Regrettably, we did not reproduce the so-called 'redox switch mechanism' [18] described in ref. [18]. As a supplement, we have built a completely identical QM model for structures A, B, C and D in all possible spin states according to the Figure 4 of the ref. [19] and execute DFT optimizations, chiefly aiming at checking the availability of the described S_2 (III, IV, IV, IV) for B.[19] We can see all the optimized structures keep consistent with the intention depicted in the paper, and spin populations are in line with the established oxidation state distributions, except for B in the S_2 state. We have imposed (III, IV, IV, IV) and corresponding unpaired spins on B in the initial guess for all spin topologies, but the subsequent wavefunction optimization results always turn into (IV, IV, IV, III), let alone the following geometry optimizations based on this (see Table SVb in the SI). It is too suspicious to be a coincidence and we think Mn1-Mn4 (III, IV, IV, IV) is not fit for the closed-cubane structure as a steady electronic structure, at least in our constructed QM model. However, it is worth to note that although the electronic configuration of the cluster is generally independent of the farther and subordinate MM region, subtle change and influence on the geometric configuration and oxidation arrangement of Mn_4CaO_5 cluster may appear due to their chosen smaller QM region and extra MM part added to the optimization. Different functional or basis set selections and energy minimization algorithm or optimization strategies may also contribute to the diversity

in geometric and electronic configurations. Additionly, the coherence of the calculated and experimental EXAFS Mn spectra and XRD data reveals certain steric rationality which is respectively characterized by distances between metals and electron-density maps for the binding motif, offering support for their model structurally from the viewpoint of experimental spectrum. In this sense, NH_3 binding terminally as an additional ligand proposed by Brudvig et al. remains optional temporarily despite our failure to imitate it. It is therefore still an open problem as to the inconformity on valence state distributions and more targeted inspections and further discussions are needed to examine its validity.

Nevertheless, according to the purpose reflected by our computation results approved by the majority, the conversion of S_2~S_3 does not undergo the so-called redox switch to (III, IV, IV, IV) of the closed-cubane form triggered by the addition of a new water Wx and carousel rearrangement of W1 and W2 around Mn4. It follows that it is in favor of the strategy suggested by Cox et al. that S_2 (IV, IV, IV, III) directly converts to S’ 3(IV, IV, IV, IV) sparked by the PCET of ET from Mn4 to Yz· and PT from W1 to Asp61 prior to Wx binding to Mn4 by the pivot mechanism.[5] Unlike the impermissibility of step2, water deprotonation to O5 is not inadmissible for step4, but the point is the nonoccurrence of valence rearrangement highlighted in the proposition and the invalidation for g≈2.0 MLS in our model. Consequently, we have attempted to search other underlying valid pathways in the framework of NH_3 addition to the dangler Mn4.

Analysis of the analogous mechanism to the Mn4 addition scheme

There remains one plausible statement for the Mn4 addition scheme that after NH_3 binding terminally as an additional ligand generating E, the water ligand (W2) *trans* to NH_3 goes away before O5 shifting to Mn4 to achieve the g≈2.0 MLS. On the face,

it satisfies the requirement for ligand addition, however, this pathway is actually equivalent to the W1 substitution scheme because both of them cause water dissociation, which violates the addition rule. So this mechanism cannot justify the feasibility for the Mn4 addition scheme. Moreover, it is difficult and worthless to distinguish the identity of the gone water belonging to W1 or W2 owing to the potential rapid interchange in the cytoplasmic matrix, leading to the ambiguous ascription for the leaving group. In spite of this, we classify this situation into the 'W1 substitution scheme' from the view of the common reaction outcomes structurally and the comparable free energy barriers for the rate-determining steps (see W1 substitution scheme) on the routes to the NH_3-altered g≈2.0 MLS structure.

Table SVa. Gibbs free energies and Mulliken spin populations for the Mn4 addition scheme:

Spin states	Spin topology (Mn1-Mn4)	Gibbs Free energy (a.u.)			
		C	TS3	E	TS4*
doublet	αββα	-3347.6421	-3347.6260	-3347.6506	-3347.6390
	βαβα	-3347.6400	-3347.6251	-3347.6494	-3347.6385
	ββαα	-3347.6390	-3347.6250	-3347.6484	-3347.6374
sextet	αααβ	-3347.6428	-3347.6277	-3347.6524	-3347.6410
octet	ααβα	-3347.6422	-3347.6271	-3347.6517	-3347.6410
	αβαα	-3347.6396	-3347.6258	-3347.6492	-3347.6376
	βααα	-3347.6419	-3347.6269	-3347.6492	-3347.6383
14-et	αααα	-3347.6423	-3347.6280	-3347.6501	-3347.6398

		F	TS5	G	TS6
doublet	αββα	-3347.6361	-3347.6044	-3347.6484	-3347.6180
	βαβα	-3347.6357	-3347.6039	-3347.6479	-3347.6181
	ββαα	-3347.6340	-3347.6035	-3347.6441	-3347.6302
sextet	αααβ	-3347.6382	-3347.6062	-3347.6500	-3347.6195
octet	ααβα	-3347.6377	-3347.6060	-3347.6496	-3347.6194
	αβαα	-3347.6345	-3347.6038	-3347.6454	-3347.6303
	βααα	-3347.6353	-3347.6043	-3347.6462	-3347.6313
14-et	αααα	-3347.6369	-3347.6054	-3347.6473	-3347.6315
		H	I	TS7	A
doublet	αββα	-3347.6453	-3347.6408	-3347.6064	-3291.1081
	βαβα	-3347.6452	\	-3347.6056	-3291.1069
	ββαα	-3347.6402	\	-3347.6059	-3291.1073
sextet	αααβ	-3347.6460	\	-3347.6083	-3291.1096
octet	ααβα	-3347.6460	-3347.6404	-3347.6078	-3291.1094
	αβαα	-3347.6399	-3347.6419	-3347.6058	-3291.1072
	βααα	-3347.6404	\	-3347.6056	-3291.1089
14-et	αααα	-3347.6411	-3347.6564	-3347.6064	-3291.1095
		TS9	J	K	TS10
doublet	αββα	-3291.0977	-3291.1104	-3347.6425	-3347.6388
	βαβα	-3291.0973	-3291.1075	-3347.6418	-3347.6489
	ββαα	-3291.0971	-3291.1127	-3347.6419	-3347.6386
sextet	αααβ	-3291.1004	-3291.1106	-3347.6445	-3347.6412
	ααβα	-3291.0992	-3291.1122	-3347.6439	-3347.6403

octet	αβαα	-3291.0963	-3291.1122	-3347.6415	-3347.6391
	βααα	-3291.0973	-3291.1138	-3347.6433	-3347.6401
14-et	αααα	-3291.1005	-3291.1149	-3347.6433	-3347.6419

Spin states	Spin topology (Mn1-Mn4)		Mulliken spin density			
			C	TS3	E	TS4*
doublet	α	Mn1	2.92	2.92	2.93	2.92
	β	Mn2	-2.93	-2.93	-2.93	-2.92
	β	Mn3	-2.80	-2.81	-2.73	-2.73
	α	Mn4	3.83	3.84	3.81	3.85
		O4	-0.09	-0.07	-0.18	-0.23
		O5	0.01	0.02	0.01	0.02
	β	Mn1	-2.92	-2.92	-2.92	-2.91
	α	Mn2	2.95	2.94	2.94	2.95
	β	Mn3	-2.77	-2.80	-2.71	-2.69
	α	Mn4	3.82	3.84	3.82	3.85
		O4	-0.11	-0.08	-0.19	-0.25
		O5	-0.01	-0.02	-0.02	0.01
	β	Mn1	-2.93	-2.93	-2.94	-2.93
	β	Mn2	-2.94	-2.94	-2.94	-2.94
	α	Mn3	2.87	2.87	2.76	2.76
	α	Mn4	3.89	3.92	3.87	3.90
		O4	0.14	0.12	0.19	0.22
		O5	-0.02	-0.02	-0.02	-0.01

sextet	α	Mn1	2.93	2.93	2.93	2.93
	α	Mn2	2.92	2.93	2.93	2.92
	α	Mn3	2.80	2.82	2.75	2.74
	β	Mn4	-3.83	-3.84	-3.82	-3.85
		O4	0.09	0.06	0.17	0.23
		O5	0.03	0.04	0.04	-0.01
octet	α	Mn1	2.93	2.93	2.94	2.93
	α	Mn2	2.95	2.95	2.95	2.95
	β	Mn3	-2.75	-2.77	-2.71	-2.70
	α	Mn4	3.82	3.84	3.81	3.85
		O4	-0.10	-0.08	-0.19	-0.24
		O5	0.03	0.03	0.01	0.02
	α	Mn1	2.92	2.93	2.92	2.91
	β	Mn2	-2.94	-2.94	-2.94	-2.94
	α	Mn3	2.89	2.90	2.82	2.77
	α	Mn4	3.89	3.92	3.87	3.90
		O4	0.13	0.11	0.18	0.25
		O5	0.01	0.02	0.02	-0.03
	β	Mn1	-2.91	-2.92	2.92	-2.91
	α	Mn2	2.93	2.93	-2.94	2.93
	α	Mn3	2.92	2.91	2.82	2.82
	α	Mn4	3.89	3.92	3.87	3.90
		O4	0.11	0.11	0.18	0.22
		O5	0.00	-0.01	-0.01	0.00
14-et	α	Mn1	2.93	2.93	-2.92	2.93

	α	Mn2	2.93	2.93	2.93	2.93
	α	Mn3	2.92	2.82	2.85	2.82
	α	Mn4	3.89	3.90	3.87	3.90
		O4	0.12	0.10	0.17	0.23
		O5	0.03	0.04	0.04	-0.02
			F	TS5	G	TS6
doublet	α	Mn1	2.90	2.74	2.94	2.94
	β	Mn2	-2.92	-2.92	-2.94	-2.94
	β	Mn3	-2.72	-2.77	-2.85	-2.84
	α	Mn4	3.86	3.83	3.87	3.87
		O4	-0.25	-0.09	-0.06	-0.08
		O5	0.01	0.28	0.02	0.02
	β	Mn1	-2.90	-2.76	-2.95	-2.94
	α	Mn2	2.95	2.92	2.93	2.94
	β	Mn3	-2.67	-2.75	-2.83	-2.81
	α	Mn4	3.86	3.83	3.87	3.87
		O4	-0.27	-0.11	-0.08	-0.11
		O5	0.03	-0.26	-0.03	-0.03
	β	Mn1	-2.92	-2.75	-2.96	-2.95
	β	Mn2	-2.94	-2.92	-2.95	-2.96
	α	Mn3	2.75	2.92	2.91	2.92
	α	Mn4	3.91	3.86	3.89	3.87
		O4	0.24	0.11	0.10	0.06
		O5	-0.01	-0.29	-0.03	-0.04

sextet	α	Mn1	2.93	2.76	2.97	2.97
	α	Mn2	2.92	2.93	2.96	2.97
	α	Mn3	2.72	2.80	2.86	2.85
	β	Mn4	-3.86	-3.83	-3.87	-3.87
		O4	0.25	0.09	0.07	0.09
		O5	-0.02	0.28	0.03	0.03
octet	α	Mn1	2.92	2.75	2.96	2.96
	α	Mn2	2.95	2.93	2.95	2.96
	β	Mn3	-2.66	-2.72	-2.83	-2.80
	α	Mn4	3.86	3.83	3.87	3.87
		O4	-0.26	-0.10	-0.07	-0.10
		O5	0.01	0.29	0.02	0.03
	α	Mn1	2.90	2.76	2.94	2.94
	β	Mn2	-2.94	-2.91	-2.93	-2.93
	α	Mn3	2.75	2.95	2.91	2.92
	α	Mn4	3.91	3.86	3.89	3.87
		O4	0.25	0.11	0.11	0.07
		O5	-0.03	0.26	0.03	0.05
	β	Mn1	-2.91	-2.75	-2.94	-2.93
	α	Mn2	2.93	2.92	2.93	2.95
	α	Mn3	2.80	2.96	2.95	2.95
	α	Mn4	3.91	3.87	3.89	3.87
		O4	0.22	0.10	0.08	0.05
		O5	0.00	-0.28	-0.03	-0.04
14-et	α	Mn1	2.92	2.76	2.97	2.96

	α	Mn2	2.92	2.93	2.96	2.97
	α	Mn3	2.81	2.98	2.95	2.95
	α	Mn4	3.91	3.87	3.89	3.87
		O4	0.23	0.09	0.09	0.06
		O5	-0.02	0.28	0.03	0.05
			H	I	TS7	A
doublet	α	Mn1	2.93	3.89	2.81	2.94
	β	Mn2	-2.93	-2.92	-2.92	-2.93
	β	Mn3	-2.85	-2.88	-2.75	-2.80
	α	Mn4	3.86	2.83	3.84	3.83
		O4	-0.15	0.00	-0.19	-0.08
		O5	0.01	0.02	0.22	0.02
	β	Mn1	-2.93	\	-2.81	-2.92
	α	Mn2	2.93	\	2.92	2.94
	β	Mn3	-2.81	\	-2.72	-2.78
	α	Mn4	3.87	\	3.84	3.83
		O4	-0.18	\	-0.20	-0.08
		O5	-0.01	\	-0.21	-0.02
	β	Mn1	-2.96	\	-2.81	-2.93
	β	Mn2	-2.95	\	-2.93	-2.94
	α	Mn3	2.87	\	2.81	2.86
	α	Mn4	3.88	\	3.88	3.90
		O4	0.10	\	0.15	0.16
		O5	-0.03	\	-0.23	-0.02

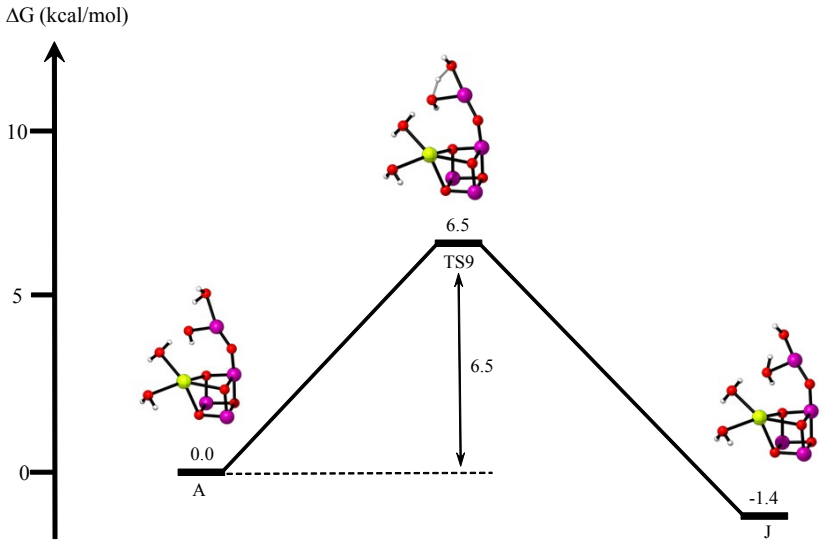
sextet	α	Mn1	2.95	\	2.81	2.92
	α	Mn2	2.96	\	2.94	2.93
	α	Mn3	2.86	\	2.78	2.81
	β	Mn4	-3.87	\	-3.84	-3.83
		O4	0.17	\	0.19	0.07
		O5	0.01	\	0.23	0.04
octet	α	Mn1	2.95	3.90	2.81	2.94
	α	Mn2	2.96	2.97	2.93	2.94
	β	Mn3	-2.81	-2.85	-2.70	-2.77
	α	Mn4	3.86	2.82	3.84	3.83
		O4	-0.17	-0.01	-0.20	-0.08
		O5	0.01	0.02	0.23	0.03
	α	Mn1	2.95	3.90	2.81	2.95
	β	Mn2	-2.93	-2.90	-2.91	-2.93
	α	Mn3	2.87	2.88	2.82	2.86
	α	Mn4	3.88	2.87	3.88	3.89
		O4	0.11	0.13	0.15	0.15
		O5	0.03	0.02	0.21	0.02
	β	Mn1	-2.94	\	-2.81	-2.92
	α	Mn2	2.95	\	2.92	2.93
	α	Mn3	2.91	\	2.86	2.89
	α	Mn4	3.88	\	3.88	3.90
		O4	0.09	\	0.14	0.15
		O5	-0.02	\	-0.21	-0.01
14-et	α	Mn1	2.97	3.93	2.82	2.95

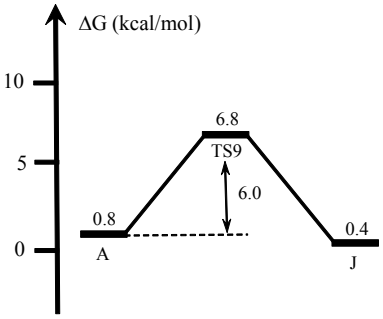
	α	Mn2	2.97	2.99	2.94	2.93
	α	Mn3	2.92	2.93	2.88	2.89
	α	Mn4	3.88	2.90	3.88	3.89
		O4	0.10	0.14	0.14	0.14
		O5	0.03	0.04	0.22	0.04
			TS9	J	K	TS10
doublet	α	Mn1	2.92	2.94	2.93	2.93
	β	Mn2	-2.93	-2.93	-2.93	-2.93
	β	Mn3	-2.79	-2.79	-2.77	-2.76
	α	Mn4	3.82	3.84	3.83	3.83
		O4	-0.07	-0.09	-0.14	-0.15
		O5	0.02	0.01	0.02	0.02
	β	Mn1	-2.92	-2.92	-2.92	-2.92
	α	Mn2	2.94	2.94	2.95	2.94
	β	Mn3	-2.78	-2.73	-2.74	-2.74
	α	Mn4	3.82	3.83	3.83	3.83
		O4	-0.07	-0.17	-0.16	-0.16
		O5	-0.02	-0.01	-0.01	-0.01
	β	Mn1	-2.93	-2.94	-2.94	-2.94
	β	Mn2	-2.94	-2.94	-2.94	-2.94
	α	Mn3	2.87	2.85	2.84	2.83
	α	Mn4	3.90	3.91	3.88	3.89
		O4	0.14	0.17	0.18	0.18
		O5	-0.02	-0.01	-0.02	-0.02

sextet	α	Mn1	2.92	2.93	2.93	2.93
	α	Mn2	2.93	2.93	2.93	2.93
	α	Mn3	2.80	2.77	2.78	2.76
	β	Mn4	-3.82	-3.83	-3.83	-3.82
		O4	0.06	0.08	0.14	0.17
		O5	0.04	-0.02	0.03	0.03
octet	α	Mn1	2.93	2.95	2.94	2.94
	α	Mn2	2.95	2.95	2.95	2.95
	β	Mn3	-2.75	-2.75	-2.73	-2.72
	α	Mn4	3.82	3.84	3.83	3.83
		O4	-0.08	-0.10	-0.15	-0.16
		O5	0.03	0.02	0.03	0.03
	α	Mn1	2.93	2.94	2.93	2.93
	β	Mn2	-2.93	-2.94	-2.93	-2.93
	α	Mn3	2.89	2.86	2.85	2.84
	α	Mn4	3.90	3.90	3.88	3.89
		O4	0.13	0.17	0.18	0.18
		O5	0.02	0.01	0.01	0.01
	β	Mn1	-2.92	-2.93	-2.93	-2.92
	α	Mn2	2.93	2.93	2.93	2.93
	α	Mn3	2.91	2.89	2.88	2.88
	α	Mn4	3.89	3.91	3.88	3.89
		O4	0.13	0.16	0.16	0.17
		O5	-0.01	0.00	-0.01	-0.01
14-et	α	Mn1	2.93	2.95	-2.93	2.93

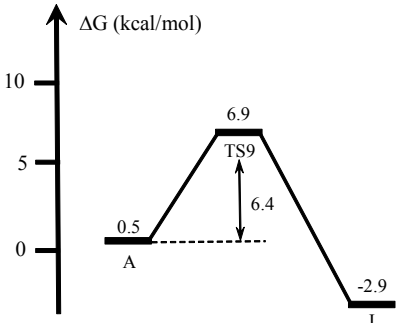
α	Mn2	2.93	2.93	2.93	2.93
α	Mn3	2.92	2.90	2.88	2.88
α	Mn4	3.90	3.90	3.88	3.89
	O4	0.12	0.16	0.16	0.16
	O5	0.04	0.03	-0.01	0.03

doublet/Mn1-Mn4(αββα) surface

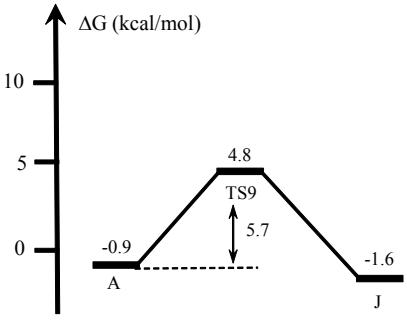




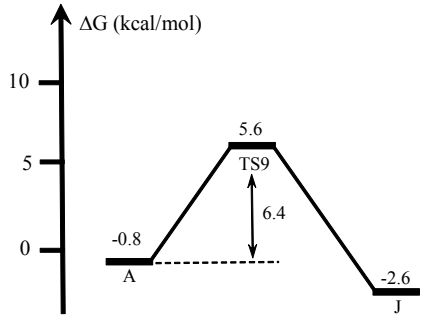
doublet/Mn1-Mn4 (βαβα) surface



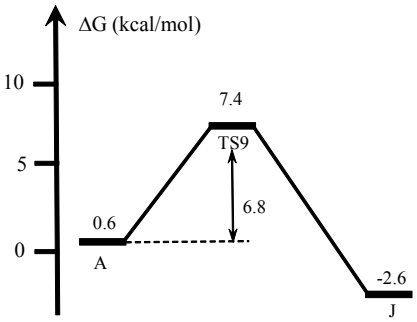
doublet/Mn1-Mn4 (ββαα) surface



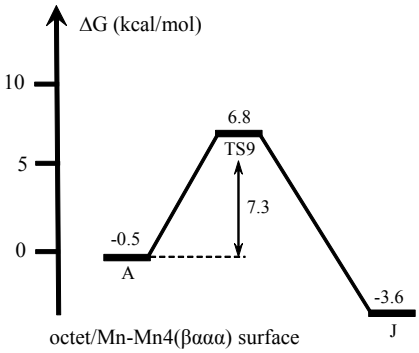
sextet/Mn1-Mn4 (αααβ) surface



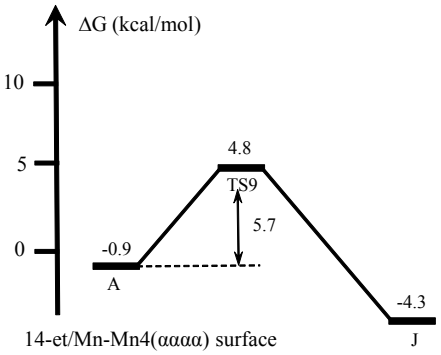
octet/Mn1-Mn4 (ααβα) surface



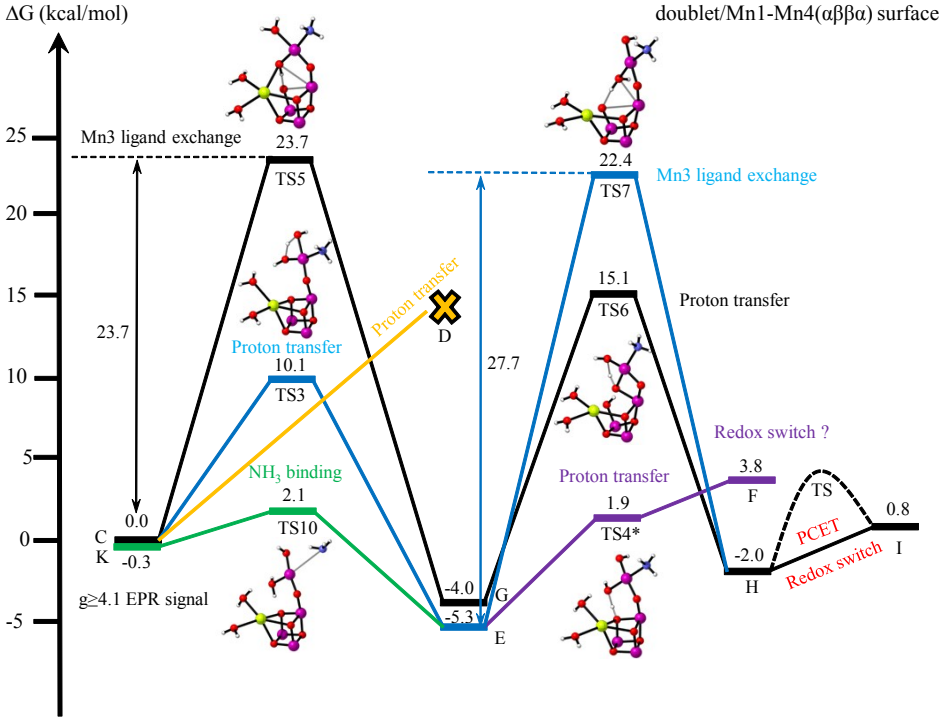
octet/Mn-Mn4(αβαα) surface

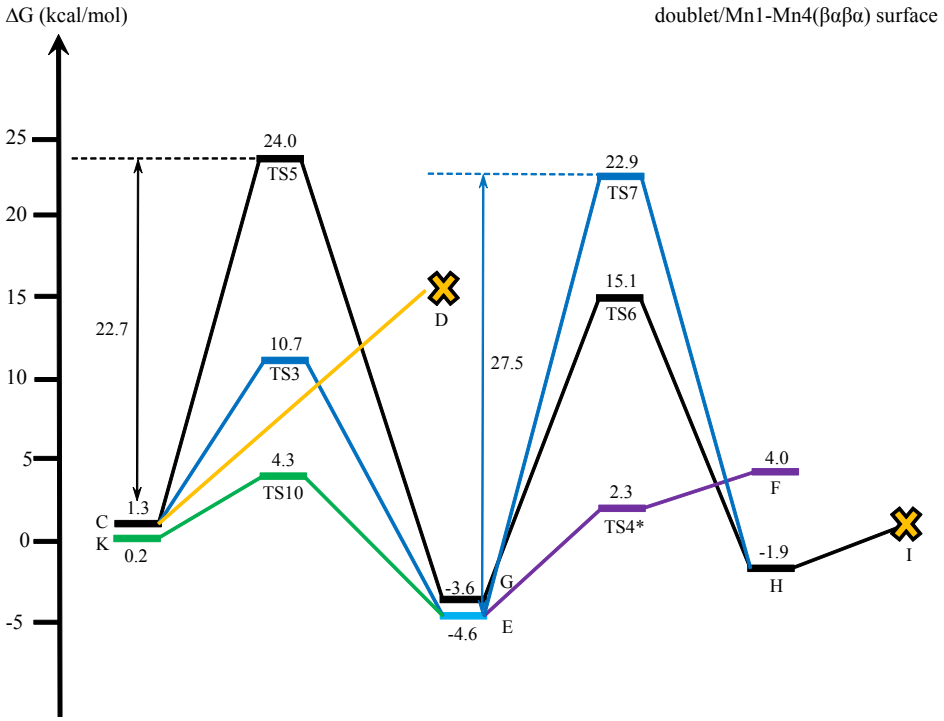


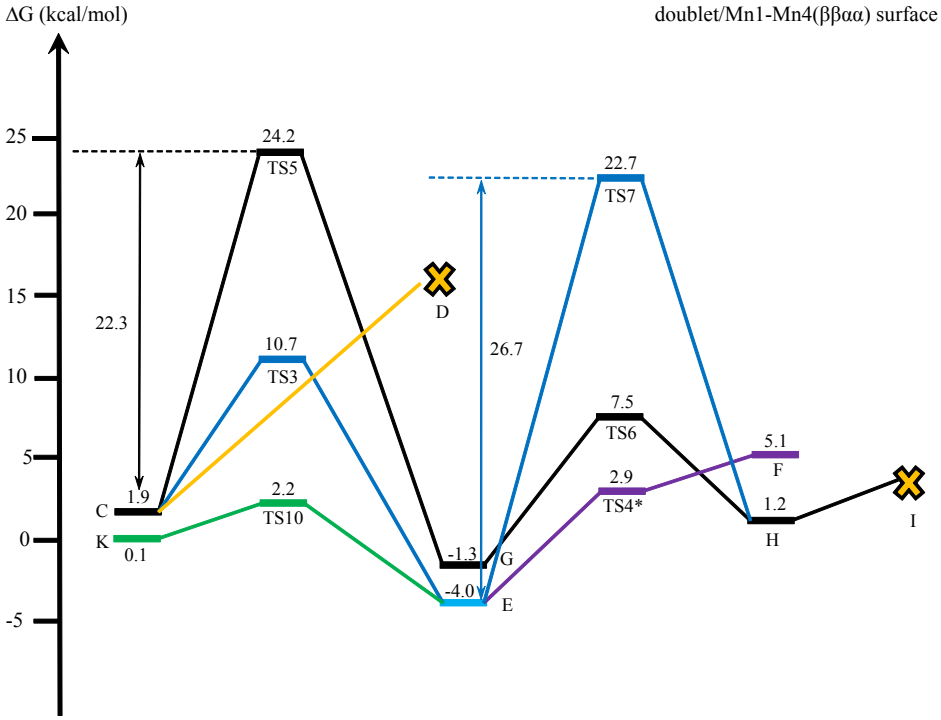
octet/Mn-Mn4(βααα) surface

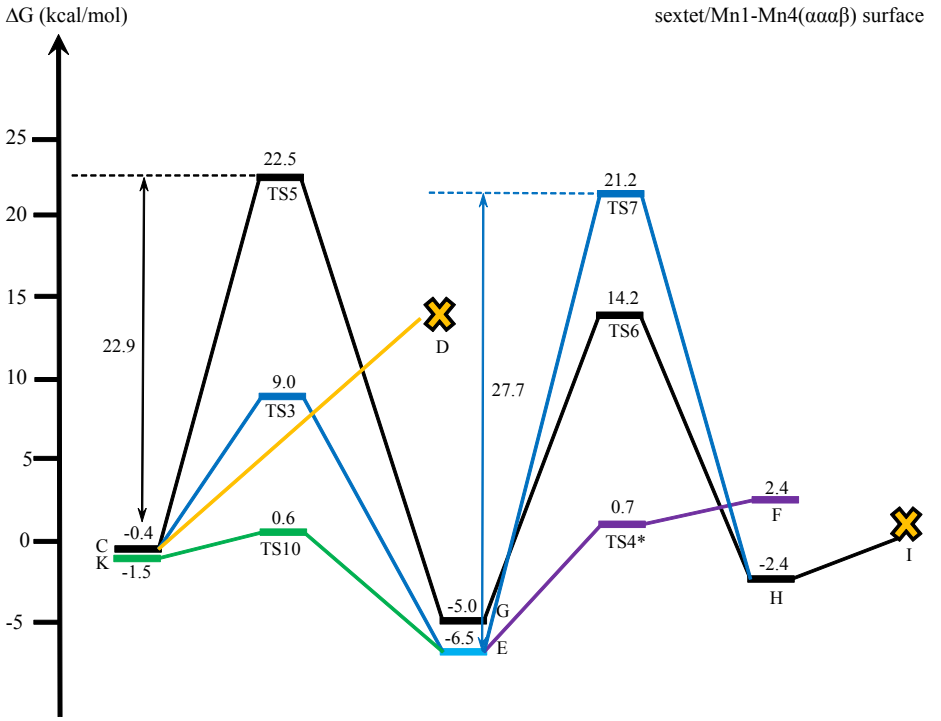


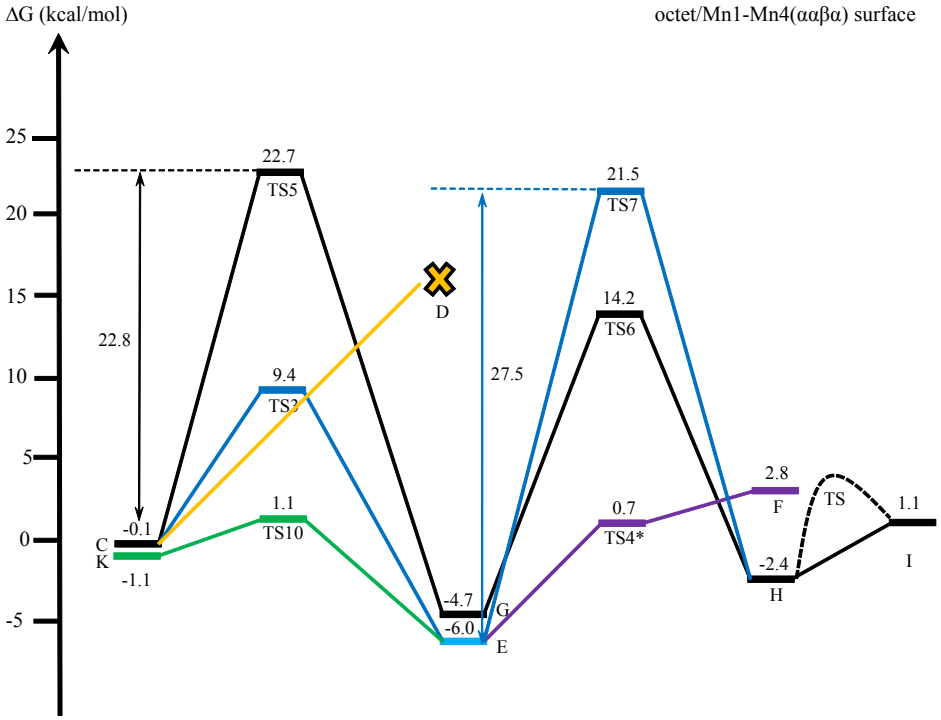
14-et/Mn-Mn4(αααα) surface

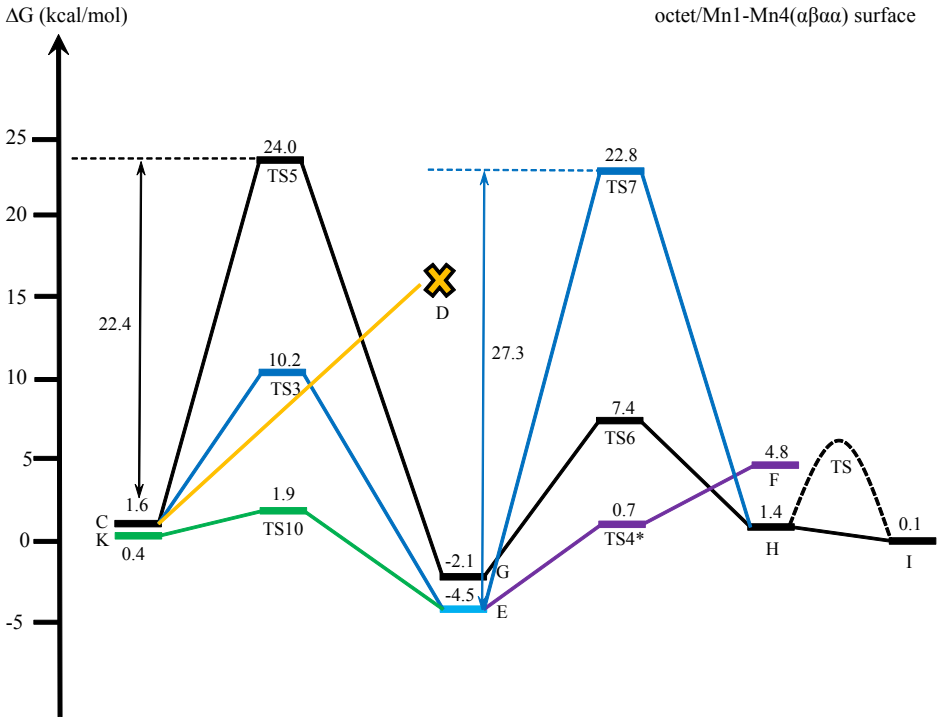

ΔG (kcal/mol)
doublet/Mn1-Mn4(αββα) surface
25
20
15
10
5
0
-5
Mn3 ligand exchange
23.7
TS5
23.7
Proton transfer
10.1
TS3
Proton transfer
D
27.7
NH3 binding
2.1
TS10
0.0
C
K
-0.3
g≥4.1 EPR signal
-4.0
G
-5.3
E
22.4
TS7
Mn3 ligand exchange
15.1
TS6
Proton transfer
Redox switch ?
Proton transfer
3.8
F
1.9
TS4*
TS
0.8
PCET
Redox switch
I
-2.0
H


ΔG (kcal/mol)
doublet/Mn1-Mn4(βαβα) surface
25
20
15
10
5
0
-5
24.0
TS5
22.7
10.7
TS3
D
27.5
4.3
TS10
1.3
C
K
0.2
-3.6
G
-4.6
E
22.9
TS7
15.1
TS6
4.0
F
2.3
TS4*
-1.9
H
I


ΔG (kcal/mol)
doublet/Mn1-Mn4(ββαα) surface
25
20
15
10
5
0
-5
24.2
TS5
22.7
TS7
22.3
D
26.7
10.7
TS3
7.5
TS6
5.1
F
2.9
TS4*
1.9
C
2.2
TS10
1.2
H
I
K
0.1
-1.3
G
-4.0
E


ΔG (kcal/mol)
sextet/Mn1-Mn4(αααβ) surface
25
20
15
10
5
0
-5
22.5
TS5
21.2
TS7
22.9
D
27.7
14.2
TS6
9.0
TS3
2.4
F
0.7
TS4*
-0.4
C
0.6
TS10
-2.4
H
I
K
-1.5
-5.0
G
-6.5
E


ΔG (kcal/mol)
octet/Mn1-Mn4(ααβα) surface
25
20
15
10
5
0
-5
22.7
TS5
21.5
TS7
14.2
TS6
9.4
TS3
1.1
TS10
0.7
TS4*
2.8
F
TS
1.1
I
-2.4
H
-4.7
G
-6.0
E
D
22.8
27.5
-0.1
C
K
-1.1


ΔG (kcal/mol)
octet/Mn1-Mn4(αβαα) surface
25
20
15
10
5
0
-5
24.0
TS5
22.8
TS7
10.2
TS3
1.9
TS10
7.4
TS6
0.7
TS4*
4.8
F
TS
0.1
I
1.4
H
-2.1
G
-4.5
E
D
22.4
27.3
1.6
C
K
0.4

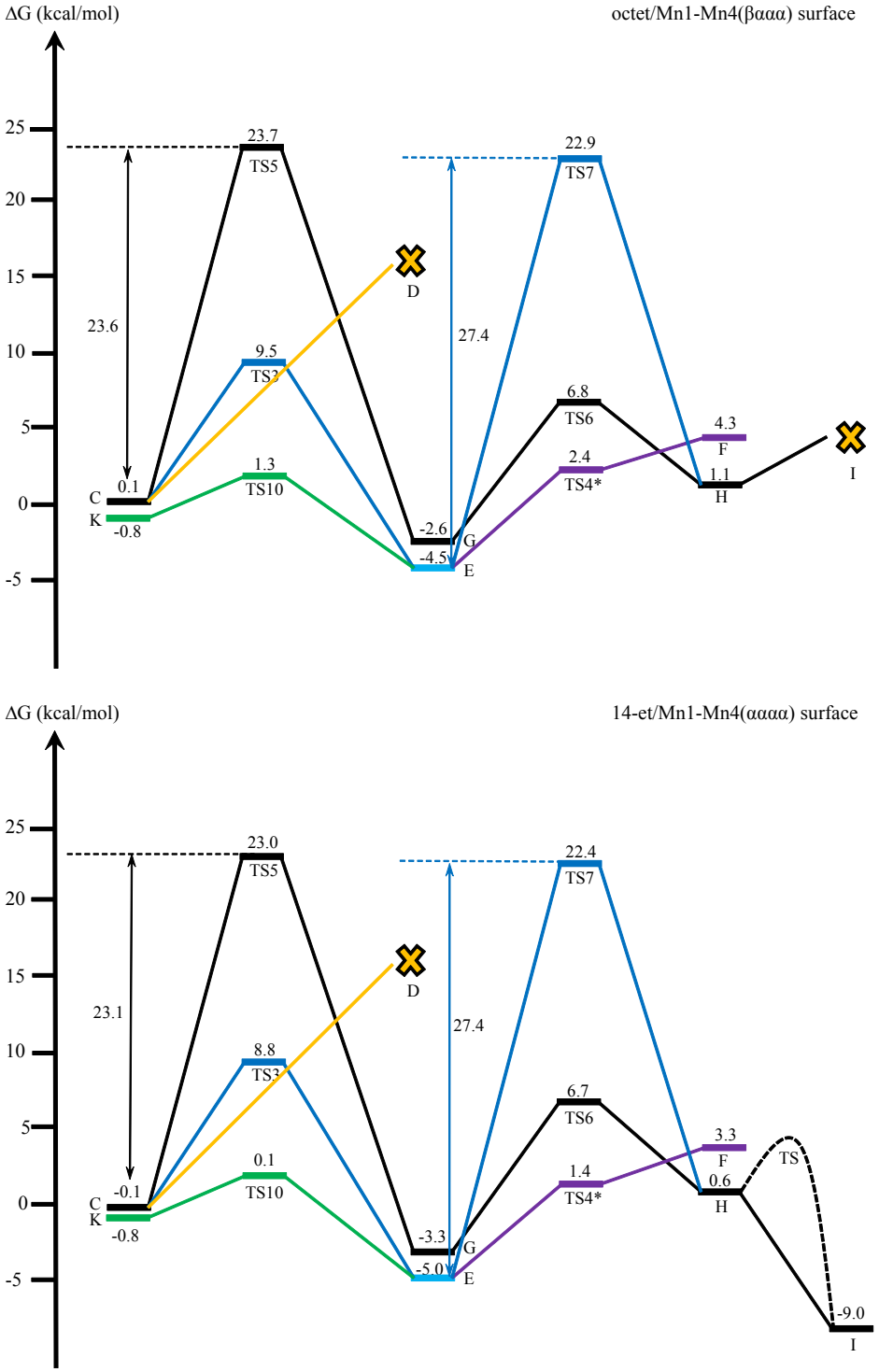


Figure SVa. Free energy profiles for the Mn4 addition scheme (only with the closed-

cubane structure) for all spin states.

The Cartesian coordinates for A to K, and TS3 to TS10:

A:

Ca	-2.58641000	0.50631300	-1.10537800	H	-0.01417100	-2.29042200	-5.13727500	H	4.21239100	3.33716400	0.43061200
Mn	0.11531000	-1.44228700	-0.70400400	H	-0.89367100	-3.56965900	-4.33413700	O	2.03226500	1.14268800	1.05253400
Mn	-1.52718000	-1.49314700	1.44022800	C	-2.14156100	-2.32426300	-5.61809400	C	2.55833300	2.01135300	0.31335700
Mn	0.00727700	0.76346100	1.09951000	H	-2.22203600	-1.26111800	-5.88521800	O	1.96376900	2.74067700	-0.56039800
Mn	0.09479700	3.26708200	-0.64058100	H	-3.08101300	-2.57979300	-5.10808500	O	0.31426400	-3.44837100	-0.28861500
O	-1.64094600	-1.67522800	-0.37321800	C	-1.99367000	-3.17181800	-6.88657500	C	-0.31039000	-4.01753500	0.66776300
O	0.30793300	-1.17579500	1.11298200	H	-1.07736100	-2.91296900	-7.43567300	O	-1.05971800	-3.45798700	1.52863300
O	-1.74132000	0.28480500	1.27070400	H	-1.94384700	-4.24339400	-6.64756600	C	-0.14695400	-5.53176600	0.76169300
O	-0.03263100	0.38374000	-0.75161100	H	-2.84262300	-3.02079500	-7.56561900	H	0.88331700	-5.77182300	0.46853800
O	-0.28314300	2.48422100	0.92013800	N	2.18237500	-1.48688700	-0.93903400	H	-0.78854200	-5.95613000	-0.02695300
O	-4.59904600	-0.05891700	-2.51025300	C	2.99458300	-0.92916900	-1.90073400	C	-0.50512200	-6.13217100	2.12219200
H	-5.01569300	-0.60208900	-1.81117800	H	2.57450000	-0.39716400	-2.74337300	H	-0.38553600	-7.22294200	2.10069800
H	-4.13453900	-0.67885800	-3.10545900	C	4.31234800	-1.17827100	-1.58739400	H	0.14108500	-5.73346300	2.91428100
O	-1.84775000	1.87571000	-3.06411700	N	4.26706000	-1.92418300	-0.41567100	H	-1.54013900	-5.89921100	2.39372800
H	-1.56843400	1.18168100	-3.68524200	H	5.07952300	-2.11479900	0.17791000	O	-4.37157600	-0.76626000	0.10868200
H	-1.08872100	2.52213700	-2.99828300	C	2.97470100	-2.06765900	-0.05069400	C	-4.39121900	-1.50303300	1.11527900
O	0.26476100	3.50028200	-2.51945500	H	2.64148000	-2.55908500	0.85125400	O	-3.35349000	-1.87901700	1.79517200
H	1.09895200	3.07375600	-2.78641500	C	5.58579300	-0.77562200	-2.28853700	C	-5.70336400	-2.04344100	1.65555600
O	0.79920000	5.54890500	-0.68804900	H	5.71278200	-1.36262100	-3.21042700	H	-6.53951000	-1.71844400	1.03054600
H	0.83307700	5.36789000	-1.65292800	H	5.47589700	0.26804900	-2.61577400	H	-5.84862100	-1.68489900	2.68226900
H	-0.12681500	5.83369800	-0.55323900	C	6.89521900	-0.92271500	-1.46645100	H	-5.66555700	-3.13891000	1.69706600
O	-3.15700600	2.70351200	-0.43143000	H	7.17380500	-1.97865700	-1.37980900	O	-1.10788800	-1.20813700	3.36502400
C	-2.78135800	3.88630900	-0.43533000	H	7.70303900	-0.41558800	-2.01171800	C	-0.40916000	-0.22756700	3.78728500
O	-1.56714700	4.27882300	-0.67224600	C	6.77494600	-0.39202800	-0.03827300	O	0.14951400	0.67202800	3.07904700
C	-3.80487300	4.98707500	-0.16945100	O	6.58888700	-1.16193200	0.91385700	C	-0.22712200	-0.13049500	5.29368600
H	-4.57305400	4.88859600	-0.95033200	N	6.79906100	0.95640700	0.11957000	H	0.35696700	-1.00820300	5.61083500
H	-4.30656300	4.71734800	0.77050500	H	6.91182000	1.53481800	-0.70406200	H	0.36456400	0.76569900	5.51293700
C	-3.26478000	6.41597900	-0.11249400	C	6.33502100	1.59205800	1.36004600	C	-1.56700600	-0.10975300	6.05132100
H	-2.79586300	6.70241300	-1.06207500	H	6.81459900	1.07366500	2.19652100	H	-2.13870800	-1.00660100	5.78066600
H	-2.51770300	6.52697900	0.68375900	H	6.69741400	2.62756900	1.35068900	H	-2.15788700	0.75417500	5.71250900
H	-4.07774800	7.12542100	0.08907000	C	4.80417700	1.53420800	1.51871300	C	-1.37332000	-0.04054400	7.56947100
O	-0.01403400	-1.80401100	-2.60332600	H	4.49274700	0.48529500	1.56590200	H	-0.81027700	-0.90938900	7.93866100
C	-1.04593700	-1.68093700	-3.37343600	H	4.53516600	1.98085200	2.48576600	H	-2.33975700	-0.02349300	8.08983600
O	-2.02851400	-0.94234900	-3.14489100	C	4.06398000	2.24886500	0.38659800	H	-0.82050600	0.86296100	7.86234500
C	-0.97365900	-2.51731800	-4.64773500	H	4.45668600	1.93144500	-0.59127200				

TS9:

Ca	-2.59412600	0.49160300	-1.04542100	H	-5.10443300	-0.61853100	-1.40071000	C	-2.64169000	4.03523600	-0.60001800
Mn	0.04510200	-1.59492400	-0.60087100	H	-4.33112500	-0.88826000	-2.73560500	O	-1.44305100	4.52569200	-0.77032600
Mn	-1.45232400	-1.33724100	1.63407200	O	-2.13068400	1.51894600	-3.24286900	C	-3.72698200	5.06299600	-0.29513700
Mn	0.09797400	0.81457400	0.91490300	H	-1.98385500	0.75255100	-3.82275500	H	-4.66403600	4.67143800	-0.70947700
Mn	0.21616900	3.57216200	-0.72524200	H	-1.25656100	2.00504500	-3.19315200	H	-3.85047800	5.05378800	0.79981600
O	-1.69017400	-1.72159600	-0.12777700	O	0.21331500	2.68576000	-2.78768400	C	-3.44801200	6.48765800	-0.77958500
O	0.36782000	-1.09924800	1.15654400	H	0.91053400	2.00860900	-2.76214800	H	-3.33592100	6.52095900	-1.87112300
O	-1.63782000	0.41303800	1.26199000	O	0.85833900	4.85720500	-2.15216600	H	-2.52796800	6.88258900	-0.33469500
O	-0.04058900	0.20477200	-0.85921700	H	0.65533000	3.86072500	-2.78128600	H	-4.27682400	7.15342400	-0.50679500
O	-0.27203900	2.50391600	0.58077600	H	0.11535400	5.46195600	-2.33542200	O	-0.25825200	-2.17980900	-2.41739000
O	-4.74068600	-0.18262000	-2.19767800	O	-2.93290500	2.83295100	-0.65666100	C	-1.34702200	-2.09131500	-3.11269400

O	-2.27336000	-1.28160500	-2.89660300	H	7.49792900	-0.44615100	-2.38796500	H	-0.37317000	-6.95675300	2.95528400
C	-1.41656000	-3.07280600	-4.27910500	C	6.70773700	-0.52463600	-0.35676500	H	0.21124200	-5.38531800	3.54461100
H	-0.48716600	-2.96352400	-4.85844200	O	6.55502800	-1.33402300	0.56806400	H	-1.49533900	-5.58512600	3.12904600
H	-1.36834800	-4.08458900	-3.84739600	N	6.78065500	0.81439300	-0.14022300	O	-4.33346400	-0.56728000	0.44790500
C	-2.64446000	-2.92327000	-5.18063000	H	6.86647800	1.42624500	-0.94268300	C	-4.32133500	-1.22628100	1.50682200
H	-2.68782900	-1.89653000	-5.57088000	C	6.40214700	1.40514700	1.14933400	O	-3.25957000	-1.61334000	2.14299100
H	-3.55392700	-3.05643100	-4.57813100	H	6.85667100	0.79283100	1.93429800	C	-5.61869300	-1.65068500	2.17220400
C	-2.64140800	-3.92283800	-6.34255000	H	6.84925100	2.40605600	1.19746400	H	-6.47894600	-1.30144100	1.59479300
H	-1.75749700	-3.78956700	-6.98208400	C	4.87566300	1.46045900	1.34524500	H	-5.66073700	-1.23685900	3.18732300
H	-2.63164500	-4.95947200	-5.97757500	H	4.47512200	0.44169500	1.30214300	H	-5.64661100	-2.74335200	2.26650300
H	-3.53085400	-3.79997900	-6.97379000	H	4.66444900	1.83518100	2.35661200	O	-0.90533800	-0.83148400	3.48283600
N	2.08340300	-1.69959600	-1.00513800	C	4.17643800	2.33858700	0.30532500	C	-0.16250500	0.17399300	3.73656300
C	2.81708600	-1.04761300	-1.97087000	H	4.53911100	2.09551000	-0.70620100	O	0.36204000	0.96825700	2.89011200
H	2.33034700	-0.45652600	-2.73454400	H	4.39997900	3.40357200	0.45327200	C	0.12915800	0.44271500	5.20513500
C	4.15679500	-1.29394500	-1.77341300	O	2.10671700	1.20499200	0.75615600	H	0.75936300	-0.38412600	5.56838000
N	4.20771700	-2.13276500	-0.66684000	C	2.65712100	2.20126600	0.22134400	H	0.71507800	1.36635100	5.27716100
H	5.06243700	-2.32909400	-0.13738500	O	2.09635400	3.13058700	-0.46075800	C	-1.14627200	0.52546900	6.06196100
C	2.94654800	-2.33341200	-0.22591900	O	0.24822300	-3.53456000	0.06301300	H	-1.71536700	-0.40453300	5.93764900
H	2.68596500	-2.91301400	0.64685700	C	-0.32662500	-3.96384700	1.11861100	H	-1.78366200	1.33695400	5.68030500
C	5.37006800	-0.81858400	-2.53245400	O	-1.01742100	-3.28202200	1.93929900	C	-0.83555500	0.76515100	7.54292000
H	5.44369000	-1.34450900	-3.49614700	C	-0.17918200	-5.45598600	1.39993300	H	-0.22387400	-0.04847200	7.95776100
H	5.21949400	0.24075200	-2.78369900	H	0.83208100	-5.75216600	1.09179100	H	-1.75807500	0.82413600	8.13497800
C	6.73538400	-0.98823900	-1.81211900	H	-0.86371700	-5.96542700	0.70318300	H	-0.28383200	1.70413700	7.69025300
H	7.02858800	-2.04383900	-1.79677700	C	-0.47775600	-5.87017600	2.84173200				

J:

Ca	-2.58223700	0.06677500	-1.20049400	O	-2.31130000	-2.31218600	-2.15385200	H	4.46565600	0.96043700	1.11072900
Mn	0.04694900	-1.60585100	0.04375800	C	-1.29825300	-4.40463000	-2.82561000	H	4.64556200	2.65003100	1.56184100
Mn	-1.49784300	-0.54472300	1.99178100	H	-0.37543500	-4.43145900	-3.42418200	C	4.16993300	2.33834400	-0.53085100
Mn	0.06586600	1.21702900	0.57721300	H	-1.17196100	-5.18977700	-2.06398200	H	4.53770800	1.73239200	-1.37357700
Mn	0.23688400	2.99635100	-2.01480700	C	-2.52537100	-4.68349400	-3.69692800	H	4.39193800	3.38114900	-0.79558600
O	-1.69653900	-1.56197800	0.49968500	H	-2.63937300	-3.87620000	-4.43457700	O	2.08818200	1.48291700	0.31641400
O	0.32809900	-0.49242700	1.49459600	H	-3.42849100	-4.65335300	-3.07136900	C	2.65352500	2.17364300	-0.56920600
O	-1.67895800	0.94164700	0.99457800	C	-2.43590800	-6.03400800	-4.41617900	O	2.10351200	2.73829600	-1.58178800
O	-0.05367400	-0.00905200	-0.88391900	H	-1.55730500	-6.07812500	-5.07484100	O	0.23558200	-3.15049200	1.36482200
O	-0.24495100	2.67942300	-0.32663200	H	-2.35383900	-6.86318900	-3.69948500	C	-0.35952200	-3.16944900	2.49639000
O	-4.73117700	-0.96749700	-2.04494100	H	-3.32506400	-6.21408800	-5.03400300	O	-1.06782800	-2.24365300	2.99874800
H	-5.12881800	-0.98733100	-1.14995400	N	2.08400600	-1.83466900	-0.27838300	C	-0.20643600	-4.45534100	3.30202000
H	-4.35085600	-1.85649100	-2.18855000	C	2.83561500	-1.60253700	-1.41286400	H	0.82219600	-4.81262500	3.16120700
O	-2.01028500	0.01547100	-3.65877400	H	2.37317400	-1.31966200	-2.35100500	H	-0.84957400	-5.20127900	2.80878100
H	-2.30687900	-0.88636500	-3.87429500	C	4.16735700	-1.77827500	-1.11458200	C	-0.56640200	-4.33123400	4.78322000
H	-1.01565100	-0.03072200	-3.77178000	N	4.19650200	-2.14355100	0.22645300	H	-0.45107200	-5.30052400	5.28471000
O	0.68557400	-0.08097200	-3.56224000	H	5.04310700	-2.13992800	0.80241100	H	0.08146600	-3.60494900	5.28953000
H	0.58387300	-0.08144100	-2.57833500	C	2.92995500	-2.14446400	0.69385100	H	-1.60063700	-3.99379000	4.90929600
O	0.65020400	2.65327900	-3.78755800	H	2.65369400	-2.35198500	1.71659100	O	-4.35821500	-0.29134600	0.54500100
H	0.85600600	0.87410300	-3.78121500	C	5.39327700	-1.63890500	-1.98094800	C	-4.36804200	-0.50340700	1.77543100
H	-0.11247700	2.88080900	-4.34962100	H	5.47159900	-2.49549400	-2.66699900	O	-3.32002500	-0.62608500	2.52751800
O	-2.85412700	2.35287900	-1.80727500	H	5.25350500	-0.75846100	-2.62329800	C	-5.67967200	-0.63890300	2.52796600
C	-2.57131300	3.50293400	-2.17588700	C	6.74889400	-1.52579100	-1.23137000	H	-6.52757300	-0.55138400	1.84325700
O	-1.36814800	3.90155300	-2.48315300	H	7.03659300	-2.49814100	-0.81621400	H	-5.74144400	0.14351500	3.29462500
C	-3.66109900	4.56148200	-2.28051000	H	7.52184200	-1.23987800	-1.95786600	H	-5.71183600	-1.60448200	3.04741200
H	-4.59580600	4.03912400	-2.51795600	C	6.70660100	-0.55036900	-0.05681700	O	-0.99177700	0.60333600	3.53846600
H	-3.78593500	4.96478100	-1.26260200	O	6.54460100	-0.95311000	1.10309000	C	-0.24559500	1.63046300	3.42483300
C	-3.38215200	5.69948300	-3.26559500	N	6.77852600	0.77277100	-0.35792400	O	0.29417800	2.06573500	2.35527200
H	-3.26954500	5.32007700	-4.28930800	H	6.86658400	1.03849400	-1.33128500	C	0.03476500	2.41024200	4.69986200
H	-2.46136900	6.23135600	-3.00264700	C	6.39094300	1.80244400	0.61344100	H	0.68267500	1.77949600	5.32875500
H	-4.21109100	6.41858800	-3.26197800	H	6.84171600	1.53154400	1.57321400	H	0.60194600	3.31019100	4.43548200
O	-0.23476100	-2.81915200	-1.42792900	H	6.83568200	2.75024900	0.28474000	C	-1.24318500	2.76558000	5.47936800
C	-1.32107100	-3.07090200	-2.08712800	C	4.86315700	1.92196300	0.76781300	H	-1.79302200	1.84094300	5.69581400

H	-1.89662500	3.37662400	4.83901700	H	-0.31159400	2.91825800	7.44994900	H	-0.40651500	4.46095500	6.57941400
C	-0.93896100	3.52022700	6.77748500	H	-1.86323200	3.76723100	7.31569200				

C:

Ca	2.79226800	-0.77450700	-0.20754800	H	1.98439500	3.65435500	-2.68446900	C	-2.69249800	-2.32440000	0.54540700
Mn	0.06743700	1.35737100	-1.02121600	C	3.64663600	3.31833500	-4.06652200	O	-2.12991600	-3.44835200	0.49558800
Mn	1.14656200	1.73202800	1.42612300	H	3.84716400	2.69648600	-4.94949900	O	-0.22362200	3.39066800	-0.93657100
Mn	-0.25035300	-0.62806000	1.02933100	H	4.34904300	2.97671100	-3.29178000	C	0.13981500	4.09918700	0.06387700
Mn	0.04636600	-3.72129600	0.12579000	C	3.91341200	4.79290400	-4.38794400	O	0.67874900	3.68024700	1.13233700
O	1.71340800	1.63810700	-0.31663400	H	3.24755900	5.15354100	-5.18468600	C	-0.08435000	5.60266100	-0.07170100
O	-0.55466600	1.30450500	0.71417300	H	3.74954100	5.42977900	-3.50708000	H	-1.06382300	5.74847900	-0.54690400
O	1.39066700	-0.02450000	1.60062400	H	4.94739800	4.94695400	-4.72296200	H	0.65503700	5.95853000	-0.80646200
O	0.20581500	-0.44463300	-0.77510400	N	-1.86095300	1.24732600	-1.78015400	C	0.03255200	6.39010100	1.23380800
O	0.36797400	-2.27037200	1.13350900	C	-2.42480600	0.24833300	-2.54286100	H	-0.12037700	7.46081600	1.04747600
O	4.62095300	0.15768500	-1.57900700	H	-1.83352000	-0.58598300	-2.89447900	H	-0.71562200	6.05899700	1.96447700
H	4.91799600	0.93874300	-1.08082600	C	-3.76124500	0.51598800	-2.72797400	H	1.01930600	6.25232800	1.68867000
H	4.20844600	0.48444400	-2.41125700	N	-3.98440100	1.71868600	-2.06729200	O	4.19571700	0.71949100	1.17624800
O	2.43917800	-1.85106500	-2.38395700	H	-4.91407200	2.06434700	-1.81486300	C	3.97293700	1.65358900	1.96929000
H	2.29246600	-1.10122800	-3.00454000	C	-2.82427700	2.11030400	-1.49537300	O	2.82105100	2.21891000	2.17501600
H	1.59474900	-2.35910100	-2.30772400	H	-2.70586600	2.99475300	-0.88774600	C	5.09361500	2.23399700	2.81505400
O	0.02769500	-2.96640800	-1.55488400	C	-4.82573100	-0.24594100	-3.47401800	H	5.08073100	3.32886400	2.76512900
H	-0.14925100	-1.99655000	-1.44776000	H	-4.72225100	-0.08325600	-4.55752700	H	6.06101700	1.84613000	2.48452200
O	-0.14292200	-5.53088000	-1.03553000	H	-4.64476900	-1.31813000	-3.31613000	H	4.93017700	1.95387700	3.86414000
H	-0.29583400	-5.04617700	-1.87388800	C	-6.29319900	0.09529800	-3.09553500	O	0.24541200	1.69691000	3.20959700
H	0.83826200	-5.66644800	-0.99244100	H	-6.57622600	1.06949900	-3.50955600	C	-0.50330800	0.73838700	3.59395200
O	3.44757700	-2.97601500	0.34101100	H	-6.95240100	-0.65628300	-3.55117600	O	-0.84987200	-0.28622400	2.92066200
C	3.23808600	-4.17808500	0.04993600	C	-6.51226500	0.18398700	-1.58636700	C	-1.03013300	0.83144600	5.01974900
O	2.07932400	-4.73031700	0.00228800	O	-6.51364100	1.27709500	-1.00527900	H	-1.76254500	0.02932100	5.16965900
C	4.45847400	-5.05348600	-0.24981300	N	-6.62957500	-0.99566000	-0.92148100	H	-0.17826700	0.63043700	5.68886200
H	5.02867900	-4.53484000	-1.03355100	H	-6.56034400	-1.85075700	-1.46002300	C	-1.63119100	2.20534800	5.35855200
H	5.09806600	-5.01921500	0.64465400	C	-6.45143800	-1.08486800	0.53219100	H	-2.46846000	2.41074700	4.67442200
C	4.16457800	-6.49865800	-0.65218300	H	-6.94567200	-0.21164700	0.96850700	H	-0.87571200	2.97749100	5.16667800
H	3.57483200	-6.54190900	-1.57690900	H	-6.98018000	-1.98299600	0.87720600	C	-2.11780900	2.28574300	6.80912900
H	3.59883000	-7.02324500	0.12782400	C	-4.96790500	-1.11638000	0.94478600	H	-2.89129200	1.53267500	7.01589100
H	5.09788400	-7.05058100	-0.82466400	H	-4.48141600	-0.19399000	0.60810200	H	-2.54617800	3.27246300	7.02831400
O	0.66479900	1.40965000	-2.84415300	H	-4.91206200	-1.11626300	2.04308200	H	-1.29259800	2.11597900	7.51505200
C	1.87538600	1.62353000	-3.27626000	C	-4.21764200	-2.32725900	0.38432800	N	-0.06357900	-4.87669900	1.89079300
O	2.70055400	0.70968300	-3.46651700	H	-4.38166900	-2.39867300	-0.70356700	H	-0.95280400	-5.36964700	1.97922400
C	2.21305200	3.07377700	-3.59024500	H	-4.59152200	-3.26761900	0.81070200	H	0.02492400	-4.19622200	2.64734600
H	1.48588100	3.41643600	-4.34325300	O	-2.13743700	-1.17531100	0.65313900	H	0.71741900	-5.53294000	1.93097700

TS3:

Ca	-2.39385100	-0.28207400	-1.34406200	H	-0.14428900	1.59006100	-3.41284800	C	-0.72851200	-4.42785100	-3.27596000
Mn	0.30451400	-1.82277400	-0.08200200	O	0.75460000	4.47092600	-3.16538100	H	0.21165200	-4.35539900	-3.84428100
Mn	-1.43455900	-1.05179900	1.83279800	H	0.75304500	3.33904200	-3.52542600	H	-0.58708500	-5.27641400	-2.58984200
Mn	-0.02875100	0.94159900	0.54148700	H	1.67654700	4.66682400	-2.91140800	C	-1.91109000	-4.67452600	-4.21547700
Mn	-0.01686100	3.38389300	-1.63181500	O	-3.28029600	1.89068000	-2.13370800	H	-2.04582800	-3.79918400	-4.86604100
O	-1.45079300	-2.01305500	0.29953100	C	-3.20180600	3.15293700	-1.94512500	H	-2.83345000	-4.75816400	-3.62274400
O	0.39231900	-0.74627000	1.42964500	O	-2.19218800	3.86270300	-2.21387700	C	-1.72888000	-5.93597800	-5.06710900
O	-1.75657700	0.44609400	0.90222200	C	-4.46015100	3.81855500	-1.38270200	H	-0.83029800	-5.86632900	-5.69627800
O	0.06711400	-0.22911500	-0.91284900	H	-5.26385400	3.63553200	-2.11130700	H	-1.62251500	-6.83087600	-4.43801600
O	-0.64809600	2.30275800	-0.39256700	H	-4.74874000	3.25209800	-0.48574600	H	-2.58873100	-6.09547800	-5.73067000
O	-4.34489400	-1.39400300	-2.52161900	C	-4.34019600	5.31096600	-1.07721700	N	2.33212400	-1.78901200	-0.45703800
H	-4.80089100	-1.57583700	-1.67411200	H	-4.01305700	5.87074600	-1.96147500	C	2.96691600	-1.04194800	-1.42749500
H	-3.81110400	-2.19105300	-2.71868800	H	-3.61494500	5.49645600	-0.27303500	H	2.39808300	-0.38094200	-2.06890500
O	-1.67895600	0.62152100	-3.68217000	H	-5.30446400	5.71982200	-0.74820600	C	4.31873200	-1.28432000	-1.36778500
H	-2.00482600	0.21784500	-4.50322500	O	0.16838800	-2.99554000	-1.62234200	N	4.48059000	-2.21182500	-0.34183200
H	-2.34246300	1.31786500	-3.39331300	C	-0.83355300	-3.16815500	-2.41925500	H	5.37004300	-2.37558000	0.13228900
O	0.56697300	2.17137100	-3.05429200	O	-1.81176600	-2.39820000	-2.53203500	C	3.26442500	-2.46998900	0.19101900

H	3.07855700	-3.13422300	1.02234800	H	4.24698500	3.68312600	0.32497400	H	-5.74911300	-1.26525500	2.97090800
C	5.45478200	-0.75028600	-2.19827300	O	1.89423200	1.50265300	0.45775600	H	-5.52865100	-2.87829200	2.28610300
H	5.56632300	-1.33987300	-3.12117900	C	2.47734400	2.53186500	-0.01453200	O	-1.14526700	0.08719900	3.44948300
H	5.18025000	0.26223200	-2.52321200	O	1.96222600	3.46893500	-0.68451700	C	-0.55659100	1.21721600	3.40723700
C	6.84223200	-0.71981200	-1.49680100	O	0.66081500	-3.39144400	1.19551300	O	-0.04200200	1.77777900	2.38585100
H	7.27151300	-1.72710300	-1.45565000	C	0.03980900	-3.52128600	2.30525200	C	-0.43920200	1.96422900	4.73006700
H	7.52418300	-0.09939200	-2.09441300	O	-0.81839500	-2.72519000	2.79578400	H	0.35396600	1.46372400	5.30869800
C	6.74749500	-0.22379900	-0.05610400	C	0.37529500	-4.77668200	3.10606100	H	-0.09269500	2.98359400	4.52073900
O	6.69482400	-1.01822300	0.88975100	H	1.47020800	-4.81457600	3.20198400	C	-1.73980900	1.97258000	5.54856900
N	6.64501900	1.12437400	0.10567400	H	0.10693900	-5.63336500	2.46986800	H	-2.06261100	0.93627400	5.70779500
H	6.63556700	1.69385100	-0.73209000	C	-0.30320400	-4.87281400	4.47227300	H	-2.53323400	2.45787500	4.96038000
C	6.10946600	1.72126000	1.33323200	H	-0.01273500	-5.80351300	4.97659200	C	-1.57812800	2.69236700	6.89146200
H	6.47133600	1.10999100	2.16517600	H	-0.02177700	-4.02972800	5.11406300	H	-0.81327300	2.20627200	7.51354600
H	6.54147400	2.72569000	1.43599300	H	-1.39434700	-4.85846000	4.37236600	H	-2.51881800	2.68960900	7.45736600
C	4.56978600	1.77137800	1.33947300	O	-4.21345400	-1.06288300	0.20235300	H	-1.27548800	3.73997500	6.75268300
H	4.17565000	0.75118300	1.26913500	C	-4.26552600	-1.37872000	1.41007300	N	-0.43819200	5.09838000	-0.45065300
H	4.23622900	2.16826900	2.30917100	O	-3.26776900	-1.39175800	2.23647000	H	0.27092700	5.83078200	-0.46367200
C	3.99279800	2.62120500	0.20405500	C	-5.58136300	-1.81062000	2.03508200	H	-0.58106500	4.77390600	0.50653500
H	4.42971600	2.31269900	-0.75989400	H	-6.41065000	-1.63812400	1.34341500	H	-1.32127500	5.44477800	-0.83211600

E:

Ca	-2.84888200	0.30271500	-0.62725300	H	-1.78540900	-4.13178500	-3.74622400	C	2.53188400	2.30105000	-0.11102700
Mn	-0.02145200	-1.62104300	-0.67734300	C	-3.27382400	-3.00039600	-4.86757800	O	1.88877400	3.27675000	-0.61244700
Mn	-1.16063700	-1.47266400	1.76024200	H	-3.40804900	-1.97054800	-5.22791400	O	0.37439500	-3.54714800	-0.13111100
Mn	0.12207300	0.80559600	0.87050300	H	-4.08595900	-3.17676700	-4.14851900	C	-0.00287500	-4.03684100	0.98983700
Mn	-0.11630300	3.80017200	-0.53262100	C	-3.39656100	-3.98173200	-6.03857200	O	-0.58052500	-3.41830700	1.93272700
O	-1.65172700	-1.85000400	0.04083900	H	-2.61532900	-3.80555500	-6.79140800	C	0.26340200	-5.52744700	1.17863100
O	0.53586000	-1.13651800	1.00977600	H	-3.29941100	-5.02260100	-5.69930300	H	1.24263100	-5.74816000	0.73327800
O	-1.51629300	0.25398500	1.47136300	H	-4.36885600	-3.88326700	-6.53817000	H	-0.47300600	-6.05043600	0.54820100
O	-0.26046900	0.19017000	-0.89470900	N	1.94318100	-1.61168400	-1.38798100	C	0.17537300	-6.01622400	2.62497000
O	-0.39025400	2.43158300	0.64132800	C	2.51624500	-0.89963800	-2.41791800	H	0.35361600	-7.09811800	2.67297400
O	-5.06230400	-0.56085800	-1.48814200	H	1.91351400	-0.28826200	-3.07579000	H	0.92032400	-5.51832000	3.25806500
H	-5.26646900	-1.03646100	-0.65782200	C	3.87504300	-1.12098900	-2.42994500	H	-0.81134600	-5.80545600	3.05084600
H	-4.67244500	-1.21827100	-2.09707300	N	4.10228400	-2.00662400	-1.38399700	O	-4.24980700	-0.91623300	1.06838500
O	-2.81949900	1.36566200	-2.90509200	H	5.02759500	-2.20769300	-0.99406700	C	-4.01790500	-1.57839000	2.10040100
H	-2.67079000	0.57817200	-3.45828600	C	2.92304600	-2.25714400	-0.77440300	O	-2.84278600	-1.88887800	2.54888000
H	-1.99245800	1.89853800	-2.95844700	H	2.80365600	-2.88322900	0.09671500	C	-5.15780100	-2.10005400	2.95803400
O	0.32892100	5.07063100	-1.77534900	C	4.95802800	-0.58421300	-3.33146300	H	-5.09023400	-3.19196300	3.04055700
H	1.30228500	5.12491900	-1.78017900	H	4.90988300	-1.07300300	-4.31615600	H	-6.12270800	-1.81453400	2.53038200
O	-0.30936800	2.31088100	-2.39121700	H	4.74879000	0.47862300	-3.51781700	H	-5.06689500	-1.69243200	3.97249700
H	0.45510600	2.67328600	-2.86993200	C	6.41385000	-0.74002600	-2.81240400	O	-0.35809400	-0.97137600	3.51174500
H	-0.06089400	1.44268900	-1.94744400	H	6.73558000	-1.78440800	-2.89030600	C	0.34310100	0.08026400	3.67980300
O	-3.28877300	2.57841400	-0.23466400	H	7.07562100	-0.14595200	-3.45749400	O	0.67118900	0.93290600	2.79277500
C	-3.12183500	3.81291100	-0.30325800	C	6.57263500	-0.34634800	-1.34451600	C	0.82486000	0.34763900	5.09910900
O	-2.00761300	4.41955500	-0.52693000	O	6.58731000	-1.20420600	-0.45187800	H	1.54205900	1.17662000	5.06901100
C	-4.35081200	4.71551200	-0.15698100	N	6.61697500	0.98379100	-1.07127800	H	-0.05081300	0.69135600	5.67277100
H	-4.88605400	4.65600000	-1.11774800	H	6.55340300	1.63247700	-1.84648600	C	1.42947800	-0.88920900	5.78275500
H	-5.01237700	4.24569300	0.58219900	C	6.38324300	1.49844500	0.28336700	H	2.29207700	-1.23965200	5.19588900
C	-4.06123200	6.17560600	0.19443100	H	6.93914200	0.85658900	0.97358200	H	0.69023900	-1.69965200	5.76299700
H	-3.40055200	6.63307600	-0.55012200	H	6.81599900	2.50585800	0.33288300	C	1.86666200	-0.60251100	7.22293800
H	-3.57084600	6.25796400	1.17455600	C	4.88995200	1.51111100	0.66134200	H	2.62384100	0.19330300	7.26243700
H	-4.99199600	6.75655400	0.23967400	H	4.50308000	0.48650900	0.63202100	H	2.29847800	-1.49698900	7.69046100
O	-0.55245800	-2.19345200	-2.45516200	H	4.79673900	1.84915000	1.70328800	H	1.01569100	-0.28138800	7.84003600
C	-1.73237400	-2.15061500	-2.98117500	C	4.05418100	2.40656900	-0.25564600	N	0.14143700	5.19629400	1.25149400
O	-2.65639700	-1.39199700	-2.61323800	H	4.25785100	2.15775100	-1.30983800	H	0.94911200	5.81582400	1.30524100
C	-1.92829000	-3.11616800	-4.14716700	H	4.32243200	3.46526900	-0.13810700	H	0.08999900	4.62666800	2.09676800
H	-1.09241800	-2.96380500	-4.84663100	O	2.06183700	1.25694800	0.42554000	H	-0.70516400	5.76251600	1.18307600

TS4:

Ca	-2.76557900	0.15679800	-0.86119200	H	-1.26064000	-4.51399200	-3.46629500	C	2.59014900	2.38539100	0.16580800
Mn	0.17540100	-1.70963600	-0.51373700	C	-2.74251000	-3.56545400	-4.75539800	O	2.06003100	3.35888900	-0.42180900
Mn	-1.18766200	-1.36503100	1.79221900	H	-2.91129700	-2.57661400	-5.20438000	O	0.60911800	-3.49940100	0.18615800
Mn	0.08356000	0.91300800	0.86600000	H	-3.58305100	-3.73282500	-4.06718700	C	0.17715500	-3.92849900	1.32510200
Mn	-0.10813800	3.58706500	-1.03082900	C	-2.74523800	-4.64160900	-5.84681200	O	-0.51753200	-3.28968200	2.15630600
O	-1.49302800	-1.91867100	0.07212000	H	-1.93372100	-4.47917500	-6.57003700	C	0.56652300	-5.36680900	1.64806200
O	0.54850500	-1.02773900	1.15150600	H	-2.61092800	-5.64517900	-5.41926600	H	1.64987500	-5.45805300	1.48391200
O	-1.59345200	0.30117300	1.33900000	H	-3.69176300	-4.63984200	-6.40234200	H	0.09970100	-5.99713600	0.87626800
O	-0.16465900	0.13655100	-0.90253100	N	2.16832100	-1.60617000	-1.14124000	C	0.17429700	-5.83187900	3.05021100
O	-0.47693100	2.46082900	0.40726600	C	2.76783000	-0.72255300	-2.01436400	H	0.47993900	-6.87478100	3.20200900
O	-4.84122900	-0.87581500	-1.86302000	H	2.19196100	0.03472400	-2.52788800	H	0.65323600	-5.21598100	3.82039100
H	-5.11046500	-1.31014400	-1.02929400	C	4.11909200	-0.97409000	-2.06595000	H	-0.90874800	-5.76195200	3.19993200
H	-4.36144000	-1.55029300	-2.38305300	N	4.31819300	-2.05077900	-1.21042000	O	-4.21616100	-1.07045600	0.78203300
O	-2.36539100	1.06897800	-3.15136300	H	5.23309600	-2.30609100	-0.82901400	C	-4.04961400	-1.63142500	1.88270400
H	-2.12336500	0.28801600	-3.67744500	C	3.12896700	-2.38284000	-0.66184000	O	-2.90480600	-1.82964600	2.46071200
H	-1.52944900	1.59946100	-3.04820200	H	2.98522100	-3.16756700	0.06526500	C	-5.23440700	-2.15112700	2.67727600
O	0.55444100	4.69285200	-2.32793900	C	5.22100800	-0.30948200	-2.84946300	H	-6.16581600	-1.98911600	2.12816300
H	1.50267700	4.79607100	-2.12218500	H	5.23382400	-0.68492900	-3.88392100	H	-5.28032000	-1.63126100	3.64246800
O	0.01404200	2.03689100	-2.35005000	H	4.98081300	0.75990500	-2.92339500	H	-5.10119800	-3.21890800	2.89012200
H	0.10513400	0.89473900	-1.66770500	C	6.65641600	-0.48324500	-2.27722800	O	-0.56343800	-0.70539600	3.55544100
H	0.66362200	2.32985600	-3.01117400	H	7.02701800	-1.49437100	-2.47915900	C	0.04605000	0.40354400	3.70886200
O	-3.44308900	2.38567000	-0.67968200	H	7.32402700	0.21811000	-2.79604300	O	0.40078500	1.21524800	2.79213100
C	-3.28006500	3.57729800	-1.04526800	C	6.70837100	-0.29098000	-0.76288800	C	0.39185600	0.79144800	5.13794500
O	-2.16408700	4.13599900	-1.31756100	O	6.67637200	-1.26280300	0.00304400	H	1.16382100	0.08767000	5.48669500
C	-4.54222700	4.43365900	-1.21359400	N	6.70614100	0.99348800	-0.31749100	H	0.83599800	1.79361600	5.12640000
H	-5.02833900	4.07984900	-2.13638300	H	6.67868900	1.73008900	-1.01234000	C	-0.81955200	0.73000400	6.08480400
H	-5.22972600	4.17185000	-0.39832400	C	6.30289100	1.33631900	1.05167700	H	-1.24823800	-0.27923200	6.04364700
C	-4.30780900	5.94298100	-1.28646000	H	6.72789700	0.57262700	1.70957700	H	-1.59777200	1.41604400	5.71863100
H	-3.61053700	6.19049900	-2.09451900	H	6.76490200	2.29933100	1.30516400	C	-0.44717700	1.09171100	7.52620600
H	-3.87925000	6.32442100	-0.34874300	C	4.77111500	1.38720100	1.21161400	H	0.30779900	0.40093400	7.92743300
H	-5.25071600	6.47863800	-1.46131900	H	4.35419900	0.40270200	0.97038100	H	-1.32506700	1.04474000	8.18341600
O	-0.21148700	-2.42862600	-2.26764400	H	4.53279200	1.57284200	2.26839800	H	-0.03549400	2.10861700	7.59161200
C	-1.35637200	-2.47407200	-2.87494900	C	4.11556300	2.45472700	0.33200200	N	-0.23757300	5.22478700	0.36443100
O	-2.32153400	-1.71816600	-2.64317500	H	4.51080800	2.40071200	-0.69488600	H	0.53268100	5.89164900	0.35979900
C	-1.43525900	-3.54512400	-3.95939200	H	4.35466500	3.46752000	0.68599900	H	-0.36769600	4.83803400	1.29979600
H	-0.57112500	-3.40237500	-4.62596400	O	2.01421400	1.32641200	0.59661100	H	-1.09905300	5.68083300	0.05811200

F:

Ca	-2.76039100	0.14530800	-0.86379900	O	-3.53164700	2.34005300	-0.65850900	H	-2.56579400	-5.62347700	-5.46332700
Mn	0.21795100	-1.73304600	-0.52141800	C	-3.38052600	3.52893500	-1.04450600	H	-3.65966900	-4.61221600	-6.42567000
Mn	-1.15581600	-1.41173700	1.78140800	O	-2.26990900	4.10434800	-1.29359300	N	2.19493300	-1.55585000	-1.17766800
Mn	0.06906900	0.91162600	0.89372300	C	-4.65658000	4.35309800	-1.26575400	C	2.76594500	-0.62010900	-2.01682300
Mn	-0.16511700	3.61340200	-0.97791500	H	-5.11014400	3.96788200	-2.19258600	H	2.17716200	0.16534100	-2.47134400
O	-1.44370600	-1.96248400	0.05817600	H	-5.36052600	4.09522500	-0.46326800	C	4.11632800	-0.85972700	-2.11695300
O	0.57342500	-1.03987600	1.14096500	C	-4.45206400	5.86508900	-1.36758100	N	4.34482800	-1.98078000	-1.32819200
O	-1.59688000	0.24602100	1.34714000	H	-3.73628200	6.10876500	-2.16048300	H	5.27019000	-2.24361900	-0.97911500
O	-0.19487500	0.13141800	-0.90025300	H	-4.05874100	6.27733500	-0.42746700	C	3.17292100	-2.35090900	-0.76741300
O	-0.54239600	2.43278900	0.43991000	H	-5.40029800	6.37646100	-1.58220100	H	3.05285300	-3.17626500	-0.08205500
O	-4.81123800	-0.91002900	-1.89078200	O	-0.17003800	-2.43766500	-2.27907000	C	5.19357900	-0.14574800	-2.89030800
H	-5.07738800	-1.36204900	-1.06556300	C	-1.31738300	-2.47619000	-2.88544500	H	5.20115400	-0.48472600	-3.93734300
H	-4.31405300	-1.56804600	-2.41595200	O	-2.28115600	-1.72292500	-2.64500800	H	4.92918800	0.91976900	-2.92374200
O	-2.25626700	1.10738900	-3.10194200	C	-1.39610100	-3.53551700	-3.98136300	C	6.63892200	-0.30987700	-2.33965800
H	-1.97898400	0.36154400	-3.65955300	H	-0.53709500	-3.37896000	-4.65152800	H	7.03232100	-1.30095800	-2.59164200
H	-1.43631000	1.66020700	-2.95400200	H	-1.21221800	-4.50910700	-3.50120000	H	7.28439800	0.43117400	-2.83048500
O	0.54591100	4.78888200	-2.19841400	C	-2.70795500	-3.55402900	-4.76981700	C	6.69861500	-0.18767300	-0.81838700
H	1.47698900	4.90461100	-1.93069000	H	-2.88605400	-2.56017700	-5.20368800	O	6.69615100	-1.19506200	-0.09921700
O	0.07425300	2.18429300	-2.30942700	H	-3.54317300	-3.73714100	-4.07901800	N	6.66880200	1.07469200	-0.31477300
H	0.15767700	0.79035200	-1.59678100	C	-2.70975800	-4.61501900	-5.87597900	H	6.61819700	1.84065900	-0.97581100
H	0.56493800	2.64980000	-3.00984500	H	-1.90390000	-4.43669200	-6.60176800	C	6.26916600	1.34889200	1.07046400

H	6.69814700	0.55433800	1.68798100	H	1.82374500	-5.38063000	1.54759700	O	0.37246000	1.19813400	2.80964900
H	6.72991300	2.29927100	1.37009900	H	0.37368400	-6.00186300	0.78859100	C	0.37245000	0.74990800	5.14985700
C	4.73791800	1.39084300	1.23882600	C	0.24799000	-5.89608300	2.96617200	H	1.15594800	0.05755200	5.49552600
H	4.31925500	0.41614600	0.96302500	H	0.61039200	-6.92029600	3.11974800	H	0.79784900	1.76015500	5.14717400
H	4.50616100	1.53845600	2.30330100	H	0.61532700	-5.27144500	3.78838200	C	-0.84094000	0.65888000	6.09217600
C	4.07702300	2.48998300	0.40334400	H	-0.84638300	-5.90385300	3.02230400	H	-1.25073100	-0.35779500	6.04209800
H	4.43469500	2.44094300	-0.63803000	O	-4.17722300	-1.16066400	0.75583000	H	-1.63038400	1.33332700	5.72863100
H	4.35250100	3.49002400	0.76564400	C	-4.00939400	-1.73365500	1.84954500	C	-0.47941000	1.01645700	7.53733900
O	1.97609800	1.35070500	0.60546500	O	-2.86490200	-1.91987600	2.43450500	H	0.28687100	0.33660700	7.93572700
C	2.54565600	2.45895600	0.28723200	C	-5.19012700	-2.28615600	2.62767800	H	-1.35835300	0.94834500	8.19121400
O	2.00281000	3.49388600	-0.15655500	H	-6.12076300	-2.12899900	2.07589300	H	-0.08681900	2.04023400	7.61160600
O	0.69148000	-3.49761000	0.15645700	H	-5.24980500	-1.78497500	3.60192500	N	-0.41367600	5.18404800	0.43589500
C	0.27502600	-3.94543400	1.29776800	H	-5.04123800	-3.35548900	2.82168200	H	0.34756800	5.85979700	0.47777800
O	-0.43930500	-3.33356400	2.12885600	O	-0.54371800	-0.75493100	3.55117700	H	-0.56710100	4.76174400	1.35220100
C	0.72570500	-5.36657300	1.61441300	C	0.03708100	0.36618700	3.71772900	H	-1.27266900	5.63263200	0.11202500

TS5:

Ca	-2.56337400	-0.81576400	-1.15352800	H	1.64433000	-5.60334900	-1.91033300	C	1.16935400	3.25613500	-0.72332000
Mn	0.89635400	-1.51385100	-0.45417300	C	0.66291600	-5.91092400	-3.82918500	O	0.21968600	3.70480500	-1.41859100
Mn	-0.79890500	-1.35102900	1.70509000	H	0.39723700	-5.30863100	-4.70995300	O	1.85204600	-2.82271600	0.94217300
Mn	-0.42794800	1.25354700	0.82987500	H	-0.28870200	-6.25473800	-3.40362200	C	1.36489400	-3.18064300	2.04763200
Mn	-1.88160100	3.00066300	-1.20871700	C	1.51552400	-7.11059600	-4.25682400	O	0.29949800	-2.71245100	2.58078000
O	-0.76067700	-2.15274200	0.12679000	H	2.46200100	-6.78805900	-4.71380900	C	2.07508500	-4.29019300	2.81636500
O	0.65961900	-0.35756900	1.07343500	H	1.76589200	-7.74918200	-3.39758400	H	3.12954000	-4.28072800	2.51420800
O	-1.74950500	0.09482400	1.06222800	H	0.98689200	-7.73304200	-4.99079200	H	1.65583100	-5.23694900	2.43987900
O	0.28618000	-0.38483700	-1.56452200	N	2.80879900	-0.81281600	-0.76058500	C	1.91664200	-4.21669000	4.33743500
O	-1.51061500	2.59974800	0.50180200	C	3.26499100	-0.16363400	-1.88535600	H	2.42195700	-5.06479400	4.81695200
O	-3.24291700	-3.12778600	-1.76824300	H	2.62604500	-0.05624300	-2.75059800	H	2.35344900	-3.29216000	4.73724400
H	-3.54061800	-3.38175400	-0.87470600	C	4.54954400	0.27504700	-1.66924900	H	0.85882700	-4.23357200	4.61979700
H	-2.38207600	-3.58369900	-1.91621600	N	4.86173000	-0.13930700	-0.37801400	O	-3.77128400	-2.02058600	0.67607000
O	-1.50687400	-1.25005500	-3.39237900	H	5.63548500	0.24344400	0.16880700	C	-3.50673100	-2.34138400	1.85264500
H	-1.33009700	-2.21676900	-3.38005800	C	3.78080900	-0.77094500	0.13627600	O	-2.35715100	-2.20319200	2.43016500
H	-0.65114000	-0.89136900	-3.04947100	H	3.71866700	-1.17065200	1.13707800	C	-4.58142000	-2.94029400	2.74473700
O	-1.54026000	1.34852000	-1.91948500	C	5.50344000	1.00786000	-2.57468100	H	-4.18124500	-3.78760300	3.31254500
H	-0.60302600	1.01726300	-1.88694800	H	5.96279300	0.30970800	-3.29111900	H	-5.44421400	-3.24887600	2.14780400
O	-2.30718600	3.59307100	-3.27151000	H	4.91789800	1.71274000	-3.18116300	H	-4.90211200	-2.18047300	3.47026400
H	-1.93077600	2.77174600	-3.65134800	C	6.65761000	1.76458500	-1.86519600	O	-0.62285800	-0.30644500	3.51692100
H	-3.25710600	3.36673600	-3.10944600	H	7.40595400	1.05513200	-1.49461000	C	-0.31914700	0.89755900	3.60306900
O	-4.44692100	0.62347700	-1.42294800	H	7.15716900	2.40909200	-2.60153400	O	-0.16484400	1.72612000	2.61054100
C	-4.85790100	1.80255800	-1.49747400	C	6.18675100	2.56807400	-0.65492100	C	-0.11017800	1.54571600	4.96363600
O	-4.11072400	2.85491700	-1.53118800	O	6.29794000	2.12104900	0.49329500	H	0.77183300	2.19721900	4.89074600
C	-6.37345000	2.01812900	-1.55774000	N	5.58857000	3.76006500	-0.91958000	H	-0.96682000	2.21983700	5.12357900
H	-6.74521900	1.41907400	-2.40166700	H	5.48131200	4.03575700	-1.88805200	C	0.02016600	0.55085400	6.12129400
H	-6.79064600	1.53905300	-0.66005900	C	4.83168700	4.49553700	0.09768800	H	0.87202000	-0.11638000	5.92976400
C	-6.84217700	3.46893900	-1.66784500	H	5.41514400	4.46124500	1.02356900	H	-0.86872500	-0.09221600	6.14486500
H	-6.44740200	3.94945200	-2.57195400	H	4.77639600	5.54212300	-0.22913400	C	0.20046600	1.25861800	7.46863700
H	-6.50921800	4.05995000	-0.80550400	C	3.42740200	3.91720100	0.34628300	H	1.10286500	1.88610400	7.47627200
H	-7.93813800	3.51945100	-1.70957200	H	3.52131900	2.89449000	0.72717000	H	0.29418300	0.53073500	8.28458600
O	1.25740800	-2.94357500	-1.69586700	H	2.95215300	4.50783100	1.14363700	H	-0.65657400	1.90746300	7.69799400
C	0.54948800	-3.82682300	-2.32060100	C	2.53886000	3.91659300	-0.90255900	N	-2.43901500	4.93566800	-0.61728100
O	-0.67605600	-3.77998500	-2.54785600	H	3.03608200	3.35034000	-1.70640900	H	-1.99030600	5.67476300	-1.15981700
C	1.37454500	-5.02126000	-2.80680600	H	2.37332200	4.93215400	-1.28570500	H	-2.19028800	5.02933200	0.36851000
H	2.32571500	-4.63801300	-3.20274300	O	1.13070300	2.26238600	0.08500700	H	-3.45517800	4.98781600	-0.72101800

G:

Ca	2.77916000	0.20797400	-0.77422800	Mn	1.08222000	-3.11496800	-1.33282600	O	-0.26360300	0.81213200	-1.89484600
Mn	-0.48234900	1.81939700	-0.38662400	O	1.20753300	1.82475700	0.27300200	O	0.83531000	-3.17919100	0.46737700
Mn	0.92224700	0.89036900	1.83105700	O	-0.60391900	0.39499100	0.86602700	O	4.17562700	2.03176600	-1.70811400
Mn	0.17427400	-1.53891800	0.65619800	O	1.65301700	-0.65642300	1.28114900	H	4.50852800	2.33590000	-0.84149400

H	3.47288200	2.66872000	-1.97793800	N	-2.54216900	1.67068900	-0.80001100	O	0.12675600	2.51567000	2.72447300	
O	1.92808700	0.15636300	-3.18379600	C	-3.12063100	1.27672200	-1.98663400	C	-1.17527000	4.51864800	2.91481200	
H	2.34525000	0.83135400	-3.74726300	H	-2.51758700	1.16259600	-2.87608000	H	-2.24665000	4.63548000	2.70323300	
H	1.06527400	0.57985100	-2.87314800	C	-4.46411900	1.06112300	-1.79154800	H	-0.68509900	5.38199500	2.43837700	
O	0.81685600	-1.32899500	-1.04939100	N	-4.68686800	1.35130200	-0.44976800	C	-0.89245500	4.49631300	4.41726200	
H	-0.20849500	-0.13921400	-1.61195100	H	-5.52526000	1.06605600	0.06306600	H	-1.24570500	5.42441000	4.88452900	
O	1.62996800	-2.67289300	-3.35245000	C	-3.50422400	1.69350700	0.11006500	H	-1.39831100	3.65338600	4.90390900	
H	1.63083700	-1.68236800	-3.43710300	H	-3.36739100	1.92308200	1.15585300	H	0.18014300	4.39271500	4.61328700	
H	2.57051200	-2.90707900	-3.15678400	C	-5.53635000	0.62757900	-2.75628700	O	4.04876900	1.30197000	0.99607400	
O	4.28056300	-1.56502200	-1.11336300	H	-5.81836700	1.46403500	-3.41380300	C	3.74206800	1.56614500	2.18129500	
C	4.34740800	-2.81916500	-1.18393400	H	-5.10595800	-0.13756700	-3.41753100	O	2.56761600	1.45008900	2.69886400	
O	3.39926700	-3.57058200	-1.60928800	C	-6.84145000	0.08585200	-2.11763800	C	4.80865200	2.04751200	3.15141500	
C	5.65368700	-3.48040400	-0.74237300	H	-7.41598600	0.90703500	-1.67447600	H	4.42410200	2.86528400	3.77059400	
H	6.45914900	-3.01705300	-1.33047700	H	-7.46069100	-0.35224200	-2.91250500	H	5.70523800	2.36248900	2.60984700	
H	5.83117800	-3.15768700	0.29386500	C	-6.59491500	-0.92072300	-0.99466100	H	5.07219800	1.22045800	3.82447700	
C	5.69838900	-5.00394100	-0.85435800	O	-6.62345400	-0.57233800	0.19308000	O	0.29390100	-0.01488100	3.49056900	
H	5.53171400	-5.33190100	-1.88796600	N	-6.29249300	-2.18915500	-1.37387100	C	-0.24705000	-1.16350700	3.50579100	
H	4.92701900	-5.46861400	-0.22753800	H	-6.23798500	-2.39469500	-2.36383800	O	-0.47356000	-1.89461800	2.49053600	
H	6.67425900	-5.38774600	-0.52907600	C	-5.79663800	-3.19161400	-0.42450200	C	-0.63947500	-1.73825600	4.85922100	
O	-0.25851100	3.38103200	-1.48847100	H	-6.40252200	-3.10420500	0.48345900	H	-1.46727700	-2.44035600	4.69656800	
C	0.76209000	3.68701300	-2.23036100	H	-5.98779200	-4.17884300	-0.86507600	H	0.21785000	-2.34554200	5.19424100	
O	1.75491800	2.96816300	-2.44191700	C	-4.30920200	-3.01937900	-0.07322500	C	-0.98691000	-0.69298600	5.92580200	
C	0.63876900	5.07538900	-2.86330700	H	-4.16242000	-2.04483700	0.40466500	H	-1.83768600	-0.08935300	5.57610900	
H	-0.34342300	5.12957700	-3.35599800	H	-4.04747200	-3.77744900	0.67932300	H	-0.14388600	0.00066600	6.03414100	
H	0.59069800	5.80531100	-2.04017200	C	-3.37589800	-3.14414000	-1.28179200	C	-1.32650700	-1.33298500	7.27625100	
C	1.76298400	5.43115700	-3.83902900	H	-3.65487400	-2.40114100	-2.04639100	H	-2.18569500	-2.01372500	7.19428200	
H	1.80406100	4.67431100	-4.63506100	H	-3.45762000	-4.13012000	-1.75878200	H	-1.57645200	-0.56950400	8.02443900	
H	2.72794000	5.37055900	-3.31715800	O	-1.64180200	-2.10102000	-0.01551700	H	-0.47915500	-1.91542600	7.66495300	
C	1.58779300	6.82520700	-4.45151300	C	-1.89466200	-2.89575900	-0.98289500	N	1.23106200	-5.22029700	-1.48995300	
H	0.64311600	6.90181900	-5.00832600	O	-1.05260200	-3.46017200	-1.73401200	H	0.71282600	-5.61736200	-2.27429100	
H	1.57683700	7.60394300	-3.67583400	O	-1.14927600	3.14215500	0.97554800	H	0.87102700	-5.61158000	-0.61824100	
H	2.40434400	7.05973200	-5.14693400	C	-0.69088900	3.28915100	2.15568900	H	2.23022100	-5.42376800	-1.57292400	

TS6:

Ca	2.78824500	0.62398000	-0.87778900	H	6.58388800	-2.07862200	-2.33573800	C	-3.64037700	1.23278700	0.25453300	
Mn	-0.69816200	1.85295600	-0.30071300	H	6.53338100	-2.18848400	-0.59229900	H	-3.50963100	1.42328100	1.30881200	
Mn	0.86849800	0.93421400	1.79042400	C	6.39225800	-4.11906800	-1.59040900	C	-5.55091200	-0.01545400	-2.62173300	
Mn	0.38139000	-1.50939300	0.47659400	H	5.98931100	-4.55040400	-2.51546300	H	-5.96730200	0.78519400	-3.25161700	
Mn	1.64317900	-3.10009700	-1.40954500	H	5.93904500	-4.65464000	-0.74726800	H	-5.02160700	-0.68950800	-3.30987300	
O	1.00999600	2.01147600	0.32471500	H	7.47386900	-4.30679200	-1.57173500	C	-6.74822800	-0.76530700	-1.98361300	
O	-0.60613900	0.31754000	0.81266300	O	-0.79173000	3.49658400	-1.27368800	H	-7.42075900	-0.05453700	-1.49007000	
O	1.74746600	-0.47737300	1.09718800	C	0.07390500	4.16102100	-1.98063800	H	-7.32013100	-1.24917700	-2.78729900	
O	-0.37027700	0.99894400	-1.87352400	O	1.26471100	3.86497200	-2.16849900	C	-6.33705900	-1.77959500	-0.91718000	
O	1.30560700	-3.01496400	0.35814700	C	-0.52979400	5.41876900	-2.61144300	O	-6.36634400	-1.48968200	0.28665100	
O	3.66094800	2.91777900	-1.24361000	H	-1.38091900	5.09856100	-3.23219800	N	-5.89612000	-2.98402900	-1.36253200	
H	3.93506300	3.06657800	-0.31946100	H	-0.97207200	6.01452700	-1.79854700	H	-5.85847200	-3.14501300	-2.36142100	
H	2.84124600	3.44806500	-1.38449100	C	0.45961800	6.25276000	-3.42854900	C	-5.27264700	-3.96642000	-0.46970100	
O	1.97595000	1.26134300	-3.13420200	H	0.89286800	5.62556400	-4.21953000	H	-5.86493300	-3.98786300	0.45121100	
H	2.11848500	2.22316400	-3.22188000	H	1.30054600	6.54683300	-2.78562400	H	-5.36180600	-4.94813000	-0.95272800	
H	1.00933100	1.22327000	-2.90260200	C	-0.19166800	7.49711200	-4.04219800	C	-3.80655200	-3.64538400	-0.13385800	
O	1.05204000	-1.18157400	-1.32949700	H	-1.01636200	7.22615300	-4.71676500	H	-3.75767300	-2.67434400	0.37067300	
H	-0.21534400	0.04862800	-1.66818900	H	-0.60432900	8.15732500	-3.26611700	H	-3.45325900	-4.39500900	0.58979100	
O	1.39902100	-2.48524800	-3.26706000	H	0.53505100	8.08014500	-4.62294800	C	-2.88442900	-3.63263100	-1.35923800	
H	0.99301100	-1.50995100	-2.42892900	N	-2.71948400	1.42648400	-0.67795000	H	-3.26480200	-2.90861200	-2.09765300	
H	2.24942700	-2.18220000	-3.63655300	C	-3.26185700	1.00777100	-1.87312500	H	-2.85294000	-4.61176900	-1.85403300	
O	4.35480700	-0.99711800	-1.49610800	H	-2.67901500	1.04783300	-2.78225800	O	-1.31588800	-2.23433100	-0.23611800	
C	4.62581900	-2.22618600	-1.51948900	C	-4.54108500	0.55270700	-1.65913200	C	-1.44348100	-3.21191100	-1.06258900	
O	3.76084300	-3.16689600	-1.55831900	N	-4.76477400	0.72451900	-0.29770000	O	-0.51416100	-3.79907200	-1.66041100	
C	6.10371800	-2.62042200	-1.50821900	H	-5.52914000	0.27570900	0.21512800	O	-1.49211000	2.95255800	1.18942200	

C	-1.01147400	3.06730900	2.36328000	O	2.44396400	1.54694100	2.73179800	C	-0.74082000	-1.17933000	5.78764000
O	-0.07724400	2.36499000	2.83970300	C	4.69456600	1.96061700	3.33269600	H	-1.58542300	-0.52138800	5.53598500
C	-1.61756800	4.15757500	3.23742200	H	4.29392900	2.64853400	4.08436200	H	0.11778000	-0.51884100	5.96190200
H	-2.70112300	4.15851900	3.05867200	H	5.59211700	2.37571700	2.86490200	C	-1.06353600	-1.97797300	7.05524300
H	-1.25030800	5.11199200	2.82886500	H	4.96695600	1.02772400	3.84542900	H	-1.93853100	-2.62723600	6.91011900
C	-1.28647400	4.04343900	4.72584400	O	0.37275100	-0.18065200	3.39340700	H	-1.28088900	-1.30937100	7.89814700
H	-1.73461100	4.87810200	5.27970500	C	-0.06839900	-1.35911900	3.31123700	H	-0.22033000	-2.61947000	7.34787300
H	-1.67123600	3.10671900	5.14763400	O	-0.22244600	-2.02880000	2.23204700	N	1.90103400	-5.22194000	-1.48742800
H	-0.20357000	4.05718300	4.88913100	C	-0.43848900	-2.08995700	4.59274300	H	1.32098000	-5.62811800	-2.22194900
O	3.99032800	1.48188000	1.08593500	H	-1.28349400	-2.75356200	4.36584100	H	1.61477900	-5.60845400	-0.58713700
C	3.64821100	1.64190200	2.27845300	H	0.41224900	-2.75229000	4.82299600	H	2.88836800	-5.42283400	-1.65174100

H:

Ca	2.81682100	0.73887900	-0.97793000	H	-1.26488200	5.98177600	-1.91530000	C	-1.33231400	-3.11042600	-1.10468300
Mn	-0.78483000	1.78169500	-0.32958600	C	-0.16353100	6.05111900	-3.79159900	O	-0.40597800	-3.64266800	-1.75646900
Mn	0.91663900	1.02151500	1.72942700	H	0.09558900	5.35954300	-4.60623900	O	-1.50301500	2.96712900	1.06872300
Mn	0.51889200	-1.47876300	0.49316900	H	0.79024900	6.35302500	-3.34027900	C	-1.01092500	3.14900300	2.23484700
Mn	1.70508600	-3.05702500	-1.58822800	C	-0.89240300	7.27410400	-4.35887800	O	-0.05633500	2.49853300	2.73080400
O	0.92507800	2.02629400	0.15113600	H	-1.83794600	6.99022200	-4.84261300	C	-1.65271000	4.26202200	3.05245700
O	-0.58785100	0.35321300	0.87253100	H	-1.13158400	7.99917700	-3.56792300	H	-2.74075800	4.16938800	2.93386500
O	1.84833700	-0.35201600	1.08502500	H	-0.27761700	7.78992900	-5.10793000	H	-1.38077200	5.20463000	2.55300500
O	-0.51286900	0.78690600	-1.91511900	N	-2.82583700	1.20929700	-0.50244500	C	-1.24176100	4.28688600	4.52480700
O	1.44244100	-2.92002700	0.28191700	C	-3.69085700	1.10632800	-1.57257100	H	-1.72555000	5.12717900	5.03858800
O	3.42773900	3.13221500	-1.34872900	H	-3.47760500	1.58469800	-2.52098300	H	-1.53228600	3.35990200	5.03382500
H	3.71456500	3.29869100	-0.43184700	C	-4.79741300	0.37347500	-1.20101300	H	-0.15648700	4.39261500	4.62865300
H	2.56775800	3.59808800	-1.46300900	N	-4.59010800	0.07201700	0.13648900	O	4.00543500	1.71719400	0.93368900
O	1.81739200	1.39063400	-3.14811300	H	-5.18310600	-0.55125800	0.69544700	C	3.67399300	1.89291600	2.12673800
H	1.75194700	2.36793400	-3.12865800	C	-3.39336400	0.57036600	0.51013800	O	2.47603100	1.78120900	2.59231400
H	0.87888000	1.13091700	-2.98275800	H	-2.93499900	0.41147100	1.47478300	C	4.72449200	2.25733500	3.16128400
O	1.10184900	-1.07601500	-1.27866800	C	-5.96916300	-0.11990700	-2.01307600	H	4.31024300	2.92929200	3.91981600
H	-1.37987200	0.69181400	-2.34480200	H	-6.54371800	0.73387000	-2.40044900	H	5.59601900	2.70712800	2.67659100
O	1.78016600	-3.10465300	-3.40105200	H	-5.57552700	-0.63809200	-2.89990900	H	5.04462800	1.33654900	3.66844500
H	0.33557300	-0.62737600	-1.73211100	C	-6.96383200	-1.05559900	-1.28028000	O	0.51551800	-0.02331400	3.37090600
H	2.66649300	-2.80457200	-3.67457700	H	-7.53771600	-0.49241600	-0.53620900	C	0.14793700	-1.23827900	3.35552200
O	4.45051200	-0.81416900	-1.53438200	H	-7.67790300	-1.43934700	-2.02193000	O	-0.01461700	-1.95689900	2.31795400
C	4.69932700	-2.04855800	-1.48831700	C	-6.30685100	-2.20979000	-0.51739100	C	-0.09986500	-1.91844600	4.69348700
O	3.82879600	-2.97950600	-1.52997600	O	-6.16619600	-2.15768600	0.71384700	H	-0.86812400	-2.68733000	4.53869600
C	6.16991000	-2.46033800	-1.38210700	N	-5.83755000	-3.25127400	-1.24495500	H	0.82906100	-2.46149700	4.93428200
H	6.69778200	-1.97080600	-2.21325700	H	-5.95895400	-3.24355300	-2.25019500	C	-0.46911900	-0.97344000	5.84257300
H	6.56123800	-1.98513500	-0.47054800	C	-5.05602900	-4.33458300	-0.63208900	H	-1.39196200	-0.43289100	5.58459700
C	6.43910400	-3.96475200	-1.37046000	H	-5.59092400	-4.65860400	0.26778700	H	0.31260300	-0.21041200	5.94436100
H	6.06984000	-4.44042700	-2.28779600	H	-5.05527500	-5.16904700	-1.34435200	C	-0.65919900	-1.72028600	7.16728800
H	5.94135300	-4.44748300	-0.52041800	C	-3.61783900	-3.93567300	-0.25767000	H	-1.45676000	-2.47311600	7.09417200
H	7.51588300	-4.16574800	-1.29342900	H	-3.64535900	-3.13482700	0.48874000	H	-0.92711400	-1.02825600	7.97608500
O	-1.09955700	3.32977600	-1.45645400	H	-3.15256200	-4.80568300	0.22924100	H	0.26121800	-2.24146300	7.46608400
C	-0.29025900	4.10048100	-2.11918500	C	-2.77002500	-3.49898000	-1.45957500	N	2.07743100	-5.18310200	-1.35475300
O	0.93446400	3.94443100	-2.26321400	H	-3.23100000	-2.61550800	-1.92807000	H	1.62926000	-5.71015100	-2.10323000
C	-0.99640100	5.30690800	-2.74448300	H	-2.72029000	-4.28967600	-2.21835400	H	1.74333200	-5.50586800	-0.44683400
H	-1.95359400	4.96509800	-3.16370100	O	-1.20462200	-2.22621100	-0.17889300	H	3.09095600	-5.29036200	-1.40744100

I:

Ca	-2.78188300	0.52854200	-1.21179800	O	-0.68549800	-0.65801800	-2.09685800	O	1.35700700	2.79647900	-3.57590100
Mn	-0.55889800	-1.90194200	-0.06776400	O	0.96594400	3.13835500	0.06662600	H	2.20353300	2.32767700	-3.69352600
Mn	-1.31243900	-0.04906700	1.79138400	O	-5.21712100	-0.11129500	-1.45195300	O	0.50667800	1.32517000	-1.37789800
Mn	0.64040000	1.44480300	0.46096200	H	-5.39109300	0.10047300	-0.51154500	H	-0.03130200	0.14010100	-2.00652100
Mn	1.12048800	2.96989100	-1.75795200	H	-5.06052000	-1.07491900	-1.50322000	H	-0.51380400	-1.16353400	-2.90574300
O	-2.05775900	-1.03015900	0.46585700	O	-3.23381000	0.12368300	-3.67691600	O	-2.22356500	2.59404900	-2.13386100
O	0.29054700	-0.51599800	0.97061500	H	-3.30762900	-0.84619100	-3.55264900	C	-1.71374800	3.72491800	-2.22187200
O	-1.13661700	1.47700100	0.80595800	H	-2.45853000	0.27666600	-4.24141600	O	-0.46136900	4.01017000	-2.12224600

C	-2.63612500	4.92002400	-2.47457600	C	4.53210300	-3.17312700	-2.43660700	C	-1.52277400	-3.33058600	5.23638800
H	-3.27662700	4.64227000	-3.32318000	H	4.35820400	-3.94545300	-3.20084600	H	-1.66646900	-4.14856500	5.95472700
H	-3.30737700	4.97392400	-1.60441600	H	4.62579400	-2.22585000	-2.98685400	H	-0.70775100	-2.69315100	5.60093200
C	-1.95397100	6.26609400	-2.71641300	C	5.88349100	-3.50249900	-1.75197300	H	-2.43117300	-2.71878600	5.21704600
H	-1.28991700	6.22208900	-3.58888300	H	5.87714900	-4.53127900	-1.37440200	O	-4.19954800	1.06145100	0.72054500
H	-1.35447900	6.56719600	-1.84871400	H	6.67672100	-3.43827700	-2.50940800	C	-4.05965000	0.95426100	1.96530700
H	-2.70275000	7.04794300	-2.89870200	C	6.18934100	-2.59911000	-0.55840300	O	-3.01803700	0.51674700	2.56961200
O	-1.54899200	-3.22456000	-1.17254900	O	5.92342300	-2.95288900	0.59778000	C	-5.18856400	1.39651400	2.88404100
C	-2.70578400	-3.12017000	-1.72209900	N	6.70569500	-1.37494700	-0.84165400	H	-4.97404600	2.41606600	3.23304800
O	-3.29200000	-2.03769200	-1.98794200	H	6.86919200	-1.13511400	-1.81161600	H	-5.24819900	0.74905600	3.76483700
C	-3.38004900	-4.45167400	-2.05062200	C	6.77225100	-0.30839600	0.16423200	H	-6.14199200	1.40831500	2.34692300
H	-2.59607100	-5.18143800	-2.29287700	H	7.13863900	-0.75924800	1.09214300	O	-0.48263100	0.78817800	3.40333600
H	-3.83474700	-4.80786600	-1.11097900	H	7.52059900	0.41800500	-0.17784100	C	0.57734600	1.47888400	3.37290000
C	-4.44154600	-4.38564800	-3.15348100	C	5.41055100	0.36190600	0.41590200	O	1.21586300	1.79751000	2.32231000
H	-3.97869400	-4.02040900	-4.08322600	H	4.70164100	-0.39395100	0.77068100	C	1.14827500	1.94668500	4.70376200
H	-5.20035800	-3.64042700	-2.88105700	H	5.52475200	1.08692300	1.23403800	H	1.68420200	1.08757900	5.13933900
C	-5.10756500	-5.74185800	-3.41005600	C	4.83941200	1.05969900	-0.82145800	H	1.89525400	2.72355700	4.50086100
H	-4.37103300	-6.49879900	-3.71422000	H	4.86903300	0.38044600	-1.68896800	C	0.08043000	2.43865200	5.69233200
H	-5.60985600	-6.11507200	-2.50651300	H	5.43352600	1.93940400	-1.10463100	H	-0.66275600	1.64415500	5.83383600
H	-5.86126200	-5.67087400	-4.20502800	O	2.66980900	0.97853000	0.19763700	H	-0.45671400	3.28955100	5.24757100
N	1.30456900	-2.71078600	-0.61644700	C	3.37856900	1.49563900	-0.69541300	C	0.68145800	2.85328600	7.03937700
C	2.06628900	-2.59792700	-1.76102500	O	3.00449100	2.35140400	-1.57938200	H	1.19647200	2.01027500	7.52179700
H	1.66199500	-2.17833500	-2.67207100	O	-0.52024300	-3.23454400	1.65472800	H	-0.09727900	3.20583200	7.72827500
C	3.33507100	-3.07379500	-1.52556300	C	-1.01530600	-2.83919100	2.75191300	H	1.41369000	3.66451500	6.92052300
N	3.31707500	-3.49583900	-0.20336800	O	-1.38333900	-1.65145000	3.02066600	N	1.99099300	4.88978900	-1.74425200
H	4.16056700	-3.70538800	0.33941300	C	-1.20821900	-3.88730900	3.84758900	H	2.94103800	4.88560700	-2.11284900
C	2.09201200	-3.24520100	0.30856600	H	-0.30575600	-4.51413900	3.85948800	H	1.99018300	5.19148200	-0.76820800
H	1.79006600	-3.44054400	1.32746600	H	-2.01953100	-4.54652500	3.50107600	H	1.39039400	5.49712700	-2.30141400

TS7:

Ca	-2.64845300	1.28071600	-0.78181200	H	-0.71964900	7.17927700	-0.58325200	C	5.46012100	-3.19882300	-1.74332600
Mn	-0.96435500	-1.52249000	-0.63292200	H	-1.86017600	7.79597300	-1.79427100	O	5.10072900	-4.00255800	-0.87181100
Mn	-1.36287900	-0.43189200	1.84494400	O	-2.24660300	-2.43968400	-1.75998100	N	6.19259300	-2.09369800	-1.44637100
Mn	0.77216700	1.06988300	0.88195700	C	-3.41012400	-2.01043400	-2.11622800	H	6.43451400	-1.45965800	-2.19790600
Mn	1.81903300	3.40508900	-0.97813300	O	-3.84272700	-0.84418900	-1.95798100	C	6.39737300	-1.65491400	-0.06096700
O	-2.30516500	-0.83229100	0.40233200	C	-4.27935800	-3.07878100	-2.77850000	H	6.54033400	-2.55825200	0.53945800
O	0.15142900	-0.83443600	0.80911300	H	-3.63763900	-3.66820700	-3.44812800	H	7.32770600	-1.07322800	-0.02808400
O	-0.94725900	1.27299000	1.30433500	H	-4.58651300	-3.77380000	-1.98023100	C	5.20556400	-0.84457500	0.48155900
O	-0.84342500	-0.13787200	-1.64968800	C	-5.50778500	-2.54202000	-3.51844600	H	4.29382400	-1.44312100	0.37498900
O	1.10154600	2.71392800	0.59715800	H	-5.18509800	-1.83379700	-4.29576300	H	5.34786600	-0.68685000	1.55997500
O	-5.12137500	1.47587200	-1.14535800	H	-6.12677300	-1.96359800	-2.81944500	C	5.02769700	0.50212400	-0.22587400
H	-5.30682900	1.44377100	-0.18370200	C	-6.34273600	-3.65985300	-4.15276600	H	5.21835100	0.39590900	-1.30640300
H	-5.24031600	0.55992400	-1.47002600	H	-5.75388800	-4.23499800	-4.88100200	H	5.75713400	1.24499100	0.12466700
O	-2.55698600	1.14890900	-3.36642700	H	-6.70787400	-4.36503800	-3.39280000	O	2.67841600	0.44693600	0.30803600
H	-3.24923500	0.46191600	-3.41852900	H	-7.21687800	-3.25328800	-4.67767900	C	3.63865700	1.14413500	-0.14224100
H	-1.74620500	0.61350700	-3.21013500	N	0.65879200	-2.44559200	-1.54252100	O	3.56179000	2.31503400	-0.62607000
O	2.62856500	4.00037100	-2.49044100	C	1.42900000	-1.96612600	-2.58264800	O	-1.05693400	-3.27636800	0.53239400
H	3.48457900	3.53789200	-2.55474500	H	1.08633300	-1.13625400	-3.18540200	C	-1.38327400	-3.30439300	1.75589700
O	1.16260000	1.36822100	-1.90330300	C	2.59001800	-2.70078500	-2.66926200	O	-1.55327100	-2.29143000	2.51021200
H	1.88130000	0.71779400	-1.84021100	N	2.48493000	-3.65851200	-1.66951600	C	-1.62627000	-4.67585700	2.37885500
H	0.31445100	0.79166900	-1.84736800	H	3.27109800	-4.22693300	-1.33786200	H	-0.94825000	-5.38747000	1.89017900
O	-1.58243600	3.30673700	-1.13008000	C	1.32525200	-3.45941200	-1.00708900	H	-2.64259000	-4.97147300	2.07315600
C	-1.01159500	4.40268600	-1.32709000	H	0.99393300	-4.02808900	-0.15154600	C	-1.49588100	-4.72357300	3.90244700
O	0.25538600	4.59010300	-1.36224700	C	3.77518900	-2.56884900	-3.59265100	H	-1.71557900	-5.73282000	4.27363500
C	-1.88697100	5.63252800	-1.58310200	H	3.49567500	-2.87696200	-4.61108600	H	-0.48026400	-4.45690800	4.22158200
H	-2.36764700	5.46504600	-2.55925000	H	4.03530000	-1.50348900	-3.66688000	H	-2.18685300	-4.01829200	4.37603800
H	-2.70144100	5.60749800	-0.84588300	C	5.04095600	-3.37808400	-3.20217300	O	-3.97931900	1.39541900	1.31040200
C	-1.16268300	6.97865400	-1.56797200	H	4.86314500	-4.45009300	-3.34481200	C	-3.87879900	0.88285600	2.44896000
H	-0.35468600	6.99681400	-2.30790500	H	5.85319300	-3.08983400	-3.88347900	O	-2.91143000	0.13395700	2.85741800

C	-4.95276500	1.13346900	3.49501000	C	1.52322800	0.58265900	4.96615800	H	2.89210400	-0.29851000	7.25891400
H	-5.30969000	0.17963300	3.90136500	H	2.60563200	0.54670800	4.78474400	H	1.48192700	-0.96562300	8.10201600
H	-5.78567600	1.69851700	3.06735100	H	1.30865400	1.60585300	5.31567900	H	1.57619000	0.77389200	7.77221200
H	-4.51826900	1.69957400	4.32895800	C	1.09255800	-0.44280700	6.02087100	N	2.58275900	5.16135100	0.23529700
O	-0.27469600	-0.16618800	3.56121100	H	1.30469800	-1.45501300	5.64800500	H	3.56006000	5.41260300	0.09292900
C	0.81862300	0.43519200	3.62699500	H	0.00449300	-0.38811000	6.15030700	H	2.40566500	5.01479100	1.22901500
O	1.43554500	0.99072700	2.63729700	C	1.80053100	-0.22072100	7.36173800	H	1.99204100	5.92294300	-0.10058700

K:

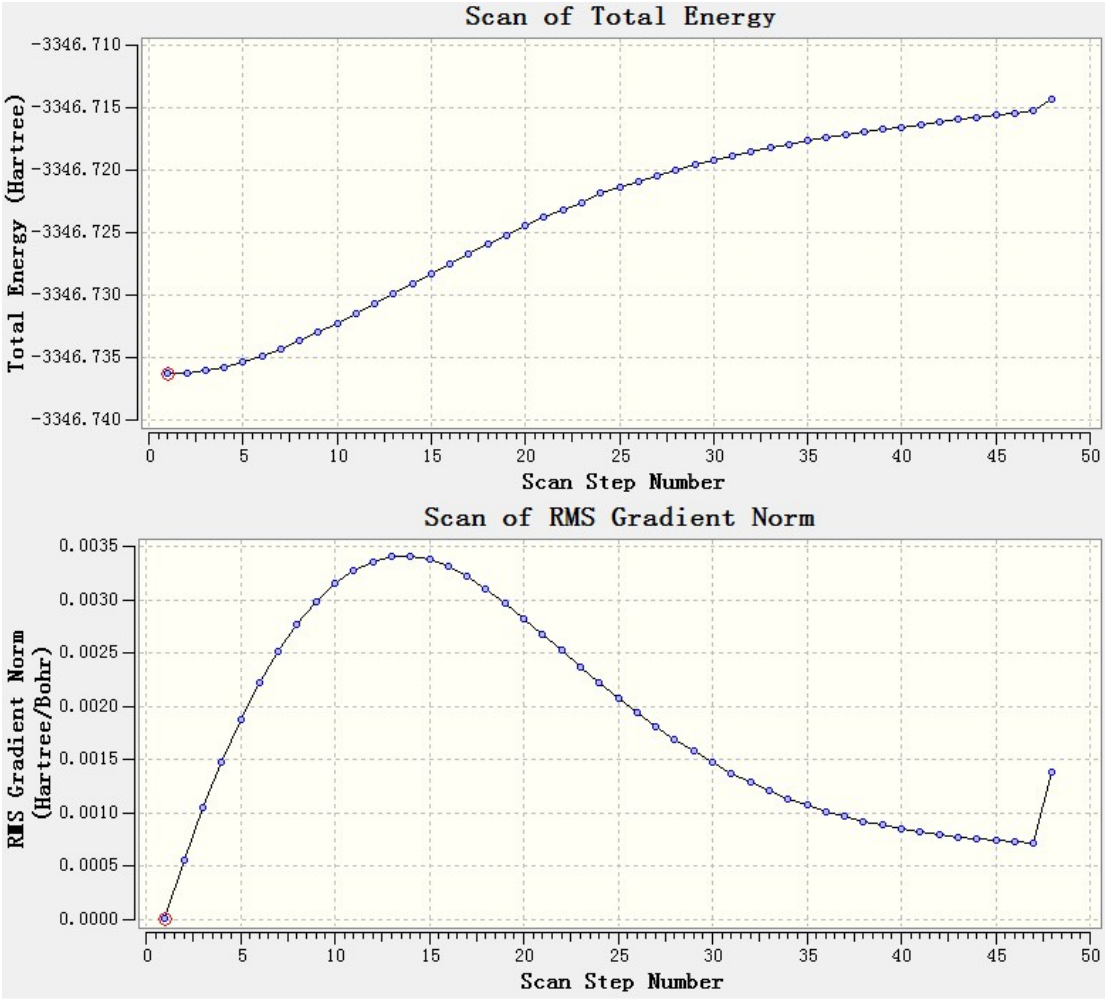
Ca	-2.59500400	0.87112300	-1.04351800	H	-2.25086300	-3.91305900	-3.77618800	C	2.94890500	1.48884100	0.09206300
Mn	-0.38383900	-1.67306900	-0.55824000	C	-3.17919100	-2.53987200	-5.19137700	O	2.58630500	2.49048000	-0.60992900
Mn	-1.77872200	-1.03130400	1.66119700	H	-2.97124800	-1.54692300	-5.61535800	O	-0.59282500	-3.57267200	0.12682000
Mn	0.17399500	0.76293200	0.88451200	H	-4.11457400	-2.43630200	-4.62413700	C	-1.23399400	-3.85582900	1.19766400
Mn	0.87325700	3.46047300	-0.81907500	C	-3.36788300	-3.55793100	-6.32151800	O	-1.75381600	-3.03367900	2.01074100
O	-2.10346500	-1.42090100	-0.09814000	H	-2.45596600	-3.65709100	-6.92694400	C	-1.38972700	-5.34353100	1.49581500
O	0.03452800	-1.19594800	1.17208000	H	-3.61115600	-4.55369300	-5.92517900	H	-0.44473800	-5.83400800	1.22725700
O	-1.62227000	0.69935000	1.23832700	H	-4.18262600	-3.25811500	-6.99294300	H	-2.13445700	-5.72198500	0.77793600
O	-0.12028800	0.12396100	-0.89611000	N	1.60406000	-2.20271700	-0.88627100	C	-1.81053900	-5.66903200	2.92953100
O	0.14533000	2.44702500	0.48989100	C	2.47204500	-1.91781000	-1.91701300	H	-1.92090000	-6.75353000	3.05636400
O	-4.80847600	0.52414800	-2.19680200	H	2.12838900	-1.42618500	-2.81725500	H	-1.06523000	-5.31417400	3.65207700
H	-5.25349000	0.20309300	-1.38653700	C	3.73460500	-2.36070600	-1.58883900	H	-2.76342900	-5.18970900	3.17803200
H	-4.54491000	-0.26874000	-2.70293800	N	3.59429700	-2.94329000	-0.33635100	O	-4.48687700	0.23411100	0.47031500
O	-2.01321200	1.68911600	-3.35653000	H	4.37998300	-3.22095000	0.26248400	C	-4.58212000	-0.37416800	1.55673100
H	-2.05367800	0.83516300	-3.82480600	C	2.31087300	-2.80908800	0.05653600	O	-3.60460100	-0.93857200	2.19159400
H	-1.06640800	1.95479600	-3.35933400	H	1.92772500	-3.12041400	1.01662300	C	-5.92313500	-0.50141000	2.25747200
O	1.85226300	4.64038400	-1.82648500	C	5.04327800	-2.26210300	-2.33399900	H	-6.71699300	-0.05300900	1.65401200
H	1.27169900	5.37507400	-2.09551300	H	5.01598900	-2.90083300	-3.22923000	H	-5.87199900	0.00229800	3.23103400
O	0.60009200	1.95337700	-2.56583800	H	5.14744300	-1.23318800	-2.70735300	H	-6.14451800	-1.55805000	2.45081000
H	0.48705400	1.11540000	-2.00250300	C	6.31721000	-2.64542100	-1.53373100	O	-1.12707500	-0.60003500	3.48746700
H	1.51759200	1.98158700	-2.89088200	H	6.35146300	-3.72802500	-1.36876400	C	-0.20422400	0.25231500	3.71226900
O	-2.39846200	3.22261000	-0.83152000	H	7.19380000	-2.37901100	-2.14002800	O	0.45840900	0.90833600	2.84470400
C	-1.90367000	4.36109000	-0.79484500	C	6.38947700	-1.99580600	-0.15058800	C	0.13557300	0.50580900	5.17239900
O	-0.64466700	4.64016800	-0.95447500	O	6.06358600	-2.62685600	0.86587700	H	0.54188100	-0.43161900	5.58227800
C	-2.81916000	5.55716600	-0.54332700	N	6.75015900	-0.69005400	-0.10295800	H	0.92542800	1.26436400	5.21681300
H	-3.71862400	5.40124100	-1.15386500	H	6.95505300	-0.21508900	-0.97397600	C	-1.09104400	0.93384200	5.99846500
H	-3.15236200	5.46541200	0.50232600	C	6.51283900	0.13323700	1.09131400	H	-1.86623500	0.16271200	5.90380400
C	-2.20646600	6.93607200	-0.79035800	H	6.87809400	-0.42849000	1.95704600	H	-1.50973800	1.85587200	5.56847000
H	-1.88995700	7.04892700	-1.83491600	H	7.12435200	1.03745100	0.98659000	C	-0.74505800	1.16169100	7.47342400
H	-1.32670600	7.09681800	-0.15702000	C	5.02642000	0.49081800	1.28101400	H	-0.35123300	0.24554600	7.93569600
H	-2.93808700	7.72468300	-0.57132000	H	4.45507500	-0.42642200	1.46218600	H	-1.63163700	1.46862400	8.04332900
O	-0.76220300	-2.23563600	-2.37402400	H	4.93564400	1.10340100	2.18956300	H	0.01516300	1.94658200	7.59022500
C	-1.80232200	-1.95555600	-3.08925400	C	4.45388700	1.24514000	0.07913200	N	5.00252200	4.55726600	-0.89310700
O	-2.55881300	-0.97616000	-2.90357500	H	4.63081400	0.65931900	-0.83839700	H	4.04226500	4.41539800	-1.22559400
C	-2.05016700	-2.93215400	-4.23509900	H	4.93828400	2.21962000	-0.08186900	H	5.45742000	5.14897800	-1.59225400
H	-1.10009300	-3.05791200	-4.77564800	O	2.19760700	0.68094500	0.71256000	H	4.90978600	5.14541900	-0.06176700

TS10:

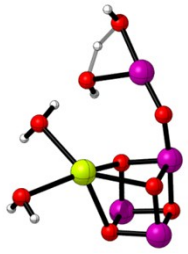
Ca	-2.58827700	0.79642300	-1.05474300	H	-4.64457500	-0.43746800	-2.49931300	C	-2.62638300	5.51227800	-0.96445800
Mn	-0.40949500	-1.73884600	-0.39486100	O	-2.11286100	1.34943200	-3.46856300	H	-3.57273800	5.33326800	-1.49186400
Mn	-1.69669700	-0.83996600	1.79900200	H	-2.19809400	0.45085100	-3.83676500	H	-2.88159500	5.52343600	0.10686900
Mn	0.25462900	0.81650600	0.76740900	H	-1.16081600	1.58343400	-3.54612300	C	-1.99825600	6.84388400	-1.37714500
Mn	0.97771800	3.27053300	-1.25841700	O	1.89420000	4.29079900	-2.48738400	H	-1.75365000	6.85365800	-2.44681000
O	-2.10233700	-1.40702200	0.10802300	H	1.27837900	4.96261200	-2.83257900	H	-1.07226700	7.03262800	-0.82235400
O	0.09228800	-1.09389900	1.25758900	O	0.53872800	1.61056000	-2.84031800	H	-2.69251900	7.67142600	-1.18129000
O	-1.52776300	0.83397600	1.18922700	H	0.44197200	0.85107400	-2.17505600	O	-0.90869600	-2.48410600	-2.11652400
O	-0.12486100	0.00387000	-0.92744400	H	1.44892500	1.59594900	-3.18670000	C	-1.97637900	-2.25087500	-2.80568800
O	0.27540700	2.44536800	0.18755900	O	-2.29392700	3.14952500	-1.09283900	O	-2.69299500	-1.23002200	-2.69771900
O	-4.86633400	0.41014000	-2.06702300	C	-1.76345000	4.26955000	-1.17243700	C	-2.31435000	-3.34174100	-3.81780400
H	-5.27729100	0.18494800	-1.20778000	O	-0.50783300	4.49244300	-1.42266500	H	-1.39791800	-3.56371000	-4.38469200

H	-2.52249000	-4.25572100	-3.23949800	N	6.72287800	-0.76475900	-0.22760000	O	-4.42645100	0.36250000	0.59433400
C	-3.47810700	-3.01876300	-4.75823400	H	6.90285400	-0.26123300	-1.08778200	C	-4.48969300	-0.13606200	1.73760300
H	-3.26106100	-2.08851900	-5.30274200	C	6.49863800	0.01401800	0.99832800	O	-3.49839200	-0.65733700	2.38727200
H	-4.37965300	-2.81724600	-4.16318100	H	6.82374800	-0.60565900	1.83961900	C	-5.80448700	-0.16683300	2.49665500
C	-3.75608300	-4.15037100	-5.75395700	H	7.15038500	0.89553300	0.95329800	H	-6.61199000	0.24498700	1.88526400
H	-2.87974400	-4.35091900	-6.38623300	C	5.02077000	0.40901000	1.17217500	H	-5.70447000	0.41990500	3.41849600
H	-4.00981400	-5.08530300	-5.23495700	H	4.41551600	-0.50420900	1.18817100	H	-6.04032200	-1.19642000	2.79216100
H	-4.59425400	-3.89859400	-6.41626500	H	4.89223600	0.87858300	2.15690200	O	-0.97346500	-0.24009500	3.54516300
N	1.54765800	-2.31908800	-0.81778700	C	4.52125900	1.35254000	0.07392300	C	-0.03166500	0.61576200	3.64690900
C	2.37168500	-1.93563200	-1.85262800	H	4.94394500	1.08344700	-0.90600300	O	0.60519400	1.16654300	2.69280000
H	1.99448200	-1.34610800	-2.67694600	H	4.83123800	2.39159900	0.25625900	C	0.37182100	1.00918900	5.05932200
C	3.64266800	-2.41458300	-1.62994200	O	2.26735400	0.69241100	0.58902700	H	0.83501300	0.12449000	5.52355400
N	3.55561600	-3.11873900	-0.43593700	C	3.01100800	1.41375200	-0.13512100	H	1.13641500	1.79167400	4.99295400
H	4.36963600	-3.42420700	0.10777100	O	2.64760800	2.19836900	-1.07149700	C	-0.82168400	1.46830600	5.91529000
C	2.29057800	-3.01904800	0.02671000	O	-0.59303000	-3.55122800	0.50084300	H	-1.57375900	0.66924300	5.92983900
H	1.94435600	-3.43456800	0.96104600	C	-1.19500500	-3.70868500	1.62066100	H	-1.29539100	2.33713300	5.43456100
C	4.90893600	-2.26041100	-2.43514000	O	-1.68378000	-2.79887700	2.35418400	C	-0.40404100	1.83183000	7.34381100
H	4.84555200	-2.85960400	-3.35573700	C	-1.34238900	-5.15313100	2.08834300	H	0.04588700	0.97077000	7.85798700
H	4.97546100	-1.21413000	-2.76536800	H	-0.40599200	-5.67471400	1.84925700	H	-1.26825600	2.15978500	7.93597300
C	6.22861200	-2.65663800	-1.71960700	H	-2.10763200	-5.60741100	1.43937800	H	0.33390300	2.64610700	7.35086000
H	6.28922500	-3.74498100	-1.60809700	C	-1.72049500	-5.31424800	3.56123900	N	3.49579400	5.16730500	-0.05740900
H	7.06929900	-2.34582800	-2.35489700	H	-1.82693100	-6.37727300	3.81238800	H	3.12040300	5.03336600	-1.00396300
C	6.35035600	-2.06734500	-0.31495900	H	-0.95439500	-4.88237900	4.21695000	H	4.49453800	5.35576000	-0.15933500
O	6.05257200	-2.73700400	0.68418600	H	-2.66576900	-4.80705800	3.78194600	H	3.07989800	6.02511000	0.30956000

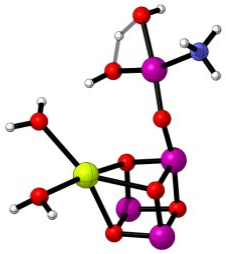
Relaxed PES scan plots for step2:



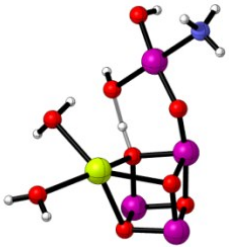
3D images for TSs:



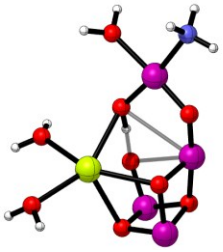
TS9



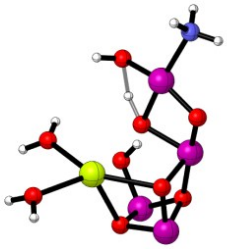
TS3



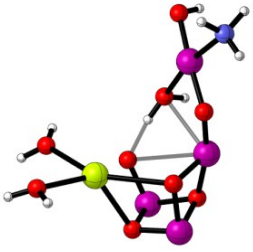
TS4*:



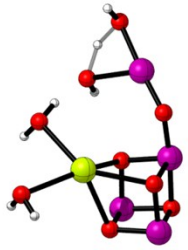
TS5



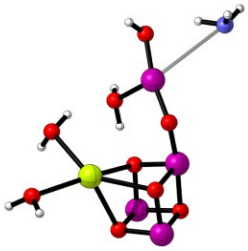
TS6



TS7



TS9



TS10

Vb. Models for Figure 4 of ref. [19]

Table SVb. Mulliken spin populations for the models of Figure 4 of ref. [19] for all spin states:

Spin states	Spin topology (Mn1-Mn4)		Mulliken spin density	
			A	B
doublet	α	Mn1	2.94	2.94
	β	Mn2	-2.93	-2.93
	β	Mn3	-2.87	-2.80
	α	Mn4	3.82	3.80
	β	Mn1	-2.94	-2.93
	α	Mn2	2.93	2.94
	β	Mn3	-2.85	-2.78
	α	Mn4	3.82	3.80
	β	Mn1	-2.93	-2.94
	β	Mn2	-2.94	-2.94
	α	Mn3	2.91	2.89
	α	Mn4	3.89	3.88
sextet	α	Mn1	2.94	2.93
	α	Mn2	2.93	2.93
	α	Mn3	2.87	2.81
	β	Mn4	-3.82	-3.80
	β	Mn1	\	-2.94
	α	Mn2	\	2.94

	α	Mn3	\	2.92
	α	Mn4	\	1.94
octet	α	Mn1	2.95	2.95
	α	Mn2	2.94	2.94
	β	Mn3	-2.84	-2.77
	α	Mn4	3.81	3.79
	α	Mn1	2.99	2.94
	β	Mn2	-2.93	-2.93
	α	Mn3	2.90	2.90
	α	Mn4	3.86	2.88
	β	Mn1	-2.93	-2.93
	α	Mn2	2.93	2.94
	α	Mn3	2.94	2.93
	α	Mn4	3.89	3.88
14-et	α	Mn1	\	2.93
	α	Mn2	\	2.93
	α	Mn3	\	2.80
	β	Mn4	\	-1.87
	α	Mn1	2.94	2.94
	α	Mn2	2.93	2.93
	α	Mn3	2.94	2.93
	α	Mn4	3.89	3.88

Spin states	Spin topology	Mulliken spin density	
		C	D

	(Mn1-Mn4)			
singlet	α	Mn1	2.93	2.94
	β	Mn2	-2.93	-2.94
	β	Mn3	-2.86	-2.92
	α	Mn4	2.78	2.86
	β	Mn1	-2.93	-2.95
	α	Mn2	2.93	2.91
	β	Mn3	-2.85	-2.91
	α	Mn4	2.78	2.85
	β	Mn1	-2.94	-2.96
	β	Mn2	-2.94	-2.94
	α	Mn3	2.90	2.92
	α	Mn4	2.85	2.88
septet	α	Mn1	2.94	2.97
	α	Mn2	2.93	2.96
	α	Mn3	2.86	2.93
	β	Mn4	-2.78	-2.85
	α	Mn1	2.94	2.96
	α	Mn2	2.94	2.94
	β	Mn3	-2.84	-2.90
	α	Mn4	2.77	2.85
	α	Mn1	2.94	2.94
	β	Mn2	-2.93	-2.93
	α	Mn3	2.91	2.91

	α	Mn4	2.86	2.86
	β	Mn1	-2.92	-2.94
	α	Mn2	2.93	2.94
	α	Mn3	2.93	2.94
	α	Mn4	2.84	2.88
13-et	α	Mn1	2.94	2.97
	α	Mn2	2.93	2.96
	α	Mn3	2.93	2.95
	α	Mn4	2.84	2.89

The Cartesian coordinates for A to D:

A:

Ca	-2.71737900	0.13471800	-1.02168700	H	-4.53014200	4.32778400	-1.93447900	H	5.08831100	-2.09572600	-2.82288700
Mn	-0.17756500	-1.85893200	-0.06984600	H	-3.30907000	5.43582500	-1.30175000	C	6.49975800	-2.63979600	-1.24933000
Mn	-1.59160400	-0.85137100	2.02423900	C	-3.36670400	5.36234300	-3.46899000	H	6.70752500	-3.52143500	-0.63335400
Mn	0.09980300	0.85449600	0.69920600	H	-3.57162400	4.64908500	-4.27799600	H	7.29393600	-2.57860000	-2.00540000
Mn	0.24305400	2.76097400	-1.76299700	H	-2.35733200	5.76559500	-3.61130200	C	6.53522400	-1.43923200	-0.30511100
O	-1.90476000	-1.68959300	0.43884400	H	-4.08000100	6.18898500	-3.56593300	O	6.32955100	-1.57633400	0.90912300
O	0.24041800	-0.88875500	1.46056900	O	-0.54356500	-2.88748500	-1.64378600	N	6.70204800	-0.21510500	-0.86608700
O	-1.63587500	0.75076400	1.16633100	C	-1.60604900	-2.89316300	-2.38682700	H	6.90372300	-0.15277000	-1.85629000
O	-0.16759100	-0.16314200	-0.82917100	O	-2.44408900	-1.96368000	-2.43190600	C	6.48574400	1.02092600	-0.10424200
O	-0.11157400	2.49757700	-0.07080400	C	-1.76404100	-4.14352100	-3.23945000	H	7.06275200	0.95695700	0.82479800
O	-4.89820200	-0.50747500	-2.00296800	H	-0.80291300	-4.32754800	-3.74233400	H	6.89801200	1.84344400	-0.70101100
H	-5.39931500	-0.64833200	-1.17553700	H	-1.88434800	-4.98622400	-2.54039700	C	5.00239400	1.26868500	0.23161300
H	-4.77144100	-1.38546700	-2.40558100	C	-2.91688700	-4.10507700	-4.24652500	H	4.65078900	0.47492000	0.89844900
O	-1.96924500	0.51430300	-3.44253400	H	-2.79053800	-3.24144700	-4.91558100	H	4.92497500	2.21431900	0.78485200
H	-1.96134500	-0.44504800	-3.63293900	H	-3.86080300	-3.93840100	-3.70901200	C	4.12008300	1.33753400	-1.01708900
H	-1.10708500	0.86163900	-3.73384700	C	-3.00984100	-5.39313400	-5.07192600	H	4.26567600	0.43475100	-1.63140000
O	1.07104200	4.17610500	1.79270800	H	-2.08940900	-5.56818700	-5.64577100	H	4.38585500	2.19541100	-1.64734600
H	0.41927900	3.80303600	1.15351600	H	-3.17134500	-6.26878300	-4.42858300	O	2.13573200	0.99821400	0.31194300
H	1.21303400	3.39028200	2.36045900	H	-3.84247200	-5.34509700	-5.78440400	C	2.62433900	1.41470000	-0.76397800
O	0.35129500	2.37673400	-3.87614200	N	1.83041300	-2.25001400	-0.35431300	O	1.94522900	1.89491700	-1.75804300
H	1.29736500	2.34825400	-4.11895500	C	2.59361100	-2.37830800	-1.49579900	O	-0.13799700	-3.51086000	1.09313400
H	-0.05055300	3.14627700	-4.32512400	H	2.14665700	-2.30771300	-2.47796800	C	-0.69947700	-3.58214700	2.23890100
O	1.32600800	4.65035600	-1.98690800	C	3.90375000	-2.61596500	-1.14188000	O	-1.28451300	-2.62935600	2.84859100
H	2.04301000	4.69397000	-1.26310200	N	3.89938000	-2.65229600	0.24630200	C	-0.67288700	-4.94326100	2.91696000
H	0.70985200	5.38697000	-1.82502100	H	4.74770400	-2.61639200	0.82329500	H	0.28419500	-5.41758500	2.66522900
O	-2.95755200	2.48288600	-1.33389800	C	2.64744500	-2.40882400	0.67977100	H	-1.44560200	-5.54466300	2.41171700
C	-2.56636100	3.53166300	-1.85553600	H	2.36273300	-2.32181000	1.71785700	C	-0.91794900	-4.91439800	4.42686800
O	-1.32325400	3.73583100	-2.23457500	C	5.14014800	-2.80498000	-1.98525400	H	-0.90313900	-5.93478800	4.82814400
C	-3.51161300	4.69721100	-2.09342400	H	5.13607700	-3.80543700	-2.44216000	H	-0.14476700	-4.33375900	4.94492100

H	-1.88736700	-4.46261600	4.66179200	O	-0.92268600	0.11036200	3.63846500	H	-0.30240800	3.74913500	4.21786200
O	-4.45636500	-0.25437700	0.69468600	C	-0.09132300	1.06950300	3.60837800	C	-0.27842400	3.78619000	6.38686300
C	-4.44571000	-0.55094100	1.90474500	O	0.48653400	1.53250800	2.55642800	H	-0.56034900	3.15295700	7.23865100
O	-3.37402700	-0.80643300	2.60143900	C	0.22155000	1.76085200	4.91948100	H	-0.84492700	4.72248800	6.46351800
C	-5.72652400	-0.65035000	2.70573200	H	-0.03918600	1.08172700	5.73895700	H	0.78777200	4.03069900	6.48904700
H	-6.58707900	-0.38472500	2.08650600	H	1.30072000	1.96269000	4.96120600	O	3.00909400	4.54542100	0.01502200
H	-5.67050100	0.01659800	3.57440000	C	-0.56374500	3.08631400	5.05432200	H	2.35866500	4.40546100	0.77510300
H	-5.84195000	-1.67160100	3.09000200	H	-1.63869400	2.87256400	4.96696200	H	3.51163800	5.34583900	0.24361500

B:

Ca	-2.80080000	0.29004700	-0.79753400	O	-2.64156900	-1.48777000	-2.62011800	H	4.52029400	3.06982800	-0.66247100
Mn	-0.10319700	-1.80502500	-0.59189600	C	-1.99204600	-3.35919400	-4.01326900	O	2.15518100	1.06931600	0.31573000
Mn	-1.31022900	-1.37105400	1.80243200	H	-1.09723600	-3.35105400	-4.65332400	C	2.69427000	2.03693600	-0.28014300
Mn	0.15773800	0.70326600	0.77131000	H	-1.98964100	-4.35105600	-3.53419100	O	2.09340400	3.04733000	-0.80500800
Mn	0.21130100	3.56461700	-0.78357700	C	-3.26544700	-3.15861000	-4.83959900	O	0.11876100	-3.65864700	0.13639000
O	-1.76593800	-1.83637100	0.10774500	H	-3.25723100	-2.15398400	-5.28715400	C	-0.31409100	-4.02709600	1.28482600
O	0.44444100	-1.17400300	1.07550600	H	-4.13789100	-3.18774600	-4.17200400	O	-0.85916200	-3.27802800	2.15441600
O	-1.51410800	0.37124400	1.34973800	C	-3.41716300	-4.21574500	-5.93887300	C	-0.16632200	-5.50516200	1.60892800
O	-0.21837300	0.02747900	-0.94851800	H	-2.57239300	-4.18759200	-6.64077100	H	0.78309000	-5.84468200	1.17521900
O	-0.24232600	2.39254500	0.41614400	H	-3.46313500	-5.22827000	-5.51526600	H	-0.95445700	-6.01765400	1.03439400
O	-5.06367800	-0.28355000	-1.64020300	H	-4.33562200	-4.05418800	-6.51636900	C	-0.27322200	-5.85077700	3.09531400
H	-5.44352000	-0.64025000	-0.81322700	N	1.87483100	-1.98825200	-1.16916700	H	-0.17776500	-6.93411300	3.23509200
H	-4.92550000	-1.04487300	-2.23261800	C	2.55234000	-1.57865700	-2.29862100	H	0.51814000	-5.36146100	3.67631300
O	-2.47914200	1.23027500	-3.12523700	H	2.02599000	-1.16425500	-3.14802100	H	-1.23591300	-5.53089700	3.50763000
H	-2.50996200	0.39935300	-3.63412300	C	3.89828500	-1.82730500	-2.13839400	O	-4.30748400	-0.60275500	0.96677200
H	-1.58044800	1.60096500	-3.26237800	N	4.00541300	-2.42155400	-0.88922500	C	-4.16284800	-1.19326900	2.05389100
O	0.26260400	3.83685000	3.02191600	H	4.89504600	-2.55221100	-0.39135400	O	-3.01740200	-1.56575000	2.55360500
H	0.50473800	2.90122200	2.83296500	C	2.78059500	-2.48089000	-0.33345600	C	-5.34970500	-1.55333200	2.92215100
H	-0.71088700	3.81388600	3.04118100	H	2.57810000	-2.84959300	0.66053900	H	-6.27317700	-1.15812200	2.49134400
O	0.65437400	5.09068100	-2.21001200	C	5.07603200	-1.55460000	-3.04170000	H	-5.20521200	-1.15244800	3.93242200
H	0.91590900	4.78459400	-3.09670300	H	5.07101200	-2.25616500	-3.88864700	H	-5.41820300	-2.64468500	3.01514100
H	-0.26282200	5.43315300	-2.29432500	H	4.94379600	-0.55627700	-3.48175900	O	-0.49479700	-0.74800500	3.53255600
O	0.64248600	5.14286100	0.71248900	C	6.48041400	-1.64330200	-2.38039500	C	0.25306600	0.26557600	3.64687200
H	1.54842200	5.49399500	0.66766000	H	6.74736200	-2.68998000	-2.19776400	O	0.65577000	1.01645900	2.67616300
H	0.54644300	4.70581300	1.61663600	H	7.21678900	-1.24021300	-3.08840600	C	0.75436600	0.64873200	5.02791300
O	-3.02706400	2.65481100	-0.57223500	C	6.56194300	-0.93512900	-1.02924100	H	1.82674300	0.39330100	5.04852000
C	-2.75735500	3.80691500	-0.93397900	O	6.41412700	-1.56130900	0.03003700	H	0.71331000	1.74525200	5.09934200
O	-1.54823000	4.23938800	-1.19261700	N	6.70686000	0.41397500	-1.04183500	C	0.02166900	-0.01740600	6.19770500
C	-3.87592200	4.82993900	-1.09598100	H	6.87527300	0.88335100	-1.92293300	H	0.08096000	-1.10782000	6.08799600
H	-4.67845600	4.32585900	-1.65103500	C	6.52612700	1.21536200	0.17397600	H	-1.04646500	0.23692900	6.14753100
H	-4.27993600	4.99667700	-0.08560200	H	7.08567600	0.73450100	0.98302000	C	0.59861500	0.41148100	7.55126300
C	-3.49758600	6.16053600	-1.74714400	H	6.97581000	2.19823400	-0.01123300	H	1.65877400	0.13640100	7.64003400
H	-3.12662600	6.01381600	-2.77024000	C	5.04520300	1.34833200	0.58055400	H	0.05991000	-0.07088700	8.37597000
H	-2.72441200	6.68273400	-1.17104300	H	4.64209900	0.35315300	0.79600400	H	0.52367300	1.49826300	7.69438700
H	-4.37488700	6.81587500	-1.80573800	H	4.99504200	1.92245700	1.51657800	O	0.16600500	1.95381600	-2.63558800
O	-0.62084000	-2.44466700	-2.31129400	C	4.20368000	2.03165900	-0.50165200	H	0.10390100	1.12885300	-2.03676300
C	-1.77552400	-2.34055200	-2.90360200	H	4.35282800	1.50722900	-1.45999800	H	1.03605100	1.88533300	-3.06598400

C

Ca	-2.72307700	0.23979600	-0.95081000	O	-4.98201000	-0.30571200	-1.80933600	H	0.11893600	5.08442700	-3.03815000
Mn	-0.06697300	-1.85664200	-0.40703100	H	-5.40728300	-0.60241400	-0.98135800	O	0.65663800	5.01693100	-0.03203900
Mn	-1.35838000	-1.13947500	1.88469500	H	-4.86185600	-1.09985700	-2.36116800	H	1.60643600	5.22800200	-0.10706700
Mn	0.18164800	0.76353400	0.67564300	O	-2.20647000	1.08918700	-3.24642700	H	0.51159600	4.71796400	0.93285300
Mn	0.31887600	3.36564500	-1.23979600	H	-2.05316100	0.32727600	-3.83078200	O	-2.86321500	2.64611300	-0.92352200
O	-1.75456200	-1.79186000	0.24754700	H	-1.34937500	1.58111400	-3.19393700	C	-2.57292800	3.74382900	-1.40432300
O	0.43417300	-1.03017700	1.20644000	O	0.25049300	2.08107500	-2.51130300	O	-1.34833300	4.14532400	-1.68230300
O	-1.51404000	0.54660200	1.21899500	H	0.30351400	1.19283400	-2.05955500	C	-3.62879800	4.78921500	-1.73828800
O	-0.13196100	-0.08208600	-0.95825500	O	0.96289500	4.63776400	-2.81972900	H	-3.39137600	5.68837900	-1.15037000
O	-0.18545600	2.44789600	0.10240100	H	1.11400600	3.98531400	-3.53255300	H	-3.48101600	5.07958500	-2.78856100

C	-5.06249600	4.32168000	-1.49015300	H	4.92830400	-0.64488700	-3.28801400	H	-0.27027700	-6.46170900	4.04031300
H	-5.21573100	4.05491000	-0.43805900	C	6.48303700	-1.74006300	-2.21595400	H	0.42451700	-4.84741900	4.29171600
H	-5.30235800	3.44083100	-2.09705100	H	6.75604900	-2.78814200	-2.05020600	H	-1.32671300	-5.03274300	4.10661500
H	-5.76859600	5.11982900	-1.74842600	H	7.21216400	-1.32388500	-2.92375600	O	-4.30506900	-0.43060400	0.84721900
O	-0.57542500	-2.68134400	-2.03484100	C	6.56147900	-1.04799200	-0.85780100	C	-4.21243600	-0.90170700	1.99575800
C	-1.70419200	-2.59642100	-2.68428200	O	6.38565400	-1.67997000	0.19315400	O	-3.09165400	-1.22447800	2.58237600
O	-2.54044500	-1.68621900	-2.53357200	N	6.73647600	0.29859800	-0.86139100	C	-5.43686800	-1.16260400	2.84666700
C	-1.91472400	-3.72069600	-3.68770700	H	6.91619800	0.76680100	-1.74087600	H	-5.52885600	-2.24020900	3.03358000
H	-1.02389100	-3.75860100	-4.33298600	C	6.53015500	1.10400600	0.34630200	H	-6.33610300	-0.79519100	2.34571500
H	-1.89445500	-4.66350300	-3.11953900	H	7.02787600	0.59631500	1.17871700	H	-5.32336500	-0.67496200	3.82199300
C	-3.19411900	-3.61154100	-4.52183200	H	7.02915200	2.06801000	0.19016700	O	-0.59594100	-0.31525100	3.56223300
H	-3.20243000	-2.64912400	-5.05317100	C	5.03650200	1.29405900	0.67694100	C	0.15758700	0.69916000	3.58715500
H	-4.06349800	-3.59696300	-3.84913200	H	4.58442400	0.31247100	0.85562900	O	0.60226900	1.32989400	2.54971900
C	-3.33344500	-4.76263900	-5.52412900	H	4.95707100	1.85796100	1.61713600	C	0.61813300	1.23079700	4.93264100
H	-2.49233100	-4.78167300	-6.23066200	C	4.28201600	2.02145200	-0.43981100	H	1.66896300	0.91517800	5.04309600
H	-4.25688700	-4.66639100	-6.10826900	H	4.48768400	1.52897800	-1.40427300	H	0.64691100	2.32772700	4.86558000
H	-3.36096000	-5.73533800	-5.01437700	H	4.61784600	3.06038100	-0.54899000	C	-0.20829400	0.76330000	6.13630900
N	1.89746200	-2.10923900	-0.95785700	O	2.17738200	1.08221200	0.25124200	H	-0.21482900	-0.33363400	6.16505300
C	2.56909800	-1.63209500	-2.06495900	C	2.76221800	2.03167100	-0.33111900	H	-1.25445800	1.07193900	5.99888300
H	2.04646400	-1.11637900	-2.85870700	O	2.20886600	3.03064500	-0.92411600	C	0.33382600	1.32559800	7.45488700
C	3.90665800	-1.93504400	-1.94928100	O	0.12951000	-3.60511800	0.56278800	H	1.36854400	1.00148400	7.63284100
N	4.01750500	-2.62500100	-0.74935900	C	-0.34758900	-3.82988400	1.72978500	H	-0.27188400	0.98423600	8.30312300
H	4.91040600	-2.77618900	-0.26508900	O	-0.92921300	-2.98053500	2.47678400	H	0.32374300	2.42428900	7.45877900
C	2.80002400	-2.69078700	-0.17682200	C	-0.21521700	-5.25374600	2.24496300	O	0.26546900	4.17496200	2.44406900
H	2.59886500	-3.13884700	0.78419600	H	0.74097800	-5.64991500	1.87979800	H	-0.70283900	4.20770600	2.54404300
C	5.07179500	-1.64742800	-2.86234900	H	-0.99430800	-5.83301500	1.72388000	H	0.46650700	3.20928700	2.44069800
H	5.05945200	-2.33955000	-3.71715500	C	-0.35676200	-5.40506300	3.76078800				

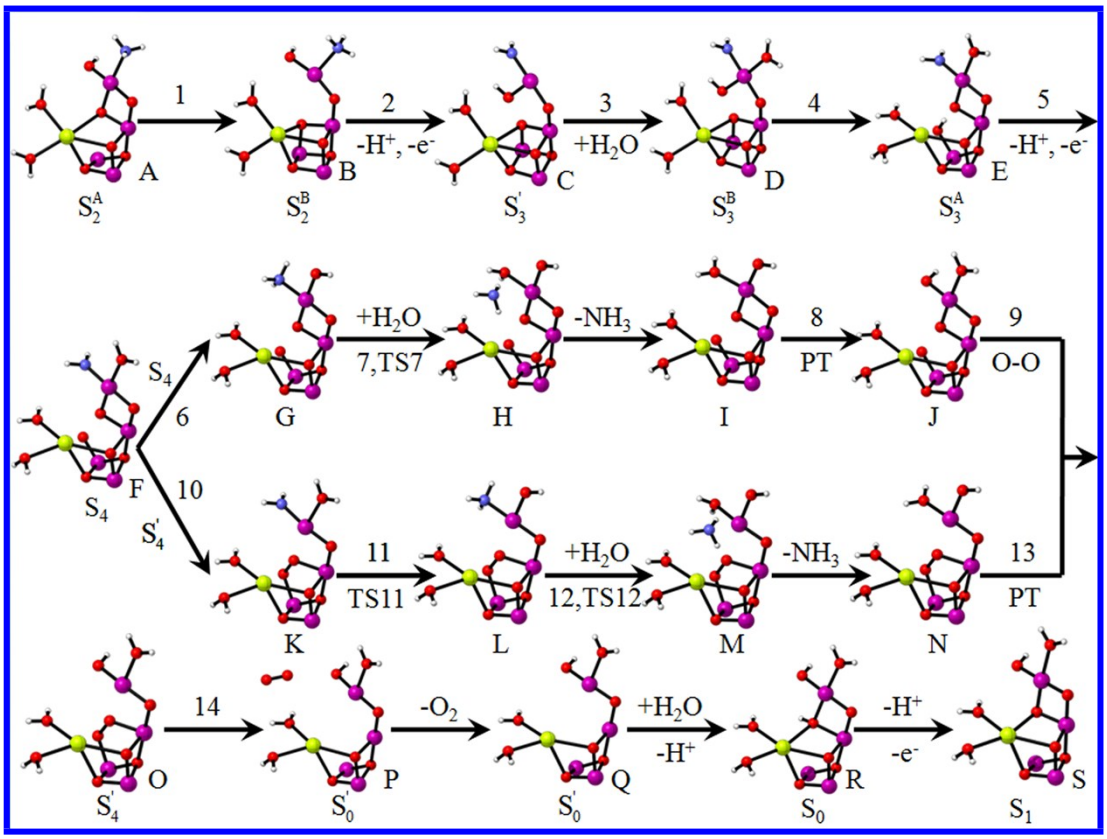
D:

Ca	2.40726900	0.18736200	-1.29436800	C	5.38864100	-3.65085800	-2.18379000	H	-7.48513100	2.04656100	-2.10075900
Mn	-0.07636500	2.07404100	0.03256500	H	5.64634400	-2.92882800	-1.40102800	C	-6.64858000	0.89833300	-0.44449500
Mn	1.31029000	0.46277000	1.86238600	H	5.46642800	-3.13719800	-3.14927400	O	-6.42822500	0.97395900	0.77251900
Mn	-0.19932300	-1.41850300	0.50860800	H	6.12913900	-4.45936600	-2.16565300	N	-6.74825000	-0.29655400	-1.08112000
Mn	-0.05189300	-2.92388000	-1.76571500	O	0.52876800	3.62089100	-0.87427600	H	-6.99259600	-0.30937400	-2.06347500
O	1.60833100	1.61526200	0.50002300	C	1.57397200	3.68130900	-1.65568500	C	-6.53069500	-1.56893800	-0.38448200
O	-0.43136600	0.45146100	1.04343100	O	2.26574500	2.70813600	-2.01069200	H	-7.10403400	-1.55008200	0.54920600
O	1.51047800	-1.07441400	0.90254600	C	1.87772200	5.09865300	-2.12612400	H	-6.94588000	-2.36118000	-1.01900200
O	-0.12904300	1.24901900	-1.62146000	H	0.99312300	5.45430000	-2.67694100	C	-5.04995800	-1.83593500	-0.06005000
O	-0.12535100	-3.18737800	-0.02701500	H	1.93360800	5.73594500	-1.23148900	H	-4.68522200	-1.05002300	0.60908800
O	4.47954100	1.14318000	-2.26795700	C	3.14143100	5.23630400	-2.97988400	H	-4.98807400	-2.78201800	0.49611400
H	5.07046300	1.08136400	-1.49304600	H	3.06587900	4.57160300	-3.85185800	C	-4.16399000	-1.90479200	-1.31002100
H	4.19341400	2.07789700	-2.31788300	H	4.00934400	4.88812900	-2.40085300	H	-4.29174800	-0.98528500	-1.90383000
O	1.23444500	0.21658600	-3.62965100	C	3.37484300	6.67933600	-3.44105400	H	-4.43995900	-2.74109200	-1.96455600
H	1.62625400	0.71863900	-4.36563300	H	2.53651800	7.04456200	-4.04999100	O	-2.20455600	-1.42328000	-0.00769400
H	0.60229000	0.83038800	-3.16073000	H	4.28569700	6.75616200	-4.04750200	C	-2.67353100	-2.00122200	-1.02146600
O	0.21931400	-1.23752900	-1.31891700	H	3.48508100	7.35957400	-2.58567200	O	-1.98472400	-2.65189900	-1.89499500
H	-0.57296800	0.38114000	-1.50682800	N	-2.09671100	2.45114800	-0.21250000	O	-0.29749200	3.18369200	1.64466500
O	0.09747200	-2.33962900	-3.78900000	C	-2.82876700	2.46066300	-1.38343200	C	0.30264700	3.01777600	2.76373100
H	0.50189700	-1.42715600	-3.80943400	H	-2.33550100	2.43632300	-2.34454900	O	0.97238200	1.99540900	3.08198500
H	0.73490200	-2.93842900	-4.22042900	C	-4.16945800	2.50211400	-1.08071600	C	0.18850800	4.15704100	3.76160700
O	-0.62024900	-4.83018900	-2.34985400	N	-4.22632100	2.53353400	0.30690400	H	-0.84738700	4.52014100	3.72687000
H	-1.59353200	-4.79649800	-2.42179700	H	-5.07803000	2.32515800	0.84151900	H	0.79933500	4.97659500	3.35135000
H	-0.41300300	-5.41824200	-1.54138300	C	-2.96885100	2.48394300	0.78917900	C	0.62521900	3.81119900	5.18559300
O	3.13803800	-1.95683000	-1.99655600	H	-2.71793500	2.44605400	1.83823500	H	0.53126500	4.69359400	5.82953200
C	2.88390600	-3.16727800	-1.97143400	C	-5.38023300	2.52957800	-1.97769400	H	0.00581300	3.01160300	5.60949800
O	1.68026400	-3.67813600	-1.96092800	H	-5.50080000	3.53192700	-2.41442300	H	1.66682800	3.47360900	5.20952000
C	3.98611000	-4.21874100	-1.96844400	H	-5.18918700	1.85579200	-2.82410500	O	4.16458700	0.29912200	0.43052600
H	3.91785000	-4.74036000	-1.00132000	C	-6.73043700	2.15324800	-1.31025700	C	4.17262800	0.37784600	1.67485100
H	3.73200200	-4.97311600	-2.72612000	H	-7.06582400	2.96284100	-0.65229800	O	3.11338400	0.43582200	2.43067100

C	5.47321500	0.41997000	2.45092800	C	-0.55431600	-2.21528400	4.66532700	H	-0.34458800	-2.61148200	7.44494800
H	5.53832600	1.36226100	3.00922200	H	-1.12367800	-1.46913800	5.24069900	H	1.08053200	-3.66520800	7.40214100
H	6.32627100	0.32880300	1.77360200	H	-1.23139500	-3.04448700	4.43112400	H	-0.43745100	-4.19920400	6.65802300
H	5.49104300	-0.39279700	3.18694300	C	0.64912100	-2.69382900	5.50106800	O	-0.13141900	-5.91415600	-0.02820200
O	0.69475100	-0.60277200	3.42633900	H	1.31212500	-1.83957600	5.68810500	H	0.77929800	-6.24770200	0.05149600
C	-0.13908300	-1.55312800	3.36798800	H	1.22904400	-3.42107700	4.91352800	H	-0.10144200	-4.99734400	0.33890700
O	-0.66561600	-1.99933800	2.28759000	C	0.21084500	-3.32822200	6.82469900				

VI. NH_3 departure time analysis

Proposed S-state cycle under NH_3 involvement



Scheme S5. Graphical expressions for the sequential conversions from the NH_3-bound S_2-A structure to the S_1 state of the next S-state cycle based on the radical coupling mechanism for O-O bond formation, with the two branches S_4 and S' 4 on F standing for the two possible departure state for NH_3. Here are specific annotations for each step: 1: interconversion from the open to closed-cubane form by O5 shifting in the S_2 state; 2: oxidation of Mn4 with simultaneous NH_3

deprotonation to Asp61; 3: water binding to Mn4 through a pivot mechanism; 4: transformation from the closed to open-cubane form by Mn3 ligand exchange in the S_3 state; 5: S_3~S_4 transition by ligand-centered oxidation; 6&11: W1 (newcomer) deprotonation to NH_2^-; 7&12: NH_3 replacement by H_2O; 8&13: W2 (newcomer) deprotonation to W1; 9&10: O-O bond formation; 14: O_2 release.

Feasibility analysis of NH_3 deprotonation to Asp61

We have enlarged our NH_3-bound model to include the side chains of Asp61 with its nearby water molecules and the peptide bonds of Asp170, in order to show the three hydrogen-bonds in the vicinity of NH_3. We have approximatively examined the relative acidity (compare the energetics) before and after NH_3 deprotonation to $Asp61^-$ in a vertical way. It turns out that the energetic difference is about 6 kcal/mol (slightly favorable for the former case), justifying the feasibility for NH_3 deprotonation to $Asp61^-$, given the thermal fluctuations in the protein matrix. We can understand this in such way. The total charge except $Asp61^-$ in our model is just 1+, while it is 1- for $Asp61^-$ (entirety neutral). So once the $[SB\ 2]^+$ state is formed after Tyr-Z is oxidized and lose its proton to His190, W1 or NH_3 on Mn4 has a tendency to deprotonate to its nearby proton acceptor $Asp61^-$, making these two parts both neutral for a more energetically lower interaction. Besides, For PCET during S_2-S_3 transition, Mn4 with its titratable ligand NH_3 is most suitable to lose electron and proton. Additionally, the chemical bond formed between O and H can compensate the energy cost for breaking N-H bond. Furthermore, hydrogen tunneling effect has been proved to be existent in many biochemical processes, which increases the possibility for NH_3 deprotonation.

VIa. NH_3 hydrolysis in the S_3 state

Theoretical study for ammonia associativity in the S_3 state

Prior to assess the candidates for NH_3 departure, we intend to examine whether ammonia is bound to Mn4 or interact in a non-bonding fasion with the OEC in the S_3 state (Scheme S3(d)). Based on the more stable S_3-A structure on the septet/Mn1-Mn4(αααβ) surface newly put forward by Cox and coworkers, we have located the TS9 (2.88 Å for Mn-N (NH_3) and 2.45 Å for Mn-O (H_2O)) for the hypothetical NH_3 replacement by H_2O in the S_3 state. It is shown in Figure SVIa that the NH_3-bound OEC is energetically more favorable than the H_2O-bound form, and it takes a barrier as high as 27.2 kcal/mol to accomplish the hydrolysis. This is believed to be almost infeasible in reactivity and suggests that ammonia is still bound to Mn4 in the S_3 state.

It should be pointed out that Boussac et al.'s EPR study[20] has uncovered the associativity for ammonia-OEC in the S_3 state, but it cannot definitely demonstrate whether ammonia is bound on Mn or just interacts with OEC in a non-bonding fasion in a short distance, the latter of which resembles the interaction between methanol and the OEC.[21] Although the latter case cannot be excluded according to the modification of S_3-state EPR signals, we advance our proposal that ammonia is still bound to Mn4 in the S_3 state, further showing the specific interaction style based on our model and computation results.

Table SVIa. Gibbs free energies and Mulliken spin populations for NH_3 hydrolysis in the S_3 state:

Spin states	Spin topology (Mn1-Mn4)	Gibbs Free energy (a.u.)		
		N	TS9	O
septet	ααaβ	-3423.4420	-3423.3987	-3423.4331

Spin states	Spin topology (Mn1-Mn4)		Mulliken spin density		
			N	TS9	O
septet	α	Mn1	2.96	2.96	2.97
	α	Mn2	2.96	2.96	2.96
	α	Mn3	2.91	2.92	2.91
	β	Mn4	-2.86	-2.90	-2.86

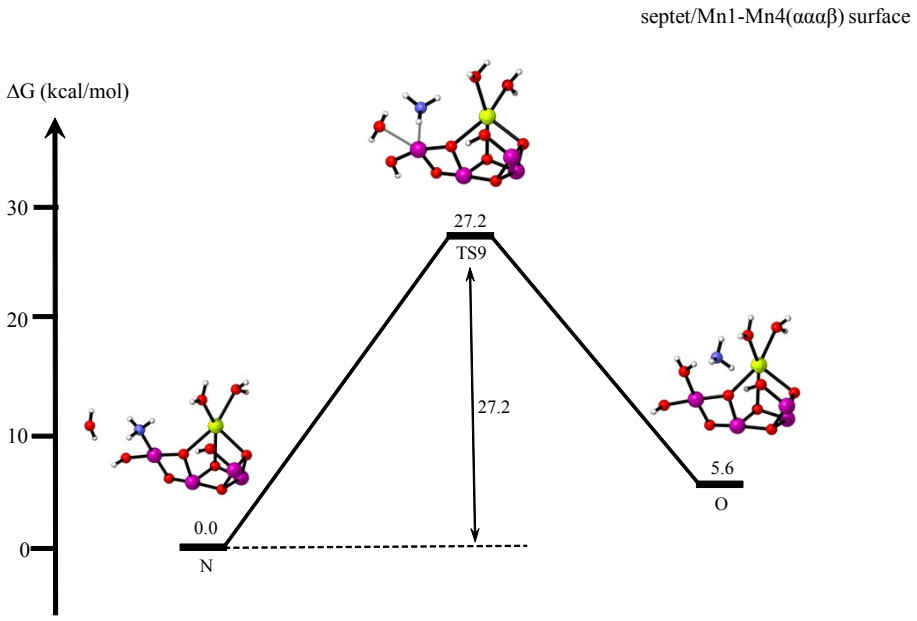


Figure SVIa. Calculated relative Gibbs free energy profile (in kcal/mol) for NH_3 replacement by H_2O in the hypothetical S_3 state on the septet/Mn1-Mn4(αααβ) surface.

The Cartesian coordinates for N, TS9 and O:

N:

Ca	-2.41841500	-0.25882200	-1.07308200	C	-1.38218800	-4.73746400	-4.81446200	O	1.14658000	-3.36713200	0.63748800
Mn	0.45329000	-1.89227500	-0.53493000	H	-0.95964000	-3.94159200	-5.44633600	C	0.64130700	-3.69455200	1.76280600
Mn	-1.02733400	-1.31121900	1.72031700	H	-2.42833000	-4.45873700	-4.63309500	O	-0.23760400	-3.04017600	2.38997400
Mn	-0.14238600	1.25886900	1.00228000	C	-1.31395300	-6.07629700	-5.55680500	C	1.14817400	-4.99538600	2.37255400
Mn	-0.87219400	3.39403300	-0.52854200	H	-0.27504100	-6.36234200	-5.77291000	H	2.24000400	-5.01014100	2.25068500
O	-1.24125800	-2.07617600	0.07139200	H	-1.76176300	-6.88461400	-4.96160400	H	0.77013900	-5.80276500	1.72648400
O	0.56949200	-0.68492500	0.91120100	H	-1.85233100	-6.02884100	-6.51238200	C	0.73906900	-5.22488000	3.82758500
O	-1.67372200	0.32015000	1.30582800	N	2.47396200	-1.61239300	-0.99587100	H	1.12557900	-6.18844600	4.18326200
O	-0.65303000	1.54681100	-0.72250600	C	3.00248800	-1.02049700	-2.12253400	H	1.13187900	-4.43526100	4.47948700
O	-0.65987500	2.95206200	1.19074100	H	2.36704600	-0.78102200	-2.96404000	H	-0.35112200	-5.22592200	3.93416300
O	-4.15940100	-1.74665700	-2.16906600	C	4.35107800	-0.81832000	-1.94239900	O	-3.99470600	-1.37804500	0.53044500
H	-4.54179900	-1.99425100	-1.30179200	N	4.62612200	-1.32178000	-0.67615800	C	-3.85364300	-1.85817300	1.67753500
H	-3.53464300	-2.46471900	-2.41332800	H	5.48861200	-1.12715700	-0.15918100	O	-2.74713400	-1.91572400	2.34262600
O	-2.19694200	-0.04343900	-3.58361900	C	3.47060400	-1.77028400	-0.13742900	C	-5.04901600	-2.43030800	2.42121000
H	-3.08612800	-0.28220700	-3.90229600	H	3.37434800	-2.17468900	0.85892100	H	-4.81401500	-3.43214600	2.79923200
H	-1.69358500	-0.88817500	-3.61110800	C	5.38392000	-0.21300600	-2.85794400	H	-5.92670800	-2.46544900	1.76975400
O	-0.86434000	5.24331600	-0.35842700	H	5.61187200	-0.90639400	-3.68143800	H	-5.26669600	-1.79697100	3.29099100
H	0.06695300	5.51424700	-0.26556400	H	4.94118000	0.67454900	-3.33176200	O	-0.54997100	-0.69215400	3.54267400
O	-2.24619700	6.09517200	-2.50833800	C	6.73271900	0.17422800	-2.19806200	C	0.06395500	0.39484900	3.78160800
H	-3.16021300	5.98179600	-2.19611300	H	7.30066800	-0.72636800	-1.93888700	O	0.42362100	1.24353100	2.90919300
H	-1.71814600	5.98028800	-1.66953400	H	7.32803800	0.73384400	-2.93254900	C	0.37400400	0.72715600	5.23300000
O	-3.68760300	1.71918100	-1.31638000	C	6.56902600	0.96884700	-0.90342500	H	1.27743600	1.35055700	5.24524300
C	-3.77156100	2.82367600	-0.74253400	O	6.62439700	0.41223000	0.20128700	H	-0.44782600	1.37542800	5.57964000
O	-2.78212700	3.58372400	-0.41379800	N	6.29960000	2.29351200	-1.03261900	C	0.51175700	-0.48673600	6.15912800
C	-5.14083500	3.37779000	-0.35338200	H	6.24571600	2.68817300	-1.96339900	H	1.32796000	-1.12840000	5.79511700
H	-5.89682000	2.80033300	-0.89733800	C	5.88603800	3.11925100	0.10721900	H	-0.40202700	-1.09072500	6.09628000
H	-5.26886600	3.15173600	0.71649600	H	6.54974800	2.87996300	0.94484100	C	0.78106000	-0.07949300	7.61183200
C	-5.30693200	4.88415300	-0.58203300	H	6.05714700	4.16683800	-0.17121800	H	1.70722300	0.50582500	7.70052400
H	-5.23174400	5.13039300	-1.65146500	C	4.42463400	2.88755700	0.52801600	H	0.88079600	-0.96133500	8.25797400
H	-4.54036100	5.44633500	-0.03762900	H	4.30187300	1.84567700	0.84227700	H	-0.03785600	0.53534700	8.01121700
H	-6.29321200	5.22131700	-0.23948000	H	4.21998200	3.50843200	1.41187500	O	0.04327000	-0.67425600	-1.81942300
O	0.27570700	-3.28306000	-1.87865000	C	3.41732600	3.21311400	-0.57998200	H	0.22063500	0.24816500	-1.50741400
C	-0.72209500	-3.46880400	-2.67764700	H	3.65591400	2.62802900	-1.48295400	N	-1.10874900	3.49833300	-2.61722100
O	-1.70517900	-2.70666700	-2.81711900	H	3.45661600	4.27127700	-0.86920700	H	-1.63376000	2.68412500	-2.94577600
C	-0.63481600	-4.76942800	-3.47676800	C	1.97031200	2.87127000	-0.23588300	H	-0.19487400	3.50201300	-3.07168900
H	0.42455400	-5.02135700	-3.61470800	O	1.75296300	1.89982800	0.53365900	H	-1.61168300	4.38260100	-2.83361000
H	-1.05250600	-5.56158500	-2.83285100	O	1.08837300	3.60269300	-0.81073700				

TS9:

Ca	2.46321400	-0.61679500	-0.95545200	O	-0.75512200	-5.24604700	0.18647000	C	1.70773300	3.17776100	-2.67624300
Mn	0.18911800	1.87887100	-0.52980600	H	-0.79368100	-5.13407600	1.15418600	O	2.46247300	2.20958700	-2.90930700
Mn	1.40408300	0.90893900	1.75357800	O	-0.69469500	-5.19021300	-2.29616200	C	1.91866900	4.51278200	-3.39294500
Mn	-0.19114900	-1.27681800	1.01449400	H	0.26544100	-5.36650500	-2.29952700	H	0.93127900	4.94267500	-3.61028200
Mn	-0.21961300	-3.61023700	-0.48562600	H	-1.02216700	-5.74937600	-1.55761100	H	2.38212200	5.19435800	-2.66053100
O	1.85699400	1.55530900	0.09780500	O	3.14373200	-2.85064000	-1.11045000	C	2.78099600	4.42521000	-4.65540000
O	-0.29805200	0.76084900	0.92038700	C	2.73344200	-4.02150900	-1.02299300	H	2.30639900	3.73755700	-5.37080300
O	1.54493100	-0.84221100	1.34580200	O	1.52803900	-4.40520100	-0.76026100	H	3.74783500	3.97309500	-4.39862500
O	0.16938700	-1.72323300	-0.68871700	C	3.73851300	-5.16298500	-1.19704000	C	2.99581000	5.79226700	-5.31401700
O	-0.12831700	-3.06971400	1.20022300	H	4.50014000	-4.81448800	-1.90557800	H	2.04082700	6.25128000	-5.60637100
O	4.45393600	0.56461300	-1.98667600	H	4.24904300	-5.26064900	-0.22588800	H	3.50091200	6.48931600	-4.63041900
H	4.87432200	0.70417400	-1.11343000	C	3.15139900	-6.51198900	-1.61619500	H	3.61392600	5.70553200	-6.21717000
H	4.01414200	1.41018500	-2.23001900	H	2.66364300	-6.44662000	-2.59911400	N	-1.82521600	2.18306000	-1.00967300
O	2.26452400	-0.49337300	-3.48601400	H	2.40830800	-6.86063500	-0.89086300	C	-2.49358700	1.75841000	-2.13740900
H	3.18469600	-0.48560100	-3.80508400	H	3.94323600	-7.26820800	-1.69217600	H	-1.94978900	1.32349100	-2.96475900
H	2.01331400	0.46168100	-3.44248700	O	0.71961900	3.19605600	-1.84378400	C	-3.84220800	1.98054500	-1.97994600

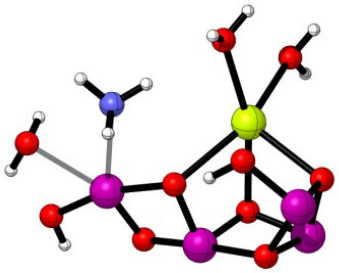
N	-3.96721900	2.56896500	-0.72692800	H	-4.21070000	-1.42609500	-1.43967400	H	5.55877800	-0.02765400	3.39954100
H	-4.85529600	2.66327000	-0.22529600	H	-4.53885700	-3.04934900	-0.82812000	O	0.74040200	0.46730800	3.56810100
C	-2.73754100	2.65456500	-0.17291400	C	-2.70323600	-2.18415400	-0.17189800	C	-0.13877600	-0.41886700	3.81229900
H	-2.53511200	3.03348900	0.81738800	O	-2.19969800	-1.34677300	0.62339000	O	-0.71270600	-1.14387200	2.94484300
C	-4.99900500	1.70013800	-2.90472600	O	-2.09120900	-3.14383700	-0.75286600	C	-0.51672400	-0.64659100	5.26822800
H	-4.99013400	2.40888200	-3.74641700	O	-0.07723400	3.49079000	0.65141500	H	-1.52176900	-1.08657500	5.28766100
H	-4.84581900	0.70766700	-3.35177600	C	0.49191100	3.66600300	1.77875100	H	0.16908300	-1.42329300	5.64550800
C	-6.41038500	1.76517100	-2.26505900	O	1.14961500	2.79200900	2.41040200	C	-0.42849500	0.60078200	6.15645500
H	-6.67698200	2.80362500	-2.03860100	C	0.36873200	5.05737200	2.38694000	H	-1.10875600	1.37180700	5.76455500
H	-7.13911000	1.39473800	-2.99906500	H	-0.66883400	5.38770400	2.24119400	H	0.58310400	1.01923200	6.08458100
C	-6.51645900	0.99557700	-0.94929200	H	0.97967000	5.72115000	1.75565200	C	-0.77681500	0.29821600	7.61782000
O	-6.42078100	1.57517900	0.14099800	C	0.79358900	5.15774800	3.85215100	H	-1.79676400	-0.10005500	7.71417400
N	-6.65521300	-0.35169800	-1.04188600	H	0.69492300	6.19178000	4.20628800	H	-0.71265200	1.20346100	8.23550500
H	-6.69830200	-0.77136000	-1.96235400	H	0.17383600	4.51565500	4.48971400	H	-0.08958200	-0.44587100	8.04470300
C	-6.51282900	-1.23095600	0.12394700	H	1.83452500	4.84253200	3.98207700	O	0.25898800	0.59315500	-1.80418700
H	-7.08209700	-0.78298500	0.94521500	O	4.27767400	0.05030500	0.66670900	H	-0.17695100	-0.24207900	-1.48782300
H	-6.98395300	-2.18837300	-0.13197500	C	4.25698100	0.56525900	1.80583100	N	0.18876900	-2.80294600	-3.21567600
C	-5.05096900	-1.43188700	0.55948200	O	3.20256600	0.98521900	2.42553200	H	0.81286100	-2.03276700	-3.47101100
H	-4.62963000	-0.46796600	0.86441800	C	5.54309000	0.72408900	2.59901400	H	-0.75401600	-2.42354700	-3.13367200
H	-5.04528200	-2.07404400	1.45170200	H	5.58192800	1.71050200	3.07416200	H	0.16176300	-3.46904900	-3.98829000
C	-4.17882000	-2.05487400	-0.53537900	H	6.41244800	0.57309600	1.95274800				

O:

Ca	-2.45104100	0.29873500	-1.15850500	H	-2.22784900	-5.73864500	-1.41777700	O	2.17806700	1.55207700	0.21635500
Mn	-0.11630600	-1.91533500	-0.12140100	C	-2.52551400	-5.46978100	-3.55247100	O	2.05439600	3.00516100	-1.51996000
Mn	-1.37448700	-0.44178700	1.84528800	H	-2.01913200	-4.96250700	-4.38753800	O	0.13916000	-3.20138200	1.40268500
Mn	0.18413600	1.55721000	0.61159700	H	-3.50869100	-4.99116200	-3.45818800	C	-0.43962500	-3.10817500	2.53603200
Mn	0.15240600	3.40538000	-1.40315800	C	-2.68986500	-6.95863000	-3.87604400	O	-1.10504400	-2.11418600	2.93889800
O	-1.79998300	-1.49022300	0.39074700	H	-1.71581400	-7.45232100	-4.00067500	C	-0.31328200	-4.31674700	3.45517100
O	0.32437500	-0.48201200	1.01867300	H	-3.22531400	-7.48384800	-3.07251600	H	0.73027400	-4.65682800	3.40692500
O	-1.55156500	1.15222200	1.02786900	H	-3.25794300	-7.10332100	-4.80428600	H	-0.90521500	-5.11900800	2.98797900
O	-0.20061600	1.53414600	-1.15710100	N	1.92360300	-2.26286800	-0.45426400	C	-0.76381800	-4.07660900	4.89622200
O	0.12279300	3.32440000	0.37252300	C	2.63557100	-2.13429000	-1.62630100	H	-0.66117000	-4.99723600	5.48467900
O	-4.48418400	-1.15724900	-1.74640500	H	2.12366400	-1.99544000	-2.56819400	H	-0.16251200	-3.29413300	5.37472600
H	-4.86707900	-0.99717300	-0.85821200	C	3.98273800	-2.20525100	-1.35489300	H	-1.81010700	-3.75441700	4.93250500
H	-4.03391800	-2.02982400	-1.71002200	N	4.06298600	-2.39916200	0.01845400	O	-4.26321000	0.11920500	0.59802700
O	-2.48981000	-0.54354800	-3.57575500	H	4.92588200	-2.29741400	0.56273000	C	-4.23628700	-0.11294800	1.82900900
H	-3.45097200	-0.57463300	-3.73620400	C	2.80906600	-2.40935300	0.52055400	O	-3.18255900	-0.38866100	2.51961700
H	-2.26984800	-1.46463800	-3.27910300	H	2.56962800	-2.49604000	1.56945700	C	-5.51843600	-0.05926000	2.64267200
O	0.61268700	5.14283700	-1.56441900	C	5.17707000	-2.10432500	-2.26983600	H	-5.54028500	0.88691200	3.20033300
H	-0.14929500	5.66037300	-1.24085700	H	5.23200600	-2.99297400	-2.91628100	H	-5.54512600	-0.87344600	3.37479200
O	0.13201000	3.16552500	-3.46594700	H	5.01935300	-1.25332500	-2.94801000	H	-6.39223900	-0.10148000	1.98593500
H	0.07058700	2.18955800	-3.81002900	C	6.55556900	-1.95568600	-1.57600100	O	-0.74198100	0.42732800	3.50337400
H	-0.65994300	3.63660100	-3.77802900	H	6.83036800	-2.88986200	-1.07338600	C	0.12769200	1.35620600	3.53230300
O	-3.12571200	2.38855600	-1.97745700	H	7.31133300	-1.76811900	-2.35106500	O	0.69792900	1.85996900	2.51956300
C	-2.86600600	3.58204000	-1.70809900	C	6.58657700	-0.86358200	-0.50668800	C	0.49645100	1.92899400	4.89235800
O	-1.69365000	4.08532700	-1.54242400	O	6.44637000	-1.13893600	0.69316900	H	1.51327300	2.33497900	4.81742800
C	-4.03125600	4.56328900	-1.57104100	N	6.71218300	0.41454700	-0.94406000	H	-0.16859300	2.79429500	5.04997300
H	-4.65758900	4.43439000	-2.46525400	H	6.79497300	0.57950700	-1.93962900	C	0.36356100	0.94786900	6.06330500
H	-4.63898000	4.18944800	-0.73332500	C	6.50202900	1.56545300	-0.05711800	H	1.02431600	0.08547900	5.88899500
C	-3.65880300	6.03008300	-1.35794500	H	7.04938300	1.36991600	0.87106300	H	-0.65892500	0.55054300	6.08293300
H	-3.06896700	6.41882400	-2.19742800	H	6.95944200	2.43638000	-0.54301600	C	0.70691300	1.59957500	7.40720400
H	-3.06518700	6.15767700	-0.44534700	C	5.01925700	1.82222100	0.26213400	H	1.73711800	1.98263900	7.41695900
H	-4.56394700	6.64428600	-1.26617100	H	4.60955900	0.95386500	0.78902600	H	0.61041000	0.88113300	8.23162500
O	-0.57902700	-3.52196700	-1.11264500	H	4.96086200	2.66997400	0.95940100	H	0.03800500	2.44497100	7.62182200
C	-1.59429700	-3.76205600	-1.86923600	C	4.17720900	2.11591600	-0.98362200	O	-0.18146700	-0.96697600	-1.67639700
O	-2.43979200	-2.92706600	-2.26435700	H	4.28789000	1.29508000	-1.71054200	H	0.19133400	-0.05601300	-1.51957700
C	-1.73168800	-5.23356200	-2.26349900	H	4.49968600	3.03438700	-1.48944100	N	0.02574400	0.66496600	-4.40172500
H	-0.72622700	-5.67044000	-2.32341900	C	2.67977600	2.23588200	-0.71976200	H	-0.94067100	0.32286600	-4.46091700

H 0.47093300 0.04332500 -3.72252600 H 0.47966100 0.52306200 -5.30471800

3D image for TS9:



VIb. NH_3 hydrolysis in the S_4, S' 4 or S' 0 state

Principle of spin topology selection for the S_4, S' 4 state

Ahead of this, we have refined the oxo-oxyl coupling mechanism[22] in the S_4 state rebuilt in our model with an elaborated spin regulation principle (paper in progress). According to the computation results, we find that besides the requirements for the antiferromagnetic coupling between Mn1 and its bonded O· radical lowering energy of the system and ferromagnetic coupling between Mn4 and the O· ensuring smooth electron transfer during O-O bond formation, which are in coincidence with Siegbahn's spin alignment rule,[23] ferromagnetic coupling between Mn1 and Mn3 is necessary to avoid production of singlet $^1O_2$ which is beyond 20 kcal/mol in energy than triplet $^3O_2$ and considered forbidden.[24] As a result, sextet/Mn1-Mn4-O·(αααββ) and doublet/Mn1-Mn4-O·(βαβαα) are screened out from 16 spin topologies for effective $^3O_2$ generation and they are regarded as the spin coupling forms for NH_3 replacement in the S_4 state. As radical character disappears and Mn4(IV) reduces to (III) upon O-O bond formation, sextet/Mn1-Mn4(αααβ) and doublet/Mn1-Mn4(βαβα) are the corresponding forms in the S' 4 state (see analysis of these two states in the main text).

S' 0 state ruled out as a candidate for NH_3 departure

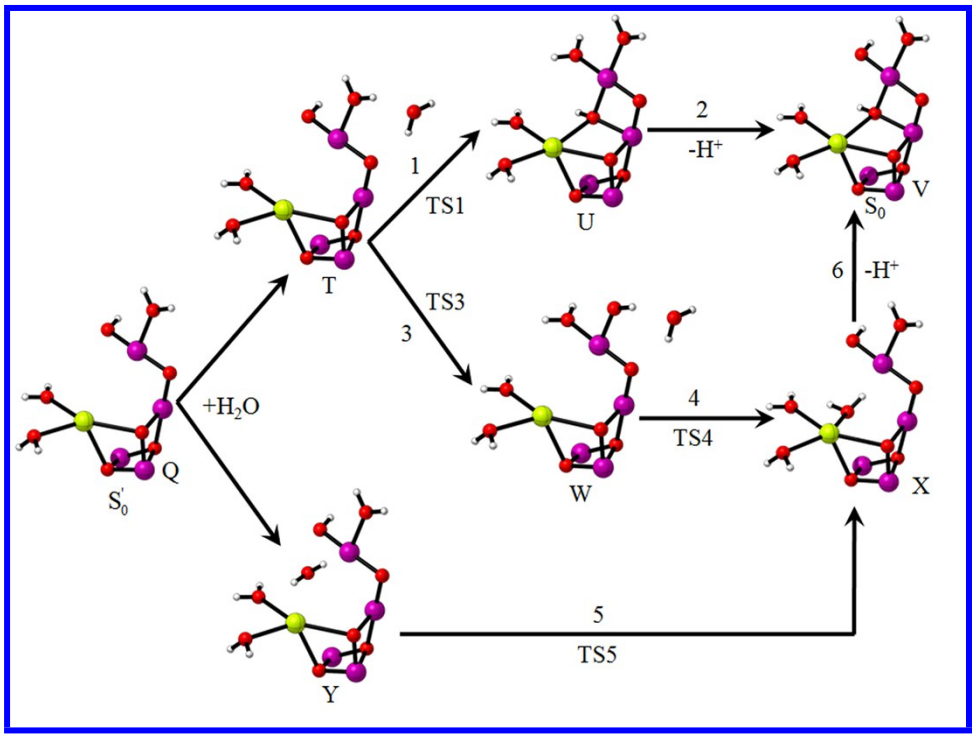
Focusing on the following S' 0 state for ammonia dissociation. This is a special and transient state between the S' 4 and S_0 states, which is after O_2 release and before water binding to the OEC.[25] It is in the oxidation arrangement of Mn1-Mn4 (III, IV, III, III) because Mn1 and Mn3 are reduced once upon O_2 release. On the view of geometric structure, there is a huge hole inside the cluster due to the gone oxygenic groups as molecular O_2. We have attempted to search the transition state for NH_3 replacement by H_2O in the S' 0 state, but unfortunately any optimizations failed because of the extreme easiness for one of the ligands sliding into the cavity and losing its association with the substitution reaction on Mn4. We do not regard the unsuccess as absolute technical difficulty, on the contrary, it precisely indicates the unsuitability for NH_3 replacement in the S' 0 state, perhaps because of the existence of the pivot Mn4 and the adjacent large vacancy that is exceedingly prone to be filled by insertion or translocation of some ligand, and this just prompts the quick formation of the S_0 state. Consequently, judging from the instantaneity and structural characteristics, we expel the possibility for ammonia departure in the S' 0 state.

VIc. NH_3 hydrolysis in the S_0 state

The S_0 state is the last candidate for ammonia dissociation. It keeps consistent in the valence distribution with the S' 0 state. Structurally, it is added with a hydroxyl as the bridging group between Mn3 and Mn4.[26] To date there is seldom theoretical or experimental researches on the water binding mode in the S' 0 state, the precursor event for the formation of hydroxyl bridge in the S_0 state. Likewise, the TS location for NH_3 replacement by H_2O in the S_0 state failed since we could not simultaneously

observe both eigenvectors with negative eigenvalues and imaginary vibrations for Mn4-N (NH_3) and Mn4-O (H_2O). However, we have searched out a reasonable judgment method after careful deliberation in conjunction with the survey on the water binding modes in the S' 0 state (Scheme S6), which plays an accessorial role in clarifying whether ammonia is still bound in the S_0 state.

Water binding modes in the S' 0 state

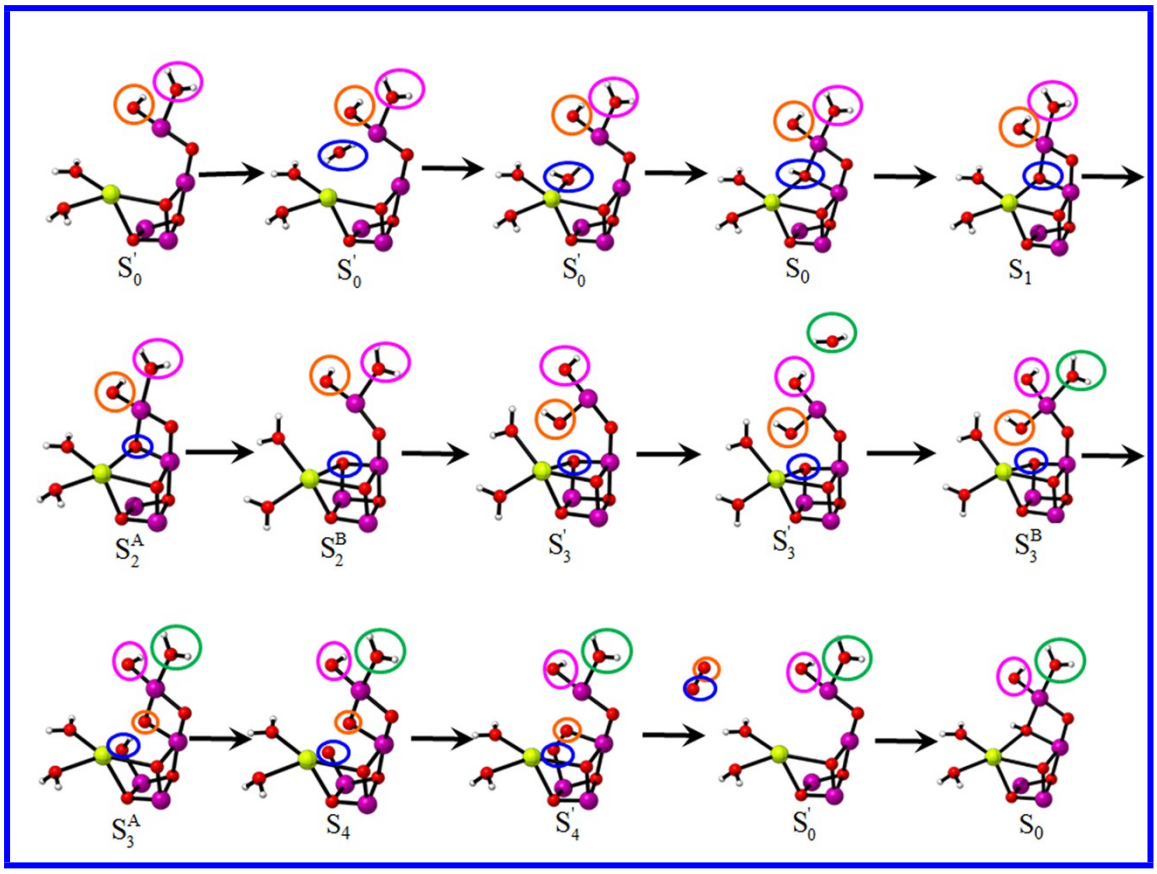


Scheme S6. Water binding in the S' 0 state and then formation of the S_0 state. Here are specific annotations for each step: 1: water binding to Mn4 in concomitance with W1 (H_2O) and W2 (OH^-) pivoting on Mn4; 2: W2 (new title after pivoting) deprotonation to lumen; 3: W1 deprotonation to W2; 4: water binding to Mn4 in concomitance with W1 (OH^-) and W2 (H_2O) pivoting on Mn4; 5: water binding to Ca(II); 6: newly bound water deprotonation to lumen.

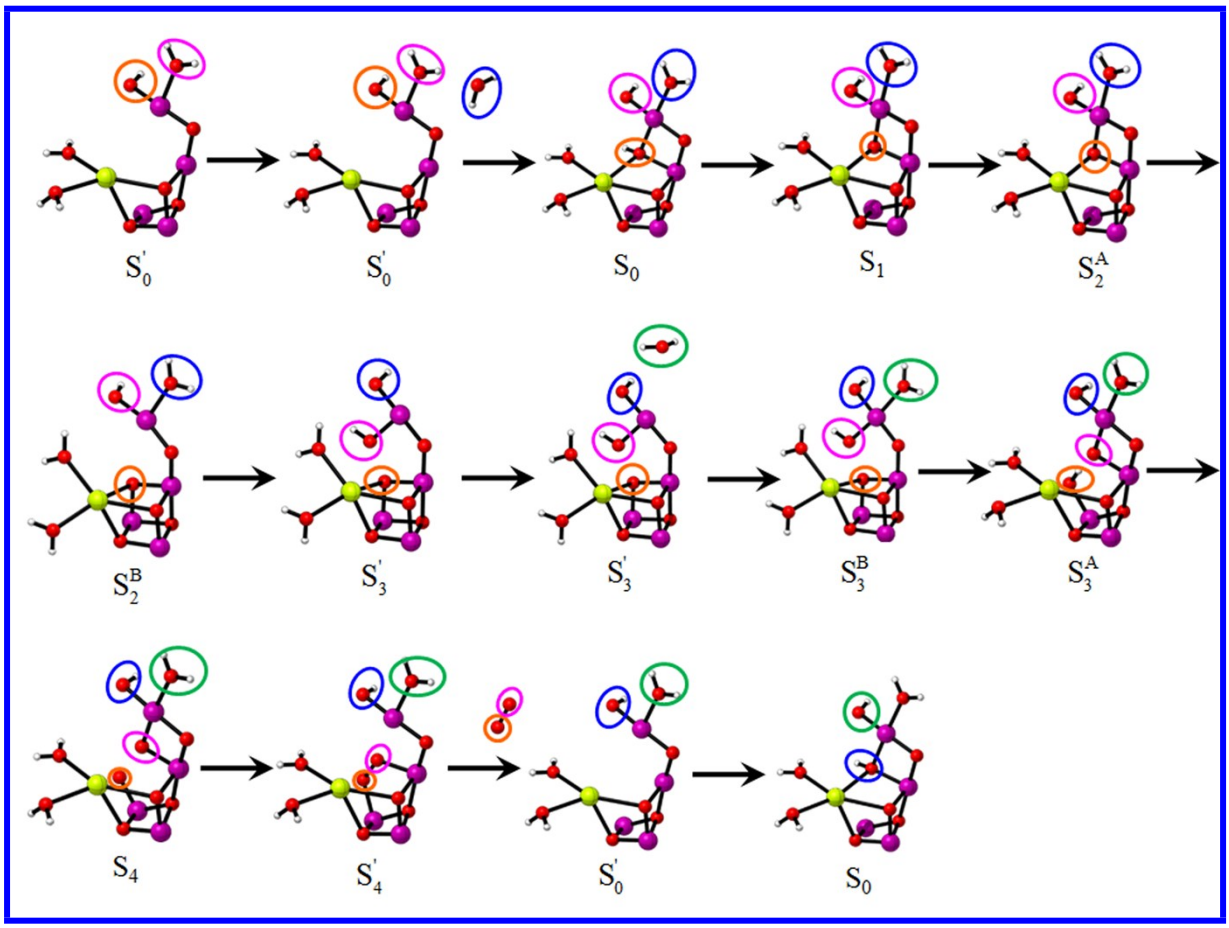
Implications for substrate identifications in the present and following S-state cycle

Inspired by the pivot mechanism for water binding in the S’ 3 state,[5] we have advised water binding to Mn4 in concomitance with the carrousel rearrangement of W1 and W2. Given the different protonation states of W1 and W2 in the S' 0 state, there are two kinds of binding microenvironment for step1 and 4, the latter of which needs a preceding proton transfer from W1 to W2 (step3). Besides, taking cognizance of the giant hole of the cluster, we suppose the newcome water may refill it through straight inserting and bind to Ca (step5). Other binding sites including Mn1, Mn3 and *trans* to W1 position of Mn4 are tried and proved to be unreliable. These pathways are expressed in Scheme S6, and proton transfer to lumen is required for the S_0 state formation.It is valuable that the choice of water binding mode in the S' 0 state has a significant impact on the sources of both substrate waters for the current and even following S-state cycles in the precondition of the pivot mechanism for water binding in the S’ 3 state and radical coupling mechanism for O-O bond formation in the S_4 state (Scheme S7). As sketched in Scheme S7(a) for water insertion mechanism in the S' 0 state, substrates for the present (n) cycle originate from the water binding in the S' 0 state (blue, becoming O5 and serving as the slow exchanging substrate water W_s in the S_0~S_3 states) and the W2 hydroxyl ligand (orange, as the fast exchanging substrate water W_f in the S_0~S_3 states). The W1 water ligand (fuchsia, n cycle) will become the W2 hydroxyl ligand and serve as the W_f substrate in the next (n+1) cycle, while the water binding in the S’ 3 state (green) will be W1 in the next (n+1) cycle and then W2 (serving as the W_f substrate) in the (n+2) cycle. Interestingly, different scenarios exist for the pivot mechanism in the S' 0 state as outlined in Scheme S7(b). It can be seen that both W1 (fuchsia) and W2 (orange) convert to O_2 in the current cycle, with W1 acting as the W_f substrate and W2 as W_s in the S_0~S_3 states. The water binding in the S' 0 state (blue) and S’ 3 state (green) will turn into O5 and W2 and act as the Ws and

W_f substrates, respectively, in the S_0~S_3 states of the next (n+1) cycle. Further customized experiments such as FTIR measurements, TR-MIMS, isotope labeling combined with site-specific mutagenesis and water exchange kinetics studies, etc. may be useful to further shed light on the substrate selectivity during the cycle.



Scheme S7(a). Graphical expressions for the water insertion mechanism of water binding to Ca in the S' 0 state and the influence on the substrate sources for the present and later S-state cycle. Circles of different colors are used to trace substrate sources (the same below).



Scheme S7(b). Graphical expressions for the pivot mechanism of water binding to Mn4 in the S' 0 state and the influence on the substrate sources for the present and later S-state cycle.

All the transition states for the key steps are managed to be located and the energy profiles are shown in Figure SVIc in the SI. We can see that water directly binding to Mn4 in concomitance with W1 (H_2O) and W2 (OH^-) pivoting on Mn4 (step1) is an endothermic process throughout (6.9, 5.5 kcal/mol on the octet/Mn1-Mn4(αααβ) and doublet/Mn1-Mn4(αβαβ) surface, respectively), while it is slightly exothermic for the W1 (OH^-) and W2 (H_2O) case (step4) with a very small barrier (ΔG = -4.0, -3.6 kcal/mol and $\Delta G^{\neq}$= 1.9, 1.4 kcal/mol on the octet/Mn1-Mn4(αααβ) and doublet/Mn1-

Mn4(αβαβ) surfaces, respectively). However, the latter case is presupposed by proton transfer (step3) with $\Delta G^{\neq}$ of 7.6 and 6.9 kcal/mol on the octet/Mn1-Mn4(αααβ) and doublet/Mn1-Mn4(αβαβ) surfaces, respectively. This promotes the barrier height of the rate-determining step for the latter, equalizing the degrees of difficulty of water binding to Mn4 with the former. Coincidentally, transition states on the electronic PESs for both binding cases have a similar Mn4-O (H_2O) distance of 3.40~3.45 Å. Pointing at the water insertion way of step5, the new water moves from ~5.0 to ~2.6 Å (~4.35 Å in the TS5*) binding to Ca(II) and the process is barrierless and exothermic by ~2.5 kcal/mol. Although none of the three water binding styles is energetically prohibited according to the calculated results, we slightly prefer the insertion mechanism of Ca(II) binding mode for its relative superiority in reactivity and simplicity of the process closely related to the structural characteristic of the S' 0 state. Strictly speaking, we cannot rule out the pivot mechanism of Mn4 binding mode, which may be concomitant or competitive with the insertion mechanism and further persuasive experiments are still needed for discrimination.

S_0 state ruled out as a candidate for NH_3 departure

Anyway fortunately, the following inference is valid as long as either of the mechanisms is proved to be feasible (satisfied as shown above), and this temporary selection ambiguity does not lead to an equivocal judgement on the associativity for the ammonia and Mn_4CaO_5 cluster. From both schemes it can be decided that the W2 (orange) ligand in the S' 0 state must be one of the substrate which constitutes the later molecular O_2 in the present cycle regardless of the water binding mode in the S' 0 state. Distinctly, this causes a decisive contradiction for the tentative hypothesis that ammonia is still bound in the S_0 state for the case of NH_3-intervention. The identity of

W2 changes into NH_2^- in the NH_3-bound OEC if it has not left until the S' 0 state, and results in the incapability for O_2 production which disagrees with the experimental observation that ammonia involvement does not inhibit the activity of O_2 evolution. Consequently, the S_0 state as candidate for ammonia dissociation is denied either, and we support ammonia leave at the S' 4 state with the formed O-O bond but unreleased O_2.

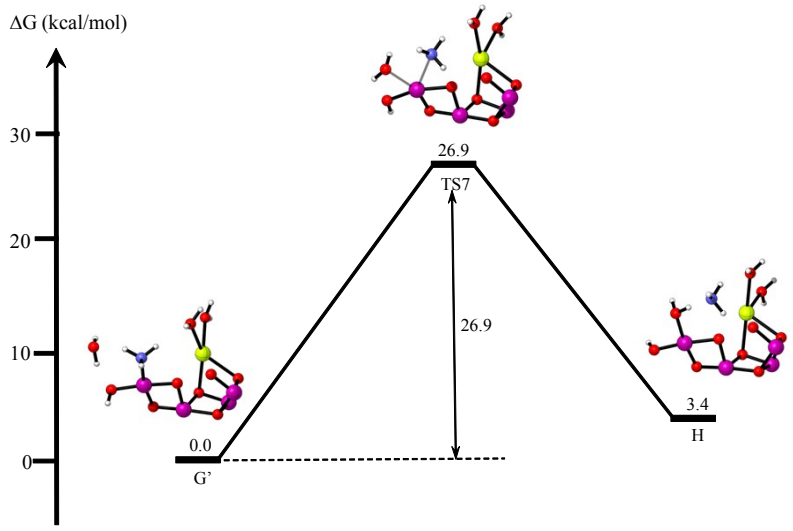
Table SVIb. Gibbs free energies and Mulliken spin populations for NH_3 hydrolysis in the S_4 and S' 4 state:

Spin states	Spin topology (Mn1-Mn4-O6·)	Gibbs Free energy (a.u.)		
		G'	TS7	H
sextet	αααββ	-3422.7736	-3422.7307	-3422.7682
doublet	βαβαα	-3422.7718	-3422.7288	-3422.7659
Spin states	Spin topology (Mn1-Mn4)	Relative Gibbs Free energy (kcal/mol)		
		L'	TS12	M
sextet	αααβ	-3422.7637	-3422.7523	-3422.7591
doublet	βαβα	-3422.7627	-3422.7511	-3422.7580
		K	TS11	L
sextet	αααβ	-3346.3383	-3346.3334	-3346.3579
doublet	βαβα	-3346.3367	-3346.3314	-3346.3561
Spin states	Spin topology	Mulliken spin density		

	(Mn1-Mn4-O6·)		G’	TS7	H
doublet	β	Mn1	-2.79	-2.79	-2.80
	α	Mn2	2.92	2.92	2.93
	β	Mn3	-2.88	-2.88	-2.88
	α	Mn4	2.86	2.91	2.86
	α	O6	0.61	0.56	0.61
		O5	0.13	0.12	0.11
sextet	α	Mn1	2.80	2.81	2.81
	α	Mn2	2.96	2.96	2.96
	α	Mn3	2.91	2.90	2.91
	β	Mn4	-2.86	-2.91	-2.86
	β	O6	-0.59	-0.55	-0.59
		O5	-0.13	-0.12	-0.11
			K	TS11	L
doublet	β	Mn1	-2.98	-2.99	-3.01
	α	Mn2	2.93	2.93	2.93
	β	Mn3	-2.80	-2.81	-2.81
	α	Mn4	3.90	3.86	3.79
sextet	α	Mn1	2.98	3.00	3.01
	α	Mn2	2.95	2.95	2.95
	α	Mn3	2.83	2.85	2.84
	β	Mn4	-3.90	-3.86	-3.80
			L’	TS12	M
doublet	β	Mn1	-2.98	-2.97	-3.00

	α	Mn2	2.93	2.93	2.93
	β	Mn3	-2.76	-2.77	-2.76
	α	Mn4	3.78	3.83	3.82
sextet	α	Mn1	3.00	2.99	3.01
	α	Mn2	2.94	2.95	2.94
	α	Mn3	2.80	2.80	2.79
	β	Mn4	-3.79	-3.83	-3.82

sextet/Mn1-Mn4-O·(αααββ) surface



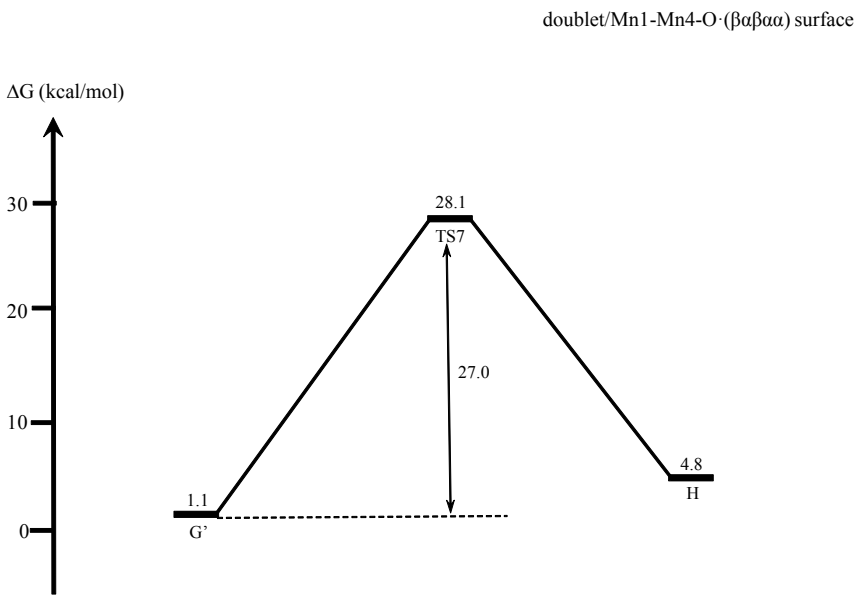
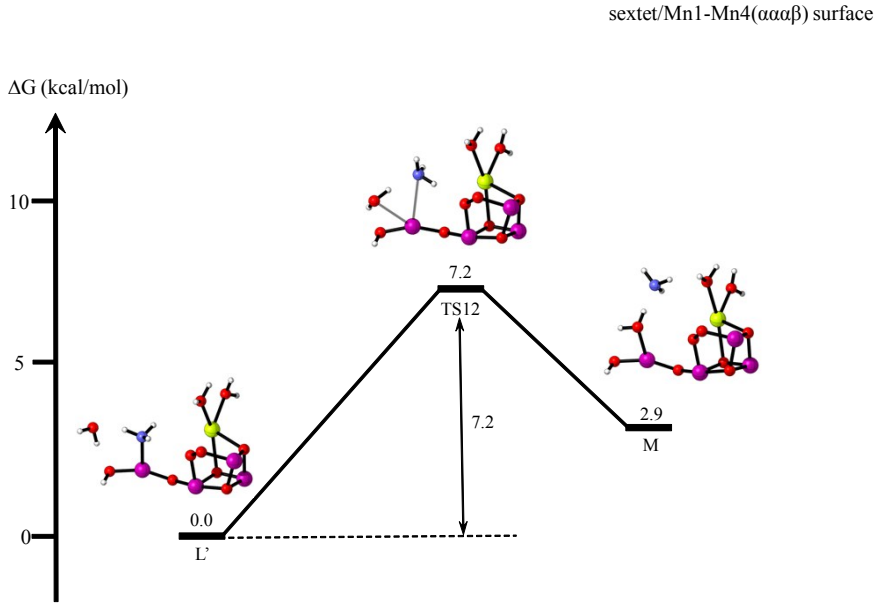


Figure SVIb1. Free energy profiles for NH_3 hydrolysis in the S_4 state.



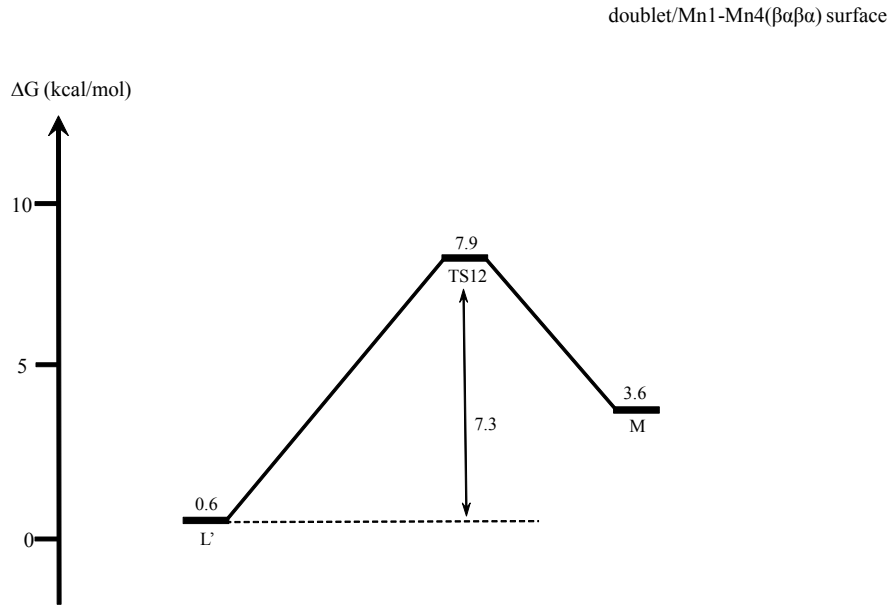
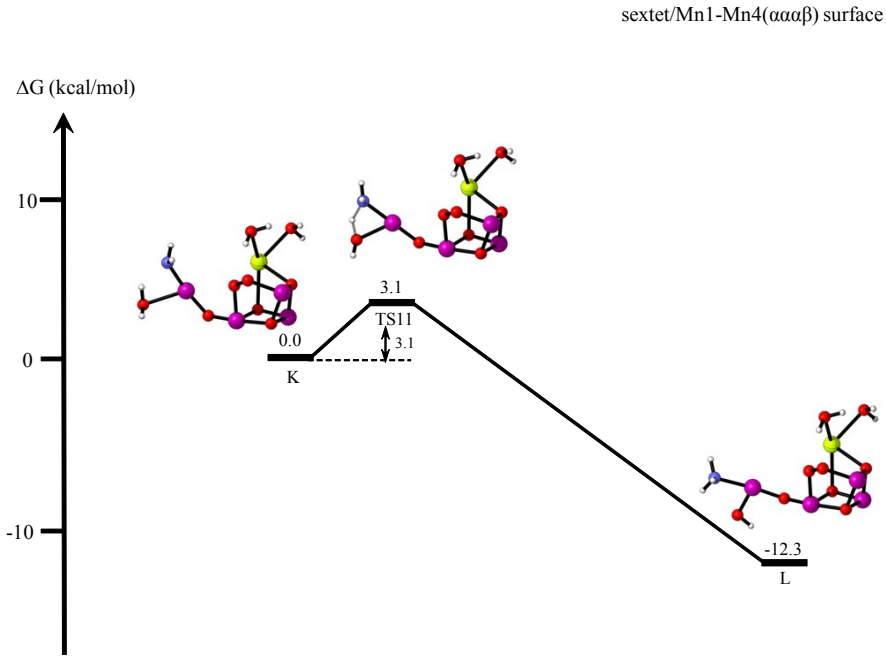


Figure SVIb2. Free energy profiles for NH_3 hydrolysis in the S' 4 state.



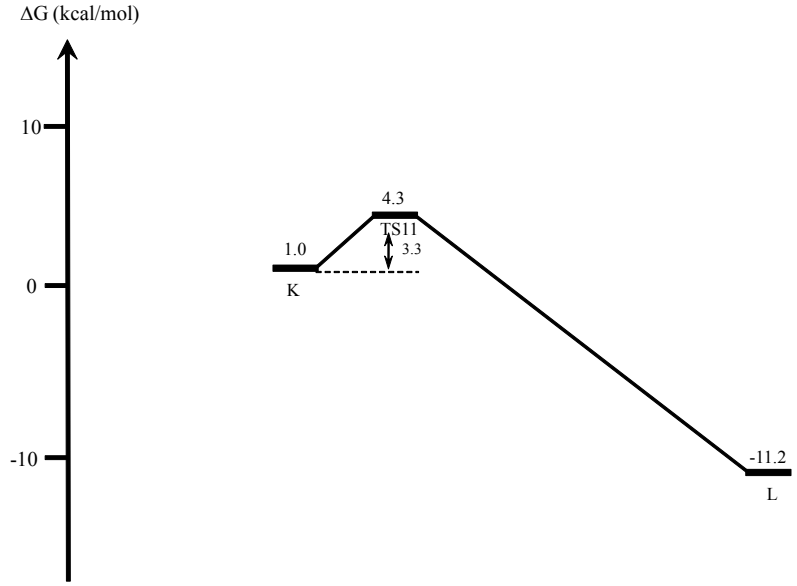


Figure SVIb3. Free energy profiles for NH_2^- protonation in the S' 4 state.

The Cartesian coordinates for G', TS7, H, L', TS12, M, K, TS11 and L:

G':

Ca	-2.38289600	-0.71457400	-1.04434900	H	-1.35947300	3.13964400	-3.87506800	H	-0.26708100	-7.10570000	-5.54463800
Mn	0.62932900	-1.81199000	-0.11184100	O	-3.88576000	0.99667100	-1.59319700	H	-0.59184500	-7.64404900	-3.88627600
Mn	-1.10436700	-1.18383800	1.93958400	C	-3.91513100	2.24222900	-1.56669600	N	2.64330300	-1.39547500	-0.48452400
Mn	-0.39256000	1.29054800	0.83016400	O	-2.89385000	3.02939900	-1.55582500	C	3.18046400	-0.83719800	-1.62438300
Mn	-0.98847200	2.91629800	-1.29555400	C	-5.26299300	2.96066200	-1.52612500	H	2.55443100	-0.63513900	-2.48262100
O	-1.06913600	-2.18152200	0.40402200	H	-6.02706500	2.24628900	-1.85309100	C	4.52490900	-0.61593600	-1.43579200
O	0.49918800	-0.49077500	1.19681500	H	-5.45770900	3.17409900	-0.46349100	N	4.78787900	-1.06968200	-0.14796000
O	-1.86687400	0.28128000	1.19784200	C	-5.32491200	4.26348700	-2.32932400	H	5.63147500	-0.82851800	0.37816600
O	-0.67833800	1.08883800	-0.93862500	H	-5.18612700	4.07116200	-3.40353000	C	3.62935900	-1.51052000	0.39218300
O	-1.05381700	2.92290200	0.49182800	H	-4.55147100	4.96321600	-1.99409300	H	3.52337900	-1.89196700	1.39643000
O	0.17917900	-0.93548100	-1.50241700	H	-6.30306800	4.74596900	-2.20976500	C	5.57056700	-0.05238300	-2.36273400
O	-3.63125100	-2.61762900	-2.10186700	O	0.78968100	-3.44145800	-1.21056900	H	5.87516300	-0.81194300	-3.09867300
H	-4.04928000	-2.88992600	-1.25994600	C	-0.03926500	-3.83798300	-2.11149700	H	5.10580100	0.75527100	-2.94523100
H	-2.86648500	-3.21712900	-2.25097500	O	-0.99962700	-3.17670700	-2.57622100	C	6.86323100	0.47451900	-1.68339400
O	-1.82564900	-0.68182400	-3.53375700	C	0.20797400	-5.26602400	-2.59964700	H	7.48180800	-0.36292100	-1.34193100
H	-2.60031400	-1.03197200	-4.00813000	H	1.26060400	-5.51740900	-2.42047000	H	7.44821100	1.02764200	-2.43092200
H	-1.23000700	-1.45868300	-3.41559700	H	-0.38137700	-5.92693600	-1.94205800	C	6.57838800	1.33377500	-0.45352100
O	-1.05958100	4.73885700	-1.64122500	C	-0.18619000	-5.50394900	-4.06232400	O	6.62936000	0.85539600	0.68662400
H	-0.15228800	5.07558800	-1.52613700	H	0.40664600	-4.83975500	-4.70941200	N	6.19778100	2.61722700	-0.68761500
N	-0.83919500	2.42163100	-3.33481100	H	-1.23450100	-5.20975800	-4.20153600	H	6.13905200	2.93167100	-1.64841600
H	0.14684300	2.44829400	-3.59728100	C	0.01688100	-6.96004300	-4.49427800	C	5.58611900	3.44867400	0.35458400
H	-1.19386900	1.47453500	-3.50916700	H	1.06641800	-7.26751900	-4.38648800	H	6.17192800	3.31080400	1.26901900

H	5.68935700	4.49529900	0.04094000	H	1.08713400	-5.34621700	2.82502300	C	-0.36469500	1.59704800	5.12276500
C	4.11350300	3.09008500	0.62279300	C	0.99838800	-4.38419600	4.77528300	H	-0.68444700	0.84701000	5.85525600
H	4.05628100	2.06078500	0.99354200	H	1.43585400	-5.23837200	5.30775200	H	0.69771700	1.81951800	5.30662100
H	3.74105200	3.73380900	1.43180600	H	1.33752900	-3.46406800	5.26715500	C	-1.18684900	2.89203700	5.25728100
C	3.22617700	3.24349500	-0.61537900	H	-0.09103300	-4.42902100	4.87791000	H	-2.24497000	2.66855800	5.05571500
H	3.62674400	2.64195700	-1.44625900	O	-3.91423300	-1.87601300	0.54542000	H	-0.86365600	3.59691300	4.48074600
H	3.20273800	4.28281600	-0.97126000	C	-3.82332500	-2.12643900	1.76721700	C	-1.04757500	3.52637300	6.64474900
O	1.49709200	2.03171000	0.52571600	O	-2.79183900	-1.89576200	2.51326700	H	-1.38762400	2.84241400	7.43493100
C	1.78154200	2.78601600	-0.43574000	C	-4.99427200	-2.74277300	2.51380600	H	-1.64367500	4.44513500	6.71926600
O	0.97264700	3.21330400	-1.33563000	H	-4.65855500	-3.61034600	3.09372000	H	-0.00169300	3.78816700	6.85934500
O	1.39374700	-3.05809400	1.33882900	H	-5.78468500	-3.03246600	1.81583500	O	-2.11004500	4.83695600	-4.13738200
C	0.82917700	-3.28223500	2.45546500	H	-5.39051900	-2.00802700	3.22669800	H	-3.05264800	4.71255600	-3.93372900
O	-0.18102400	-2.66627700	2.91140500	O	-0.88054600	-0.21104300	3.65002200	H	-1.72008800	4.99667300	-3.23415300
C	1.41124900	-4.40818500	3.30290000	C	-0.46789400	0.99014000	3.73357400				
H	2.50272000	-4.37870900	3.18581200	O	-0.13320600	1.72812600	2.75624800				

TS7:

Ca	-2.51873800	0.38005300	-0.96151500	H	-1.28547700	-5.57942400	-2.17383200	C	2.77604200	1.83153500	-0.54168800
Mn	-0.23267600	-1.86122600	-0.06140600	H	-2.85553000	-5.37840900	-1.40824000	O	2.20516800	2.54878100	-1.43397300
Mn	-1.43256300	-0.50305100	2.02368200	C	-2.90941600	-5.10070500	-3.56071200	O	0.02395500	-3.26326900	1.43546700
Mn	0.19928800	1.37281400	0.76214800	H	-2.25191600	-4.70044200	-4.34731800	C	-0.52180300	-3.19521200	2.58069000
Mn	0.38046000	3.17518900	-1.38290800	H	-3.80251700	-4.46262600	-3.55528400	O	-1.16283200	-2.20059500	3.03777400
O	-1.89831400	-1.46485500	0.54011700	C	-3.29331500	-6.54580600	-3.89580500	C	-0.41400700	-4.43095700	3.46744400
O	0.28041400	-0.56454200	1.19169500	H	-2.40921200	-7.19762400	-3.93134900	H	0.57249600	-4.87950100	3.29096200
O	-1.54423000	1.11087500	1.21496900	H	-3.79262400	-6.60777700	-4.87151100	H	-1.14468600	-5.15373700	3.07094600
O	-0.16130400	1.27426500	-0.96881700	H	-3.97906600	-6.96006700	-3.14329800	C	-0.66405000	-4.17740200	4.95496200
O	0.19783700	3.15373100	0.37087400	N	1.74637900	-2.34308700	-0.52831300	H	-0.59622700	-5.11665800	5.51862800
O	-0.34173300	-0.89924800	-1.46718700	C	2.41340200	-2.07018300	-1.70311200	H	0.07333400	-3.47722700	5.36701200
O	-4.64883000	-0.85101600	-1.68848800	H	1.89121500	-1.62888100	-2.54064900	H	-1.65614900	-3.74296700	5.11701900
H	-5.02903000	-0.75260000	-0.79006600	C	3.73270200	-2.43819300	-1.57678200	O	-4.31564000	0.12995500	0.79689900
H	-4.24797500	-1.74684500	-1.72776700	N	3.84078900	-2.95647900	-0.29122400	C	-4.28262700	-0.12720100	2.02044300
O	-2.55280200	-0.18168100	-3.46320600	H	4.73184000	-3.09776700	0.19177600	O	-3.22173000	-0.40645800	2.70435800
H	-3.51235300	-0.16099200	-3.63278300	C	2.63247000	-2.86296100	0.30802800	C	-5.55903600	-0.11146800	2.84396000
H	-2.36549400	-1.13192300	-3.27285800	H	2.42314300	-3.16157700	1.32395100	H	-5.61606100	-1.00561500	3.47502000
O	0.99463300	4.89918100	-1.20647400	C	4.87325800	-2.36795700	-2.55898600	H	-6.43535700	-0.04461000	2.19311000
H	0.89721200	5.10709400	-0.25820100	H	4.78749200	-3.17796000	-3.29910900	H	-5.53931800	0.75962900	3.51208700
N	-0.02197600	1.51342100	-3.63880700	H	4.77149900	-1.43375300	-3.12863400	O	-0.74199100	0.34308800	3.67540800
H	0.46297300	0.82292200	-3.06588900	C	6.29813500	-2.45154800	-1.94845700	C	0.12488100	1.27624300	3.69068400
H	-0.90229800	1.07324800	-3.91779700	H	6.51362000	-3.47582800	-1.62442300	O	0.68183900	1.78336900	2.67123500
H	0.54214800	1.69856400	-4.46802700	H	7.02642400	-2.19736100	-2.73071200	C	0.54031700	1.80648400	5.05448400
O	-3.08563400	2.55083600	-1.62491600	C	6.47090900	-1.56195400	-0.71905800	H	-0.14835700	1.40075800	5.80483700
C	-2.57429400	3.63025000	-1.97447000	O	6.36963300	-2.02510700	0.42438200	H	1.53866300	1.39201400	5.26906300
O	-1.32133800	3.93785200	-1.94193100	N	6.66571200	-0.23780100	-0.95288500	C	0.59913100	3.34108400	5.11819300
C	-3.49481500	4.74768300	-2.47073800	H	6.69311100	0.07936100	-1.91430500	H	-0.39595900	3.74951400	4.88740400
H	-4.33221500	4.26654000	-2.99151400	C	6.51504500	0.76758400	0.10471100	H	1.27218800	3.70217000	4.33041200
H	-3.92436200	5.20321900	-1.56445400	H	7.01874400	0.38097900	0.99634800	C	1.06158100	3.84827300	6.48798700
C	-2.83495200	5.82321900	-3.33527700	H	7.04829100	1.66941000	-0.22202600	H	0.38623300	3.51528400	7.28852600
H	-2.42490900	5.39514800	-4.26057900	C	5.04347400	1.07925900	0.43164000	H	1.09264200	4.94533700	6.51300600
H	-2.01605400	6.31313000	-2.79741700	H	4.56009400	0.17227600	0.81156700	H	2.06883800	3.47997400	6.72959500
H	-3.56824600	6.58795900	-3.62180700	H	5.01758900	1.81220700	1.25001400	O	0.94626300	4.05025700	-3.54117800
O	-0.81587100	-3.44501100	-1.06118700	C	4.26778200	1.61619800	-0.77377400	H	-0.00883900	4.10639600	-3.73117800
C	-1.86202300	-3.54507500	-1.80523500	H	4.33807600	0.91220200	-1.61736600	H	1.15099000	4.88509900	-3.06782900
O	-2.59003100	-2.59796800	-2.18477500	H	4.68168300	2.56807400	-1.13339700				
C	-2.20428800	-4.98062300	-2.20459700	O	2.22358200	1.29802300	0.45297300				

H:

Ca	-2.51873800	0.38005300	-0.96151500	Mn	0.19928800	1.37281400	0.76214800	O	0.28041400	-0.56454200	1.19169500
Mn	-0.23267600	-1.86122600	-0.06140600	Mn	0.38046000	3.17518900	-1.38290800	O	-1.54423000	1.11087500	1.21496900
Mn	-1.43256300	-0.50305100	2.02368200	O	-1.89831400	-1.46485500	0.54011700	O	-0.16130400	1.27426500	-0.96881700

O	0.19783700	3.15373100	0.37087400	H	-2.40921200	-7.19762400	-3.93134900	C	-0.52180300	-3.19521200	2.58069000
O	-0.34173300	-0.89924800	-1.46718700	H	-3.79262400	-6.60777700	-4.87151100	O	-1.16283200	-2.20059500	3.03777400
O	-4.64883000	-0.85101600	-1.68848800	H	-3.97906600	-6.96006700	-3.14329800	C	-0.41400700	-4.43095700	3.46744400
H	-5.02903000	-0.75260000	-0.79006600	N	1.74637900	-2.34308700	-0.52831300	H	0.57249600	-4.87950100	3.29096200
H	-4.24797500	-1.74684500	-1.72776700	C	2.41340200	-2.07018300	-1.70311200	H	-1.14468600	-5.15373700	3.07094600
O	-2.55280200	-0.18168100	-3.46320600	H	1.89121500	-1.62888100	-2.54064900	C	-0.66405000	-4.17740200	4.95496200
H	-3.51235300	-0.16099200	-3.63278300	C	3.73270200	-2.43819300	-1.57678200	H	-0.59622700	-5.11665800	5.51862800
H	-2.36549400	-1.13192300	-3.27285800	N	3.84078900	-2.95647900	-0.29122400	H	0.07333400	-3.47722700	5.36701200
O	0.99463300	4.89918100	-1.20647400	H	4.73184000	-3.09776700	0.19177600	H	-1.65614900	-3.74296700	5.11701900
H	0.89721200	5.10709400	-0.25820100	C	2.63247000	-2.86296100	0.30802800	O	-4.31564000	0.12995500	0.79689900
N	-0.02197600	1.51342100	-3.63880700	H	2.42314300	-3.16157700	1.32395100	C	-4.28262700	-0.12720100	2.02044300
H	0.46297300	0.82292200	-3.06588900	C	4.87325800	-2.36795700	-2.55898600	O	-3.22173000	-0.40645800	2.70435800
H	-0.90229800	1.07324800	-3.91779700	H	4.78749200	-3.17796000	-3.29910900	C	-5.55903600	-0.11146800	2.84396000
H	0.54214800	1.69856400	-4.46802700	H	4.77149900	-1.43375300	-3.12863400	H	-5.61606100	-1.00561500	3.47502000
O	-3.08563400	2.55083600	-1.62491600	C	6.29813500	-2.45154800	-1.94845700	H	-6.43535700	-0.04461000	2.19311000
C	-2.57429400	3.63025000	-1.97447000	H	6.51362000	-3.47582800	-1.62442300	H	-5.53931800	0.75962900	3.51208700
O	-1.32133800	3.93785200	-1.94193100	H	7.02642400	-2.19736100	-2.73071200	O	-0.74199100	0.34308800	3.67540800
C	-3.49481500	4.74768300	-2.47073800	C	6.47090900	-1.56195400	-0.71905800	C	0.12488100	1.27624300	3.69068400
H	-4.33221500	4.26654000	-2.99151400	O	6.36963300	-2.02510700	0.42438200	O	0.68183900	1.78336900	2.67123500
H	-3.92436200	5.20321900	-1.56445400	N	6.66571200	-0.23780100	-0.95288500	C	0.54031700	1.80648400	5.05448400
C	-2.83495200	5.82321900	-3.33527700	H	6.69311100	0.07936100	-1.91430500	H	-0.14835700	1.40075800	5.80483700
H	-2.42490900	5.39514800	-4.26057900	C	6.51504500	0.76758400	0.10471100	H	1.53866300	1.39201400	5.26906300
H	-2.01605400	6.31313000	-2.79741700	H	7.01874400	0.38097900	0.99634800	C	0.59913100	3.34108400	5.11819300
H	-3.56824600	6.58795900	-3.62180700	H	7.04829100	1.66941000	-0.22202600	H	-0.39595900	3.74951400	4.88740400
O	-0.81587100	-3.44501100	-1.06118700	C	5.04347400	1.07925900	0.43164000	H	1.27218800	3.70217000	4.33041200
C	-1.86202300	-3.54507500	-1.80523500	H	4.56009400	0.17227600	0.81156700	C	1.06158100	3.84827300	6.48798700
O	-2.59003100	-2.59796800	-2.18477500	H	5.01758900	1.81220700	1.25001400	H	0.38623300	3.51528400	7.28852600
C	-2.20428800	-4.98062300	-2.20459700	C	4.26778200	1.61619800	-0.77377400	H	1.09264200	4.94533700	6.51300600
H	-1.28547700	-5.57942400	-2.17383200	H	4.33807600	0.91220200	-1.61736600	H	2.06883800	3.47997400	6.72959500
H	-2.85553000	-5.37840900	-1.40824000	H	4.68168300	2.56807400	-1.13339700	O	0.94626300	4.05025700	-3.54117800
C	-2.90941600	-5.10070500	-3.56071200	O	2.22358200	1.29802300	0.45297300	H	-0.00883900	4.10639600	-3.73117800
H	-2.25191600	-4.70044200	-4.34731800	C	2.77604200	1.83153500	-0.54168800	H	1.15099000	4.88509900	-3.06782900
H	-3.80251700	-4.46262600	-3.55528400	O	2.20516800	2.54878100	-1.43397300				
C	-3.29331500	-6.54580600	-3.89580500	O	0.02395500	-3.26326900	1.43546700				

L':

Ca	-0.23234000	-2.83706200	-0.91770100	O	-2.53543500	-3.34462100	-0.97116900	N	1.72750600	2.33982500	-1.31308800
Mn	1.73691300	0.28071300	-0.88016500	C	-3.67540600	-3.44829600	-0.44619300	C	0.95496500	2.99267600	-2.24982200
Mn	1.35161200	-1.11051400	1.45663600	O	-4.48804000	-2.47645200	-0.23651900	H	0.39859700	2.43927100	-2.99312600
Mn	-1.09644600	0.01402700	0.77420100	C	-4.16327600	-4.83528800	-0.03660600	C	1.02172200	4.34829700	-2.03574400
Mn	-4.11018700	-0.56378400	-0.32563500	H	-4.04068100	-5.48480600	-0.91535500	N	1.87600900	4.50169200	-0.94953100
O	1.78714600	-1.43245400	-0.32268200	H	-3.43972800	-5.20700000	0.70544500	H	1.92095600	5.35255000	-0.38331700
O	0.86631400	0.56230500	0.75230800	C	-5.58944900	-4.90211900	0.50922900	C	2.25764500	3.27178700	-0.53552500
O	-0.32522000	-1.60605700	1.20047200	H	-6.31386900	-4.54947400	-0.23402200	H	2.88557400	3.08271300	0.32192000
O	-0.93378400	-0.43065200	-1.05244000	H	-5.70090700	-4.27345600	1.39993600	C	0.36665700	5.48929700	-2.76702500
O	-2.66107500	-0.73078100	0.73566800	H	-5.84622200	-5.93469300	0.77940200	H	0.93139600	5.73573800	-3.67907800
O	0.07334900	0.29056800	-1.73402800	O	2.64928400	-0.07352900	-2.53592500	H	-0.61724300	5.14176600	-3.11061800
O	1.39066100	-4.39069700	-1.97547900	C	3.28084000	-1.15797500	-2.89444800	C	0.20087100	6.80428300	-1.95789800
H	1.78796300	-4.72147900	-1.14773700	O	2.72334900	-2.22963400	-3.19912300	H	1.16289200	7.32259100	-1.87709100
H	2.07649000	-3.83763000	-2.41149200	C	4.79345300	-1.01070600	-2.97738300	H	-0.48006400	7.46790600	-2.50818500
O	-0.02146100	-2.01804500	-3.24966200	H	4.99839600	-0.16515000	-3.65251700	C	-0.28243700	6.57248700	-0.52758600
H	0.93896700	-2.15120800	-3.44929200	H	5.12972200	-0.67082700	-1.98568800	O	0.52035900	6.51823000	0.41310000
H	-0.05715800	-1.05085100	-3.08450700	C	5.54522700	-2.26544500	-3.42639800	N	-1.61639300	6.37361100	-0.36226900
O	-5.89325000	-0.22187400	-0.72225300	H	5.15908800	-2.58773000	-4.40304300	H	-2.21018000	6.39331700	-1.18229800
H	-5.99564000	0.74773500	-0.71949400	H	5.32590300	-3.08714400	-2.73007100	C	-2.18159100	5.88100100	0.89759200
N	-3.46203300	-0.75038800	-2.45472200	C	7.05936700	-2.04188800	-3.50729500	H	-1.59479700	6.33297900	1.70318500
H	-2.80850500	-0.03977000	-2.78076700	H	7.30815200	-1.24636800	-4.22389400	H	-3.20929400	6.26043200	0.97252100
H	-2.98627300	-1.65363300	-2.51203800	H	7.47342600	-1.74857500	-2.53204100	C	-2.14647200	4.35030100	1.01867000
H	-4.31053400	-0.77607700	-3.04493100	H	7.57931300	-2.95369300	-3.82863100	H	-1.11177400	4.00052200	0.93891600

H	-2.48940800	4.07980200	2.02842400	H	6.74393100	0.50488400	3.16122100	H	-1.20631500	1.30568000	5.02166200
C	-3.00460000	3.62667800	-0.02309500	H	5.06486600	0.84419400	3.63664200	H	-0.92600500	-0.38163500	5.44923700
H	-2.66685700	3.90522400	-1.03592400	H	5.53340800	-0.80048100	3.19058300	C	0.80447900	0.88617700	5.78179200
H	-4.06452600	3.90049800	0.04342300	O	0.89053500	-4.25930300	0.72603600	H	1.27300000	1.76377900	5.31155500
C	-2.87123500	2.09825600	0.04501000	C	1.53232300	-4.00050600	1.77030500	H	1.53262800	0.06932100	5.70395200
O	-1.79692100	1.68490300	0.39442500	O	1.88286200	-2.82371900	2.16638000	C	0.49893600	1.18856800	7.25261600
O	-3.87647100	1.46298500	-0.28171100	C	1.95131300	-5.12561600	2.70049100	H	-0.21199900	2.02074000	7.35314100
O	3.53101300	0.68827300	-0.02876400	H	1.93847500	-6.08369100	2.17273600	H	1.41170400	1.46230200	7.79746300
C	3.92460400	0.21646800	1.09204600	H	1.23557300	-5.17384000	3.53278300	H	0.05972400	0.31540000	7.75531800
O	3.23900900	-0.50804200	1.86442500	H	2.94082600	-4.92970200	3.12631300	O	-6.20388300	-0.93476900	-3.33683500
C	5.35559700	0.55380800	1.49569400	O	0.87777600	-0.46786200	3.27188700	H	-6.63180400	-0.16018800	-3.73720300
H	5.52984400	1.60877200	1.24400100	C	-0.20210100	0.15145200	3.53601900	H	-6.26234600	-0.76830600	-2.35670700
H	6.00930300	-0.02089800	0.82090300	O	-1.10388800	0.48338200	2.70246500				
C	5.69457700	0.25734000	2.95689700	C	-0.45633300	0.50562400	4.99350900				

TS12:

Ca	0.78656400	-2.75326900	-1.01820400	H	4.97124300	1.62055900	-3.36411900	O	-2.27081000	0.92609200	0.29784500
Mn	1.59626600	0.83832800	-0.80732000	H	5.17427800	1.16217100	-1.69087600	O	-4.21888800	0.03465600	-0.19026400
Mn	1.58160700	-0.68293200	1.48130300	C	6.20489400	-0.15983000	-3.09869000	O	3.08469600	1.80165800	0.16578300
Mn	-1.05993800	-0.42015400	0.67126900	H	6.01421200	-0.57712200	-4.09681300	C	3.55310300	1.45446200	1.30333900
Mn	-3.81802600	-1.90156300	-0.35448500	H	6.24594500	-1.01991600	-2.41552000	O	3.11950800	0.50777300	2.01615000
O	2.19248000	-0.77795600	-0.26673600	C	7.54699200	0.58022900	-3.08573100	C	4.75059300	2.25114600	1.80740000
O	0.58911100	0.75038400	0.77089600	H	7.54365900	1.42635500	-3.78730700	H	4.56030200	3.30983200	1.58469200
O	0.18228400	-1.70216300	1.11392100	H	7.77401500	0.98038900	-2.08727800	H	5.60122100	1.96509500	1.16899100
O	-0.66729500	-0.72252700	-1.15812100	H	8.37091000	-0.08613500	-3.37206100	C	5.08679300	2.03530300	3.28331700
O	-2.27063900	-1.65733100	0.52523700	N	0.90294200	2.77446500	-1.22996600	H	5.96953800	2.62474000	3.56132500
O	0.09165000	0.30502500	-1.77147000	C	-0.03711000	3.12396000	-2.17688600	H	4.25358300	2.34011900	3.92809200
O	2.90257500	-3.64845300	-1.96269700	H	-0.37154900	2.41156700	-2.91731300	H	5.29314100	0.97954000	3.48912100
H	3.32865200	-3.86485000	-1.11179300	C	-0.43360200	4.42270200	-1.97149700	O	2.20883800	-3.78418200	0.68922500
H	3.39821100	-2.88543100	-2.33442700	N	0.30874100	4.86069900	-0.88047400	C	2.68153300	-3.36068000	1.76911800
O	0.90481800	-1.84068300	-3.32035300	H	0.05194900	5.67605400	-0.31792700	O	2.61365200	-2.14367500	2.19456300
H	1.86610700	-1.62956800	-3.43146100	C	1.08026300	3.83460900	-0.45482500	C	3.39804700	-4.31289400	2.71007600
H	0.52220600	-0.94993300	-3.16852800	H	1.72897000	3.87293500	0.40712200	H	3.70388400	-5.21884700	2.17895000
O	-5.60976100	-2.20722500	-0.50367300	C	-1.43188500	5.26768500	-2.71636000	H	2.70577600	-4.59353600	3.51580400
H	-6.06644800	-1.34994000	-0.40573700	H	-0.97325000	5.69508200	-3.62098500	H	4.26155500	-3.82386800	3.17295600
N	-2.52465500	-1.84068000	-3.22168700	H	-2.22842200	4.60046300	-3.07229000	O	0.81909700	-0.30090500	3.27520200
H	-1.90456100	-1.26009800	-2.64949200	C	-2.05545100	6.44296200	-1.91547600	C	-0.41728800	-0.08782600	3.48043300
H	-2.20603600	-2.79942400	-3.07393000	H	-1.33557600	7.26424600	-1.82566100	O	-1.33252700	-0.05129800	2.59542300
H	-2.33825900	-1.61025400	-4.19952800	H	-2.91804700	6.82682000	-2.47691000	C	-0.85750600	0.11520600	4.92196600
O	-1.25264800	-3.94856000	-1.22138700	C	-2.44428400	6.05583700	-0.49055000	H	-1.83124700	0.62022900	4.91109600
C	-2.34311200	-4.41628500	-0.81381200	O	-1.67731600	6.27247200	0.45734500	H	-1.03072800	-0.89171700	5.33625200
O	-3.44365700	-3.75394200	-0.70020700	N	-3.63326000	5.41688000	-0.33720600	C	0.15815700	0.86662200	5.79373000
C	-2.41416500	-5.89630800	-0.44792200	H	-4.19401300	5.23806800	-1.16143800	H	0.33425600	1.86412900	5.36404400
H	-2.00730500	-6.45385800	-1.30404500	C	-4.00822700	4.76097500	0.91845900	H	1.11958800	0.33971500	5.75429900
H	-1.68724900	-6.04200700	0.36625000	H	-3.59945500	5.37489700	1.72682500	C	-0.31461800	1.00402100	7.24481300
C	-3.79399900	-6.41825400	-0.04788900	H	-5.10332200	4.78393800	0.99437700	H	-1.26613000	1.55040300	7.30803900
H	-4.51748700	-6.29092800	-0.86130200	C	-3.47686600	3.32408900	1.03054000	H	0.42248700	1.54721300	7.85010700
H	-4.18344300	-5.87908400	0.82300300	H	-2.38597500	3.32934900	0.93117700	H	-0.46659400	0.01934400	7.70879500
H	-3.73866700	-7.48572000	0.20163900	H	-3.69757300	2.95778500	2.04443700	O	-5.23960100	-0.95919800	-3.04152200
O	2.67849900	0.86487000	-2.39175500	C	-4.07510400	2.36300900	-0.00176600	H	-4.33781200	-1.33541200	-3.18368200
C	3.66987100	0.07591000	-2.70962000	H	-3.86867300	2.73574400	-1.01912100	H	-5.65801100	-1.62378400	-2.46177200
O	3.54040100	-1.11586600	-3.04715700	H	-5.16368200	2.27376800	0.08737700				
C	5.03666400	0.74442800	-2.70014500	C	-3.44657200	0.96775800	0.04577900				

M:

Ca	-2.63716500	1.04802500	-0.83180600	Mn	0.37747400	1.12145900	0.75309600	O	0.36117900	-0.92348800	0.76330400
Mn	-0.19869900	-1.69941000	-0.83895400	Mn	0.67974000	4.11631600	-0.46067700	O	-1.38098800	0.83027800	1.24601000
Mn	-1.35441300	-0.91420400	1.52497000	O	-1.84371700	-1.27038100	-0.23404600	O	-0.15661900	1.06518000	-1.05150500

O	0.08761300	2.82582600	0.67440400	H	-3.53169000	-6.69044500	-3.62872400	C	-0.78228000	-3.75892300	1.18581300	
O	0.23377500	-0.10961300	-1.72645500	H	-3.91570100	-6.54903200	-1.90405800	O	-1.27292200	-2.89073200	1.95814100	
O	-4.62761600	-0.02551600	-1.86501600	H	-5.20153900	-6.38703200	-3.11439200	C	-0.81743600	-5.21939800	1.62314700	
H	-5.03935500	-0.29401300	-1.02089600	N	1.75780100	-2.25674500	-1.36670800	H	0.15360600	-5.66431100	1.36589300	
H	-4.31602200	-0.85181700	-2.29723800	C	2.56542700	-1.64414500	-2.30228900	H	-1.55073000	-5.71971100	0.97135700	
O	-1.96983200	0.55455600	-3.20235100	H	2.16826000	-0.89549600	-2.97305700	C	-1.16536000	-5.43814200	3.09579200	
H	-2.36576800	-0.34248400	-3.36976300	C	3.84868800	-2.11784500	-2.17981700	H	-1.18999400	-6.51101800	3.32512000	
H	-1.02399900	0.33851600	-3.03033300	N	3.79492600	-3.05206700	-1.15084700	H	-0.42591400	-4.96337900	3.75201100	
O	1.46728100	5.69185000	-0.97164400	H	4.62010100	-3.37039400	-0.63774100	H	-2.14303000	-5.00714800	3.33684500	
H	2.43229200	5.56770500	-0.90621600	C	2.52753900	-3.08688200	-0.67860400	O	-4.28830700	0.34386000	0.83177600	
N	-1.61886600	3.40236100	-3.86373600	H	2.20017500	-3.69139100	0.15369300	C	-4.18742600	-0.32833900	1.88539900	
H	-1.81446500	2.40458600	-4.00394000	C	5.09422700	-1.77698500	-2.95224900	O	-3.13148500	-0.95145700	2.28288300	
H	-2.26733400	3.71761500	-3.13929000	H	5.13473200	-2.35233300	-3.88979200	C	-5.37458500	-0.44181900	2.82627400	
H	-1.82834300	3.90304300	-4.72737500	H	5.01795700	-0.72306700	-3.25205300	H	-6.30395900	-0.20054300	2.30210000	
O	-2.60662100	3.40659700	-0.92733200	C	6.43605000	-2.01267200	-2.20661600	H	-5.23849100	0.27595700	3.64698200	
C	-2.26209300	4.51911400	-0.44227800	H	6.67422000	-3.08200600	-2.18362300	H	-5.42614200	-1.44259500	3.26740800	
O	-1.07271900	4.99287300	-0.43357300	H	7.23863800	-1.51308000	-2.76620000	O	-0.55323000	-0.60824600	3.31011600	
C	-3.34835600	5.40210900	0.16892300	C	6.39743600	-1.54968400	-0.75186300	C	0.34127100	0.26966100	3.53547900	
H	-4.18044000	5.43402800	-0.54895500	O	6.15837000	-2.34922400	0.16222600	O	0.88220200	1.03289300	2.67472900	
H	-3.73431200	4.84559900	1.03745600	N	6.57865700	-0.22010600	-0.53584200	C	0.78756000	0.44153800	4.97970300	
C	-2.90710700	6.80686200	0.57922000	H	6.72026100	0.37944600	-1.33973200	H	1.74732200	0.97254900	4.97694700	
H	-2.53624800	7.37437600	-0.28255200	C	6.28613200	0.40934300	0.75520200	H	0.05449300	1.11600800	5.45203100	
H	-2.09667600	6.76485400	1.31523500	H	6.55027800	-0.32138300	1.52566800	C	0.87063500	-0.86894200	5.77497100	
H	-3.74826300	7.35843000	1.01903100	H	6.95371500	1.27448500	0.86469400	H	1.59350800	-1.54101400	5.28851300	
O	-0.87977500	-2.48493400	-2.46981300	C	4.81469000	0.82347000	0.90395100	H	-0.10152800	-1.37517700	5.72811600	
C	-2.11544700	-2.79241700	-2.74432700	H	4.17368200	-0.05713600	0.78889700	C	1.28029700	-0.63685500	7.23317100	
O	-2.97964100	-1.96398900	-3.09983400	H	4.66343500	1.18593800	1.93168200	H	2.26336100	-0.15018500	7.30226800	
C	-2.44325300	-4.27606900	-2.66966900	C	4.37122000	1.90228000	-0.08819300	H	1.33839600	-1.58515100	7.78304300	
H	-1.76011300	-4.78913900	-3.36508100	H	4.52908600	1.54650700	-1.12047200	H	0.55550300	0.00590500	7.75242300	
H	-2.13775200	-4.61565900	-1.66868000	H	4.94535700	2.83090100	0.01614700	O	0.76981900	3.63417700	-2.62006100	
C	-3.89952200	-4.63836900	-2.96862200	C	2.87267500	2.22172300	-0.00108100	H	-0.12057800	3.53621500	-3.11764400	
H	-4.17092500	-4.25508800	-3.96161300	O	2.16425700	1.30683200	0.33111300	H	1.07668100	4.54169900	-2.81511600	
H	-4.55524800	-4.11909100	-2.25512100	O	2.55919000	3.37698400	-0.29173300					
C	-4.15157600	-6.14868200	-2.90037500	O	-0.26569000	-3.52835800	0.03927000					

K:

Ca	-2.58341000	0.97434600	-1.30064500	H	-3.57630800	5.48352000	-2.46274000	N	3.60777400	-3.20816700	0.06408300	
Mn	-0.29403100	-1.72364600	-0.49378400	H	-3.34565300	5.56017200	-0.72955600	H	4.38100500	-3.36731100	0.71588500	
Mn	-1.65454000	-0.47428700	1.54587400	C	-2.08088200	6.94822100	-1.83212200	C	2.32618100	-2.95885000	0.41477200	
Mn	0.31027700	1.28431400	0.68038000	H	-1.56450400	7.01844200	-2.79720100	H	1.92315800	-3.10877800	1.40517600	
Mn	0.86489300	3.42247300	-1.44289100	H	-1.32774800	7.07472500	-1.04659800	C	5.08026200	-2.93453000	-2.01333400	
O	-1.96508600	-1.12661300	-0.17178400	H	-2.79571800	7.77872400	-1.76597700	H	5.05818900	-3.80061400	-2.69189200	
O	0.12557800	-0.72439500	1.01972000	O	-0.76660000	-2.77511100	-2.03546600	H	5.16846900	-2.05193600	-2.66207900	
O	-1.50829500	1.20310800	0.96337400	C	-1.95404800	-3.15155600	-2.42655600	C	6.35664000	-3.06686800	-1.14010300	
O	-0.04499900	0.96132000	-1.16708400	O	-2.77892400	-2.39841600	-2.97736300	H	6.41937000	-4.07244000	-0.70953500	
O	0.38788900	2.95958700	0.27986100	C	-2.25551800	-4.62821900	-2.21763100	H	7.23448100	-2.93497500	-1.78733500	
O	-4.49110600	-0.27284800	-2.28470100	H	-1.46133400	-5.19421300	-2.72956400	C	6.38699200	-2.09374700	0.03723100	
H	-5.00410900	-0.38863600	-1.46320500	H	-2.10307800	-4.83040000	-1.14646100	O	6.05161900	-2.45481600	1.17323800	
H	-4.15588600	-1.16236700	-2.53378900	C	-3.63971000	-5.08118200	-2.68683800	N	6.73232400	-0.81055100	-0.24171200	
O	-1.68894100	0.09848900	-3.42929700	H	-3.76025200	-4.83187500	-3.74985500	H	6.96419300	-0.56960700	-1.19748200	
H	-2.07589600	-0.81063900	-3.48169400	H	-4.40901600	-4.50482200	-2.15365100	C	6.54486900	0.27333500	0.72889100	
H	-0.76156400	-0.07997400	-3.16393300	C	-3.86889800	-6.58088100	-2.46889300	H	6.90567700	-0.08784100	1.69757800	
O	2.27351500	5.33234200	-1.42836500	H	-3.13200000	-7.18199300	-3.02019600	H	7.18932600	1.10488300	0.41648100	
H	2.19198200	5.09803300	-2.39252200	H	-3.78393800	-6.84867200	-1.40602700	C	5.07981400	0.72599400	0.85917100	
H	3.10775000	4.90598300	-1.16104600	H	-4.86739800	-6.88421300	-2.80942800	H	4.47546200	-0.11012700	1.22693700	
O	-2.47409800	3.24243800	-1.76060100	N	1.65570600	-2.47299700	-0.61819000	H	5.03141300	1.50995800	1.62855300	
C	-1.92536000	4.36684500	-1.73499400	C	2.54254500	-2.38101300	-1.66793300	C	4.49253600	1.24793000	-0.45562800	
O	-0.65604500	4.56821000	-1.74948400	H	2.22947500	-1.99697500	-2.62918700	H	4.56866200	0.47033900	-1.23233900	
C	-2.80688400	5.61073300	-1.68831900	C	3.77870900	-2.82713600	-1.26206400	H	5.04665500	2.11890000	-0.83026100	

C	3.01379700	1.62493000	-0.40182300	O	-4.41715500	0.72491800	0.29287800	C	-0.07986500	2.78831700	5.23397500
O	2.28438700	1.01875900	0.43274400	C	-4.46008900	0.30261500	1.46986700	H	-1.14916700	2.96392300	5.04516400
O	2.64295200	2.50078000	-1.24958700	O	-3.48681700	-0.26657900	2.09900100	H	0.47224000	3.41133400	4.51830200
O	-0.61038200	-3.35949000	0.65995200	C	-5.73006200	0.45519100	2.28823000	C	0.26616100	3.19434500	6.66994500
C	-1.27538700	-3.35710900	1.75078300	H	-5.60854100	1.31301300	2.96378500	H	-0.29435600	2.59597300	7.40161200
O	-1.77552900	-2.33976100	2.30658600	H	-5.90079700	-0.43122700	2.90811200	H	0.02651000	4.25055500	6.84825200
C	-1.49036600	-4.71585000	2.40801900	H	-6.58646500	0.64232200	1.63409800	H	1.33680100	3.05489800	6.87565300
H	-0.56105700	-5.28928300	2.29255900	O	-1.03105000	0.09501600	3.33960000	O	0.34608100	-0.33999300	-1.58970400
H	-2.23969200	-5.23911200	1.79306100	C	-0.08238900	0.92407800	3.52101400	N	1.31927200	3.60043500	-3.30415900
C	-1.94240100	-4.65397100	3.86770200	O	0.61366400	1.48335600	2.61303600	H	1.84045400	2.78881400	-3.64358500
H	-2.09826400	-5.66672400	4.26031300	C	0.24349100	1.30700800	4.95364000	H	0.49549200	3.72261500	-3.89610800
H	-1.19247100	-4.15533900	4.49402500	H	-0.31930000	0.65082000	5.62743300				
H	-2.87791300	-4.09310100	3.96558000	H	1.31728000	1.13178600	5.11351000				

TS11:

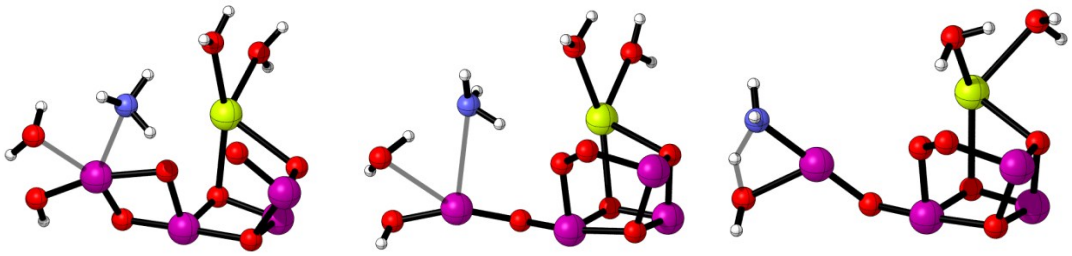
Ca	-2.27694700	1.48893800	-1.35602900	H	-4.74394700	-3.91925600	-3.75405100	O	-1.37694600	-3.16614400	0.68324300
Mn	-0.68432900	-1.66093400	-0.49325200	H	-5.31302100	-3.42110700	-2.17161200	C	-2.02972100	-2.99489300	1.76646900
Mn	-1.74204000	-0.10615500	1.51830800	C	-5.27568200	-5.57101000	-2.44987000	O	-2.28530700	-1.88012200	2.30361300
Mn	0.57694200	1.14501500	0.64467700	H	-4.69629800	-6.33847900	-2.98238900	C	-2.55648700	-4.25612700	2.44172600
Mn	1.74799800	3.34705200	-1.27081600	H	-5.26693800	-5.83295800	-1.38222800	H	-1.78427700	-5.03032300	2.34190200
O	-2.17689300	-0.69234200	-0.19670800	H	-6.31414200	-5.63571100	-2.79967300	H	-3.40378500	-4.60154000	1.82831300
O	-0.05385400	-0.75191500	1.01151500	N	1.04255400	-2.83456500	-0.57218300	C	-2.98878000	-4.06856400	3.89667400
O	-1.21215600	1.48484700	0.91727000	C	1.89697600	-3.03991700	-1.63216800	H	-3.37653600	-5.01155800	4.30230800
O	0.17680500	0.88205400	-1.19299100	H	1.64735700	-2.69083900	-2.62494200	H	-2.14674100	-3.74730700	4.52205000
O	1.00887400	2.78506900	0.26991500	C	3.01656400	-3.70790200	-1.19319100	H	-3.76958300	-3.30508500	3.97913900
O	-4.41038500	0.70164100	-2.35326600	N	2.80349800	-3.91598500	0.16487700	O	-4.14089800	1.67402800	0.21502200
H	-4.94049800	0.71756400	-1.53444200	H	3.53634000	-4.19414700	0.82353600	C	-4.29345200	1.28755000	1.39505700
H	-4.28785900	-0.24419300	-2.58920800	C	1.61866100	-3.35766200	0.49880400	O	-3.48273300	0.52035900	2.04462700
O	-1.59150500	0.40575500	-3.46695800	H	1.22306800	-3.31620500	1.50278600	C	-5.50541100	1.73484300	2.19294700
H	-2.16928700	-0.39676100	-3.50623300	C	4.24377600	-4.16380500	-1.93910100	H	-5.20197700	2.55646200	2.85622400
H	-0.72404900	0.03249900	-3.20439200	H	4.01144100	-5.04931000	-2.54968700	H	-5.87658200	0.92075800	2.82425200
O	3.28995200	4.81143300	-0.93178800	H	4.51639600	-3.37459500	-2.65367600	H	-6.29128100	2.09670500	1.52372800
H	3.27025500	4.50183500	-2.15393200	C	5.47433200	-4.51858000	-1.06321800	O	-1.02014500	0.33284800	3.31112500
H	4.06204800	4.40333000	-0.50264600	H	5.31576900	-5.47670500	-0.55600700	C	0.09515600	0.91994600	3.49158800
O	-1.64426100	3.66871000	-1.80518100	H	6.34512300	-4.63955800	-1.72203000	O	0.90983900	1.28422800	2.58353700
C	-0.89908800	4.67231700	-1.76856600	C	5.75388800	-3.49482000	0.03645500	C	0.48878600	1.24245500	4.92196300
O	0.38514900	4.64236100	-1.73157000	O	5.38665800	-3.69359400	1.20242200	H	-0.20790300	0.73547800	5.59944200
C	-1.53896200	6.05819900	-1.76774700	N	6.35910400	-2.34101900	-0.34363200	H	1.49762100	0.84023800	5.09360900
H	-2.34297700	6.04061700	-2.51612200	H	6.60742900	-2.22231700	-1.31804300	C	0.49416500	2.76297900	5.17902300
H	-2.04494500	6.15094100	-0.79386700	C	6.46720700	-1.18603200	0.55439200	H	-0.50999600	3.16421400	4.97780900
C	-0.58512700	7.23211300	-1.99001000	H	6.80557100	-1.55611000	1.52811300	H	1.17325200	3.23997500	4.46035200
H	-0.09916100	7.16918000	-2.97176000	H	7.25151700	-0.53404900	0.14947800	C	0.91150900	3.10577400	6.61253700
H	0.20513200	7.24695300	-1.23171300	C	5.14628700	-0.41616700	0.72753500	H	0.22947900	2.65532200	7.34706500
H	-1.13258400	8.18245500	-1.94322400	H	4.40453500	-1.06999800	1.19831500	H	0.90684300	4.19145500	6.77386100
O	-1.36570200	-2.60020600	-2.02561500	H	5.32812900	0.41070200	1.42936900	H	1.92473800	2.73967000	6.83010100
C	-2.60518300	-2.69106500	-2.42818000	C	4.58879600	0.13204500	-0.59148700	O	0.27073400	-0.47442600	-1.58692200
O	-3.22214900	-1.77210300	-2.99829800	H	4.38370400	-0.70215700	-1.28085200	N	2.63130000	3.82583700	-3.02209600
C	-3.24927900	-4.05081400	-2.20394700	H	5.30842000	0.79398200	-1.09009200	H	3.11447700	3.05578300	-3.48272900
H	-2.60605600	-4.79691300	-2.69665100	C	3.27209800	0.89293400	-0.45647900	H	2.03943100	4.33559200	-3.67667600
H	-3.15997100	-4.26509800	-1.12800700	O	2.44003900	0.46422900	0.39564800				
C	-4.69646400	-4.17179500	-2.68601700	O	3.12168400	1.87772000	-1.24702800				

L:

Ca	-1.41500600	2.53487200	-1.00050500	O	-0.41230300	-0.72403300	0.97203000	H	-4.00537200	1.98897600	-2.25001900
Mn	-1.41235200	-1.08892700	-0.56423300	O	-0.48495200	1.78356900	1.17666300	O	-1.34139900	1.50883400	-3.25792300
Mn	-1.64105600	0.52471700	1.65037600	O	0.46748200	0.87892400	-1.07141200	H	-2.21048800	1.03998600	-3.32665400
Mn	0.98105200	0.74946100	0.73298500	O	1.99336200	2.15873900	0.58243200	H	-0.71219200	0.77461700	-3.10125500
Mn	3.29698300	2.62122400	-0.54054400	O	-3.70320300	2.86252500	-1.91619100	O	4.52559200	2.92460600	0.78456100
O	-2.31424600	0.39620800	-0.08524400	H	-4.15144500	3.00251400	-1.06111300	H	5.71905300	3.28265700	-1.23201100

H	4.08457300	2.75277500	1.63598100	C	0.00116000	-3.65643200	0.15927400	C	-4.51774700	-2.70308200	3.70255200
O	0.16781000	4.16038600	-1.52541500	H	-0.24983400	-3.49654200	1.19754700	H	-5.27595800	-3.42106400	4.04027100
C	1.26851500	4.42866500	-2.05558000	C	1.82889400	-5.36871200	-2.52620700	H	-3.62056700	-2.83625400	4.31945800
O	2.36164800	3.76897800	-1.90565400	H	1.19822000	-6.02280900	-3.14695300	H	-4.89158200	-1.68939700	3.88207700
C	1.32604000	5.64770600	-2.98088900	H	2.37493000	-4.72720600	-3.23228500	O	-2.97225600	3.34897600	0.70144200
H	0.59334900	5.46584000	-3.78085200	C	2.83180700	-6.27789600	-1.76972400	C	-3.27993700	2.92310700	1.83759000
H	0.92567000	6.49561600	-2.40695300	H	2.30240000	-7.10273200	-1.28010700	O	-2.92149800	1.78935300	2.33985000
C	2.69723900	5.98438100	-3.56570700	H	3.51839600	-6.72208400	-2.50350400	C	-4.13562500	3.77375900	2.76028500
H	3.07990000	5.15796000	-4.17819600	C	3.60409000	-5.55458600	-0.66589100	H	-3.47485600	4.28302300	3.47532000
H	3.42755900	6.18593900	-2.77155000	O	3.28128200	-5.67597900	0.52372100	H	-4.82712500	3.14921800	3.33530800
H	2.63744000	6.87587000	-4.20352000	N	4.61049300	-4.73564900	-1.06196000	H	-4.67971000	4.53035800	2.18742900
O	-2.45716400	-1.46019000	-2.13804300	H	4.79713500	-4.64277600	-2.05282100	O	-0.77124800	0.38433300	3.42387600
C	-3.60792100	-0.94275700	-2.47213800	C	5.28497100	-3.82145400	-0.13343900	C	0.49299100	0.37791300	3.58629200
O	-3.75559700	0.21737100	-2.90072000	H	5.52083100	-4.38888300	0.77346800	O	1.37093200	0.47298300	2.67347400
C	-4.79047200	-1.89321800	-2.35542600	H	6.23214000	-3.52823500	-0.60397100	C	0.98817600	0.20926800	5.01608000
H	-4.55009800	-2.78328800	-2.95798800	C	4.45226600	-2.58199000	0.23680500	H	0.16376600	0.47095000	5.69044200
H	-4.80157300	-2.24947300	-1.31397000	H	3.55837800	-2.89390600	0.78728200	H	1.18298700	-0.86679100	5.15711500
C	-6.14148500	-1.30304600	-2.76481300	H	5.05311800	-1.97385200	0.92903800	C	2.25670700	1.01039600	5.34057900
H	-6.07613800	-0.93199700	-3.79676800	C	4.04172300	-1.73665300	-0.97679300	H	2.05942100	2.07994900	5.17595900
H	-6.35520800	-0.42301100	-2.14192900	H	3.37225400	-2.32340100	-1.62443200	H	3.04620100	0.72919300	4.63224300
C	-7.28398000	-2.31732000	-2.64184000	H	4.91534400	-1.44979600	-1.57636400	C	2.73131800	0.78676100	6.78031900
H	-7.11115300	-3.19372900	-3.28249300	C	3.28461600	-0.45712900	-0.61977200	H	1.96312300	1.08541100	7.50727600
H	-7.38817400	-2.67945800	-1.60909100	O	2.37891000	-0.57607500	0.27465700	H	3.63625700	1.37054600	6.99311100
H	-8.24364200	-1.87343900	-2.93703900	O	3.60108900	0.59428900	-1.23915500	H	2.96625700	-0.27158200	6.96263100
N	-0.38159800	-2.88491400	-0.84579600	O	-2.69207800	-2.26474200	0.50297300	O	-0.04087700	-0.32853400	-1.58687300
C	0.21121100	-3.37978000	-1.98496500	C	-3.18232500	-1.95058200	1.63738700	N	4.94498000	2.95877100	-1.81333700
H	0.05244200	-2.90852500	-2.94555100	O	-2.90303000	-0.90936900	2.29718700	H	5.18106000	2.06103500	-2.23881000
C	0.97063200	-4.48095300	-1.66284900	C	-4.20623300	-2.91841200	2.22098300	H	4.71326700	3.64431900	-2.53244800
N	0.80137100	-4.64758600	-0.29292400	H	-3.84454800	-3.93657900	2.02456200				
H	1.38391800	-5.25465300	0.29006100	H	-5.11784200	-2.80593600	1.61311400				

3D images for TSs:



TS7 TS12 TS11:

Table SVIc. Gibbs free energies and Mulliken spin populations for water binding in the S' 0 state:

Spin states	Spin	Gibbs Free energy (a.u.)

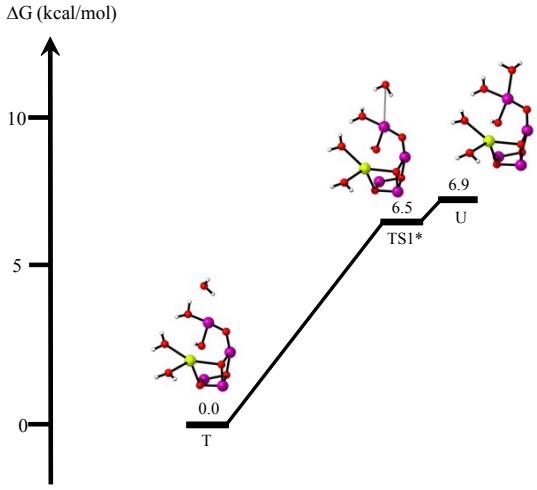
	topology (Mn1-Mn4)	T	TS1*	U
Octet	ααaβ	-3292.3588	-3292.3484	-3292.3478
Doublet	αβαβ	-3292.3593	-3292.3511	-3292.3505
		T’	TS3’	W’
Octet	ααaβ	-3215.9252	-3215.9131	-3215.9313
Doublet	αβαβ	-3215.9261	-3215.9152	-3215.9325
		W	TS4	X
Octet	ααaβ	-3292.3403	-3292.3373	-3292.3466
Doublet	αβαβ	-3292.3415	-3292.3394	-3292.3473
		Y	TS5*	
Octet	ααaβ	-3292.3425	-3292.3463	
Doublet	αβαβ	-3292.3434	-3292.3467	

Spin states	Spin topology (Mn1-Mn4)		Mulliken spin density		
			T	TS1	U
octet	α	Mn1	3.91	3.87	3.86
	α	Mn2	2.98	2.98	2.98
	α	Mn3	3.85	2.85	3.85
	β	Mn4	-3.82	-3.80	-3.82
doublet	α	Mn1	3.91	3.87	3.86
	β	Mn2	-2.87	-2.87	-2.87
	α	Mn3	3.84	3.83	3.82
	β	Mn4	-3.81	-3.80	-3.82

			T’	TS3’	W’
octet	α	Mn1	3.85	3.86	3.84
	α	Mn2	3.00	2.99	3.00
	α	Mn3	3.80	3.82	3.80
	β	Mn4	-3.82	-3.79	-3.81
doublet	α	Mn1	3.85	3.87	3.84
	β	Mn2	-2.89	-2.89	-2.90
	α	Mn3	3.78	3.80	3.78
	β	Mn4	-3.82	-3.80	-3.83
			W	TS4	X
octet	α	Mn1	3.90	3.90	3.90
	α	Mn2	3.00	3.01	3.00
	α	Mn3	3.81	3.81	3.80
	β	Mn4	-3.82	-3.82	-3.81
doublet	α	Mn1	3.89	3.89	3.89
	β	Mn2	-2.89	-2.89	-2.89
	α	Mn3	3.78	3.78	3.77
	β	Mn4	-3.82	-3.82	-3.81
			Y	TS5	
octet	α	Mn1	3.85	3.86	
	α	Mn2	3.01	3.01	
	α	Mn3	3.80	3.79	
	β	Mn4	-3.82	-3.82	
doublet	α	Mn1	3.84	3.85	

	β	Mn2	-2.90	-2.90
	α	Mn3	3.77	3.77
	β	Mn4	-3.81	-3.81

octet/Mn1-Mn4(αααβ) surface



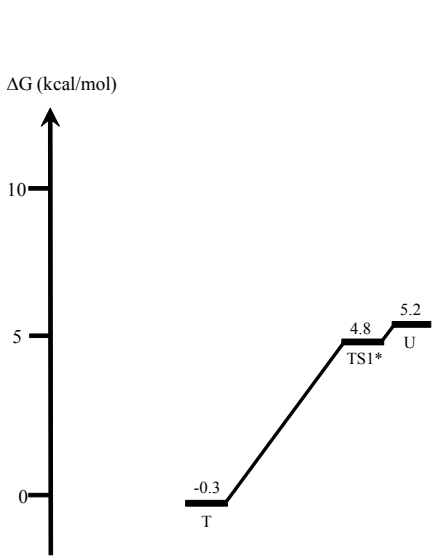
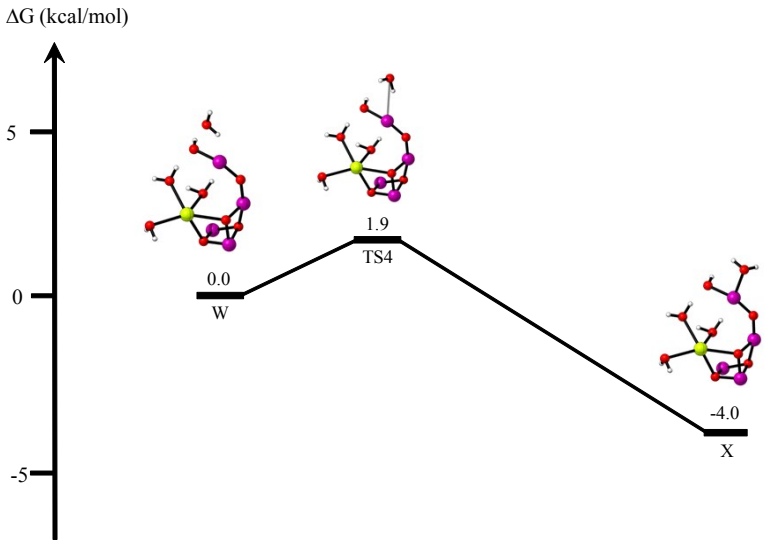
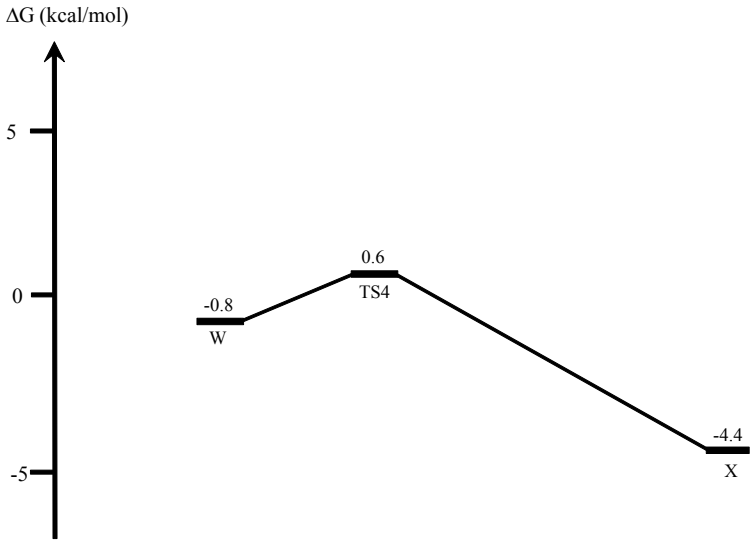


Figure SVIc1-1. Free energy profiles for water binding in the S' 0 state by pivot mechanism with W1=H_2O, W2=OH^-.

octet/Mn1-Mn4(αααβ) surface



doublet/Mn1-Mn4(αβαβ) surface



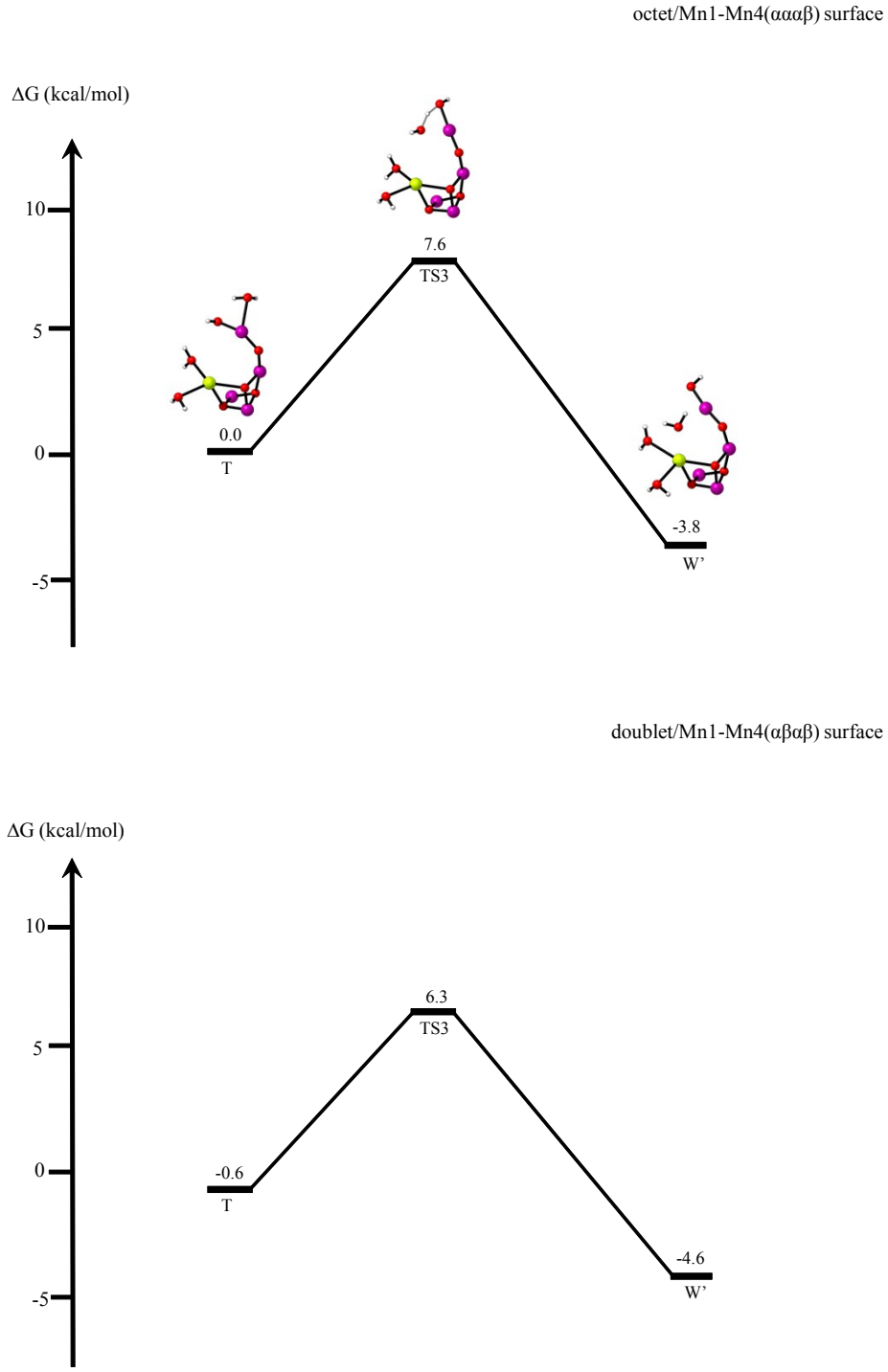
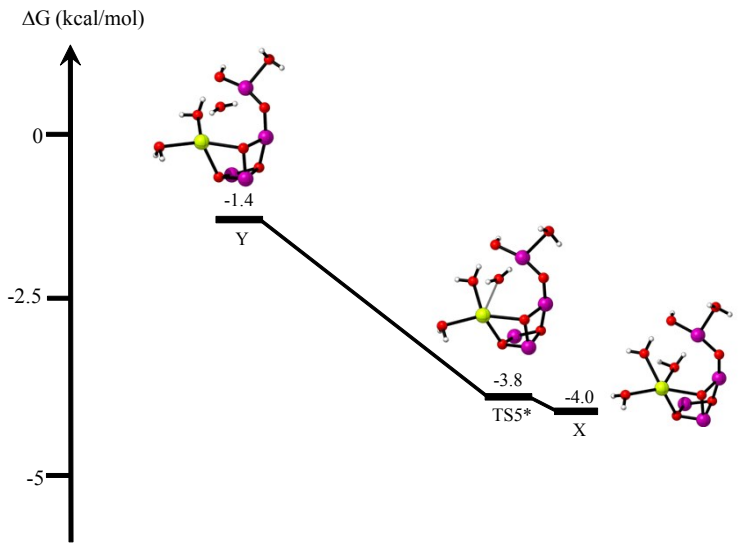


Figure SVIc1-2. Free energy profiles for water binding in the S' 0 state by pivot

mechanism with W1=OH^-, W2=H_2O and the previous proton transfer from W1 to W2.

octet/Mn1-Mn4(ααaβ) surface



doublet/Mn1-Mn4(αβαβ) surface

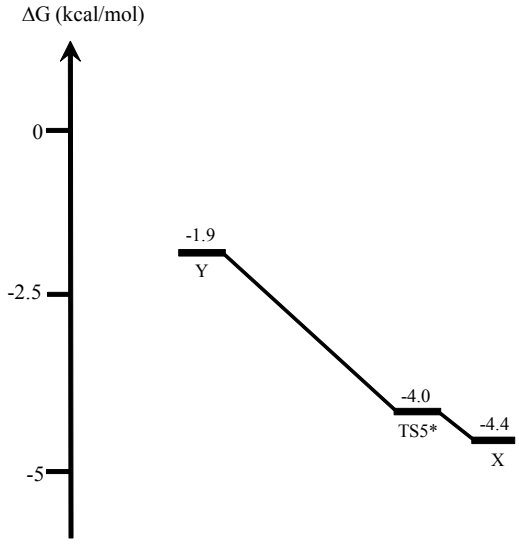


Figure SVIc2. Free energy profiles for water binding in the S' 0 state by water insertion mechanism.

The Cartesian coordinates for T, U, W, X, W', Y, TS1*, TS3, TS4 and TS5*:

T:

Ca	-2.67513600	0.35653400	-0.55863600	C	-2.21068300	2.00812300	-7.13700300	O	-0.43358600	-4.00388000	-0.40955300
Mn	0.28627000	-1.13821300	-1.61050800	H	-1.74948500	3.00584400	-7.09258300	C	0.47984700	-5.50930200	-2.02863400
Mn	-1.05052500	-2.29733400	0.47807400	H	-1.58420800	1.37946800	-7.78652400	H	1.53884300	-5.57218700	-2.31669700
Mn	0.10715800	0.00828900	1.53889000	H	-3.19120400	2.11292400	-7.62130800	H	-0.08484100	-5.56921500	-2.97264200
Mn	-0.58094500	2.76626500	0.97608200	N	2.29604100	-0.65648700	-1.81091900	C	0.08415800	-6.64839800	-1.08835600
O	-1.40741000	-1.57652600	-1.20758500	C	2.97748800	0.37729900	-2.41848500	H	0.24981100	-7.62037200	-1.57426500
O	0.60761700	-1.47298600	0.25806300	H	2.46523900	1.08023400	-3.06201900	H	0.67533100	-6.62138100	-0.16277500
O	-1.55128400	-0.77199300	1.29536300	C	4.30777500	0.31899200	-2.06770900	H	-0.97256700	-6.57410000	-0.80355200
O	-0.68170000	1.55016900	2.20557100	N	4.41301200	-0.80031100	-1.25224000	O	-4.20490000	-1.47326400	-0.05142400
O	-4.79319600	0.34374000	-1.89543200	H	5.25305500	-1.05997600	-0.72439200	C	-3.97721400	-2.63771500	0.37577300
H	-5.07115500	-0.49834300	-1.47000700	C	3.18819200	-1.34420500	-1.10773100	O	-2.82622400	-3.12372500	0.65271400
H	-4.59280200	0.13864000	-2.82432600	H	2.95688200	-2.18818000	-0.47434000	C	-5.14667800	-3.59183500	0.56341200
O	-2.56404700	3.74851700	-2.04795900	C	5.45345000	1.24509600	-2.39488500	H	-6.03946500	-3.04021600	0.87611500
H	-3.11397600	3.43379000	-1.29656600	H	5.64013000	1.24014400	-3.47857100	H	-4.90206100	-4.37165500	1.29128900
H	-2.37996300	2.92029300	-2.54905900	H	5.14532200	2.27306300	-2.15289600	H	-5.36388700	-4.07663400	-0.40107800
O	-0.43432700	1.32360900	-0.39586300	C	6.80235400	0.94360500	-1.69247800	O	-0.50887400	-3.11117300	2.17541100
H	0.07167900	1.70337200	-1.13314800	H	7.23472400	0.01450200	-2.07977400	C	0.14570200	-2.53908300	3.12252800
O	-3.34367900	2.47765200	0.38008000	H	7.50116400	1.75621700	-1.93465800	O	0.57264200	-1.35470800	3.12034200
C	-3.26127400	3.33731100	1.31642300	C	6.68475300	0.76324200	-0.17802300	C	0.40141400	-3.41433000	4.34308000
O	-2.14984800	3.81610800	1.71794500	O	6.65524900	-0.36653800	0.33017700	H	0.98284700	-4.28943200	4.01293200
C	-4.54761900	3.81816300	1.96706300	N	6.54538600	1.88675100	0.57002800	H	1.01380100	-2.84489700	5.05317900
H	-5.18620900	4.21128700	1.16230500	H	6.55870100	2.78713000	0.10710300	C	-0.90273500	-3.89632400	5.00561600
H	-5.06251600	2.91503500	2.32754000	C	6.17135100	1.82288500	1.98942400	H	-1.50192700	-4.43038400	4.25605600
C	-4.37562300	4.83713200	3.09229900	H	6.79809100	1.05840500	2.46007100	H	-1.49334600	-3.02012700	5.31520500
H	-3.86940900	5.74251700	2.73413700	H	6.42577600	2.79191100	2.43687000	C	-0.64272400	-4.79669300	6.21777300
H	-3.77506300	4.42064100	3.91038400	C	4.68655500	1.47852900	2.20603900	H	-0.08346700	-5.69774100	5.93025500
H	-5.35571200	5.12900000	3.49527800	H	4.47442000	0.50751300	1.74668800	H	-1.58382200	-5.12199300	6.67857300
O	-0.10352900	-0.06169900	-3.25020300	H	4.51331900	1.35527700	3.28436600	H	-0.05729400	-4.27488200	6.98716400
C	-1.07808400	0.69009900	-3.61360600	C	3.73768700	2.53763800	1.64195800	O	-0.36382900	4.07025100	-0.59273800
O	-2.04661000	1.03611900	-2.88176700	H	4.03122900	2.79545200	0.61121600	H	-0.07081200	4.94828500	-0.22731400
C	-0.99332800	1.23231500	-5.03864800	H	3.79292200	3.47424200	2.21368100	H	-1.18456000	4.13106800	-1.17700900
H	-0.49166400	2.21353200	-4.97817300	C	2.26587000	2.13792600	1.54375900	O	0.88876700	5.79918200	1.01590900
H	-0.32769900	0.57992500	-5.61749300	O	1.96449900	0.91230400	1.56963300	H	0.34329600	6.01007300	1.79263100
C	-2.34811500	1.40244900	-5.73641700	O	1.44980600	3.10951300	1.37241700	H	1.36186400	4.96914100	1.25856700
H	-2.99392400	2.03087000	-5.11406700	O	0.73457200	-3.13885700	-2.14740900				
H	-2.84246500	0.42414700	-5.80850500	C	0.24309400	-4.10285800	-1.48189700				

TS1*:

Ca	-2.58578800	-0.98828500	0.30364300	O	-0.27273500	-0.93508300	-2.64303800	H	0.38063000	-1.81549300	0.62140600
Mn	0.04972000	0.67470400	1.88285000	O	-4.66995900	-1.72720700	1.48141500	O	-2.92805600	-2.84233300	-1.18790100
Mn	-1.49860700	2.09380300	0.12123400	H	-5.11231400	-0.87579100	1.26604900	C	-2.65588300	-3.30535600	-2.34092600
Mn	0.10105000	0.44773000	-1.45437400	H	-4.55124300	-1.74581000	2.44573900	O	-1.47004500	-3.38278100	-2.80266100
Mn	-0.00193300	-2.44174100	-1.84716300	O	-1.69374600	-4.47944600	0.77905100	C	-3.79747800	-3.80064200	-3.21330800
O	-1.69735700	0.87359900	1.52657700	H	-2.34815400	-4.12750100	0.13216100	H	-4.40328300	-4.47916800	-2.59566700
O	0.29306600	1.56444400	0.19337300	H	-1.70104900	-3.80305500	1.49661300	H	-4.43979000	-2.92501100	-3.39457700
O	-1.68753000	0.79234700	-1.11289900	O	-0.22913100	-1.47212500	-0.05107200	C	-3.37964700	-4.45489300	-4.52997200

H	-2.76407100	-5.34513800	-4.35371000	H	7.09294200	0.78505300	2.35821900	O	-4.43795200	0.59524500	0.21582200	
H	-2.79108400	-3.76315100	-5.14268600	H	7.70960700	-0.75995900	1.75938200	C	-4.43338500	1.85231700	0.13061100	
H	-4.26548400	-4.75852000	-5.10203100	C	6.71030400	0.50380100	0.29422900	O	-3.39160000	2.59643200	0.09035900	
O	-0.10579200	-0.88025900	3.12533200	O	6.43671400	1.69917400	0.11330200	C	-5.75569000	2.59433800	0.02791200	
C	-0.96842400	-1.82282300	3.25828300	N	6.81312000	-0.36841600	-0.73926200	H	-6.00778600	2.70836700	-1.03560000	
O	-1.83185000	-2.14433100	2.39742800	H	7.02838200	-1.33785700	-0.54145700	H	-5.67759500	3.59422800	0.46514700	
C	-0.88134100	-2.58884200	4.57660500	C	6.40755900	0.00537700	-2.10196400	H	-6.55632000	2.02311600	0.50856300	
H	0.15445800	-2.94720100	4.68286100	H	6.87321300	0.96870300	-2.33472800	O	-1.13107200	3.44176500	-1.24199800	
H	-1.00838200	-1.84817800	5.38118500	H	6.82585300	-0.74645700	-2.78246100	C	-0.37983100	3.29904100	-2.27747200	
C	-1.87549400	-3.74209300	4.73792300	C	4.87995800	0.11741300	-2.25831000	O	0.27712900	2.26985700	-2.57865300	
H	-1.73772400	-4.46646500	3.92257700	H	4.50821800	0.88558100	-1.57255800	C	-0.30533500	4.51784000	-3.18890300	
H	-2.89833800	-3.35591600	4.62640000	H	4.65892100	0.47529500	-3.27324100	H	0.19909500	5.32055100	-2.62865500	
C	-1.73166300	-4.45081900	6.08937900	C	4.15661800	-1.20573300	-2.00035300	H	0.32497600	4.26125400	-4.04863800	
H	-0.72576000	-4.87623300	6.21271900	H	4.54202100	-1.67626200	-1.08127800	C	-1.68878400	5.01272500	-3.64553300	
H	-1.90164500	-3.75714600	6.92462000	H	4.34048000	-1.93072200	-2.80538000	H	-2.29518000	5.23040500	-2.75708900	
H	-2.45377900	-5.27159400	6.18463700	C	2.64562000	-1.11673500	-1.80306800	H	-2.20101800	4.20111400	-4.18394300	
N	2.12040800	0.53346800	2.02627500	O	2.11300900	0.00480800	-1.59428900	C	-1.59840900	6.25051100	-4.54400200	
C	2.99963000	-0.47301800	2.36954600	O	2.03588100	-2.24748800	-1.81535000	H	-1.11743100	7.08818400	-4.01913300	
H	2.64332100	-1.40317600	2.79229800	O	0.10056800	2.47335000	2.97613700	H	-2.59543100	6.58394200	-4.86080500	
C	4.28909700	-0.06839800	2.10227900	C	-0.57049700	3.47788600	2.57940000	H	-1.01135900	6.04610100	-5.45044700	
N	4.16201100	1.22548700	1.61533500	O	-1.21436100	3.56208000	1.48680400	O	0.34983400	-4.26129900	-0.84466400	
H	4.93107900	1.77588300	1.21619900	C	-0.60440500	4.68916500	3.50840600	H	1.20678300	-4.23759300	-0.38344500	
C	2.85314800	1.54180800	1.56732200	H	0.43142900	4.88513000	3.81950000	H	-0.38680900	-4.40855700	-0.14663400	
H	2.45398500	2.46270800	1.16771800	H	-1.12697900	4.36282100	4.42077700	O	2.12815200	-4.83012500	-3.12111400	
C	5.59982700	-0.80867400	2.21878700	C	-1.25913500	5.94096500	2.92421000	H	1.33988300	-5.09723300	-2.61885200	
H	5.78234600	-1.07821800	3.26910200	H	-1.25070700	6.75586800	3.65989000	H	2.32517900	-3.93911900	-2.77701600	
H	5.50687800	-1.76346000	1.68014700	H	-0.72966200	6.28241900	2.02653800					
C	6.86062900	-0.06451500	1.70661500	H	-2.29731700	5.74389500	2.63476100					

U:

Ca	-2.60129800	-0.77503500	0.69388100	O	-1.55426000	-2.16942000	2.48540300	C	6.10864900	-0.71069200	-2.76063700	
Mn	0.43669500	0.56337500	1.91525300	C	-0.29066200	-2.92469800	4.40325400	H	6.62530200	0.19090600	-3.10616800	
Mn	-1.18805300	2.15203100	0.37214500	H	0.71386300	-3.35595500	4.26762300	H	6.35519800	-1.52734000	-3.45070500	
Mn	-0.00257800	0.39318300	-1.43602500	H	-0.20844300	-2.29110600	5.29959300	C	4.59112000	-0.45524900	-2.71856500	
Mn	-0.53536300	-2.38894500	-2.09931100	C	-1.33113600	-4.02873400	4.61061200	H	4.38777100	0.39567700	-2.06043800	
O	-1.31535100	0.91792200	1.78841900	H	-1.39896300	-4.64824200	3.70526700	H	4.26581500	-0.15441900	-3.72435200	
O	0.52341500	1.41827400	0.19110400	H	-2.32294600	-3.57224000	4.73433800	C	3.79011300	-1.67352600	-2.25398500	
O	-1.69820400	0.93339100	-0.83722700	C	-1.00939500	-4.91333200	5.82031900	H	4.19198300	-2.04038200	-1.29521500	
O	-0.64490500	-0.78288400	-2.72336200	H	-0.03527200	-5.40961200	5.70556800	H	3.87616500	-2.50770500	-2.96304600	
O	-4.46743500	-1.17976800	2.32916200	H	-0.97260400	-4.32482200	6.74779300	C	2.29880600	-1.43727600	-2.00901900	
H	-4.83954600	-0.29270300	2.12283100	H	-1.76769700	-5.69572500	5.95134600	O	1.91287400	-0.25731800	-1.75253900	
H	-4.19292300	-1.15502200	3.26057500	N	2.48952000	0.26120000	1.78025600	O	1.56885600	-2.47920200	-2.03372500	
O	-2.04235900	-4.35155600	0.66656400	C	3.33189500	-0.79408800	2.06147600	O	0.79051500	2.29241500	3.03296200	
H	-2.74630400	-3.83176600	0.20595100	H	2.95983400	-1.68629000	2.54713800	C	0.18541600	3.37227700	2.73297000	
H	-1.79085500	-3.76391900	1.41511500	C	4.60827200	-0.48651300	1.64519500	O	-0.55791400	3.55234400	1.72158000	
O	-0.51083900	-1.58212200	-0.22617300	N	4.51458700	0.79997200	1.12987700	C	0.38166200	4.54915900	3.68602900	
H	0.19151300	-1.99485900	0.30143900	H	5.26651900	1.28429600	0.62810100	H	1.46281400	4.64608700	3.85990300	
O	-3.63060400	-2.43605100	-0.68650900	C	3.23142400	1.20373800	1.21025500	H	-0.04280800	4.23803100	4.65284700	
C	-3.61327700	-2.69125900	-1.93290400	H	2.85109900	2.13702900	0.82096500	C	-0.22970700	5.87091900	3.22141300	
O	-2.55337500	-2.93608600	-2.58854500	C	5.87341800	-1.30968400	1.65193100	H	-0.05332100	6.65750000	3.96686700	
C	-4.94958700	-2.71271400	-2.66566600	H	6.16920200	-1.53278600	2.68743100	H	0.20600200	6.19518300	2.26874600	
H	-5.60290700	-3.40737200	-2.11827200	H	5.65281800	-2.28416300	1.19142900	H	-1.31016000	5.77247600	3.06798000	
H	-5.39726800	-1.71867300	-2.51705700	C	7.10316600	-0.68333800	0.94456800	O	-4.24839100	1.02474700	0.87738300	
C	-4.88139500	-3.06265700	-4.15168100	H	7.48098100	0.16876000	1.52020600	C	-4.09948700	2.27370300	0.80208100	
H	-4.46781100	-4.06741700	-4.30566700	H	7.90090400	-1.43839000	0.91539200	O	-2.98925700	2.88538200	0.62518000	
H	-4.24926000	-2.35049100	-4.69543500	C	6.80535000	-0.15284500	-0.45959100	C	-5.32195500	3.17313500	0.88905100	
H	-5.88353200	-3.03867600	-4.59828700	O	6.63071700	1.05756900	-0.65948700	H	-5.69840500	3.34595700	-0.12880900	
O	0.32688100	-1.06258700	3.06897800	N	6.67047600	-1.06909800	-1.45033800	H	-5.06285000	4.14405600	1.32192400	
C	-0.55066700	-1.98956300	3.22289000	H	6.79196800	-2.04893000	-1.22558000	H	-6.11539100	2.69006000	1.46827900	

O	-0.85257200	3.50546700	-0.98562300	H	-1.99015300	5.47203400	-2.28312800	H	0.58614400	-4.39093700	-1.03003400
C	-0.25574700	3.32773000	-2.11401700	H	-2.18579500	4.50540500	-3.74304600	H	-0.94669600	-4.40930000	-0.50695300
O	0.23721000	2.25011500	-2.52801300	C	-1.40945500	6.49428200	-4.10977800	O	-0.46881500	-3.49919700	-4.10451300
C	-0.15938100	4.57396700	-2.98657800	H	-0.77823200	7.25146200	-3.62310900	H	-1.43455500	-3.36920600	-4.21783100
H	0.49531500	5.29230200	-2.46880600	H	-2.39478200	6.94550100	-4.28675300	H	-0.39643100	-4.41140400	-3.76563700
H	0.32857300	4.29236600	-3.92730300	H	-0.96379700	6.27122900	-5.08948100				
C	-1.52487700	5.23273800	-3.24786200	O	-0.33982400	-4.33696400	-1.33000200				

W:

Ca	-2.24609000	1.21219400	-1.13228000	C	-2.42390700	-1.07225200	-7.54837400	O	-1.75325500	-3.41025700	0.61135400
Mn	0.02197700	-1.50112500	-1.25628700	H	-1.47193600	-0.96716600	-8.08768000	C	-1.27378900	-5.59559200	-0.23658900
Mn	-1.74723100	-1.41050700	0.84847400	H	-2.68732300	-2.13915800	-7.54912600	H	-0.28160800	-6.06789400	-0.25203500
Mn	0.12648000	0.47297800	1.58204300	H	-3.19275100	-0.53864400	-8.12208000	H	-1.72095500	-5.82131100	-1.21710900
Mn	0.38553100	3.42648500	0.66592600	N	2.07981900	-1.75789500	-1.36888000	C	-2.14029100	-6.14971300	0.89455600
O	-1.72857900	-1.17388300	-0.96722100	C	3.03803700	-1.14507400	-2.14806000	H	-2.26178700	-7.23576200	0.78778100
O	0.12956400	-1.28430000	0.68637800	H	2.75694000	-0.50501700	-2.97367500	H	-1.68857800	-5.94913700	1.87375000
O	-1.65351000	0.37868600	1.13261400	C	4.29028400	-1.49830400	-1.69851200	H	-3.13286900	-5.68597900	0.89298400
O	0.11934300	2.25319300	1.93623900	N	4.05819600	-2.36406700	-0.63655500	O	-4.33825500	0.18304000	-0.45017700
O	-4.09019600	1.56787000	-2.79526500	H	4.77993100	-2.68593900	0.01544200	C	-4.57206300	-0.78273200	0.32002800
H	-4.70370100	0.99930200	-2.28452600	C	2.72431000	-2.47849800	-0.46061100	O	-3.69490700	-1.47996200	0.94627600
H	-3.66370600	0.98395100	-3.45690700	H	2.25093500	-3.04435900	0.32885200	C	-6.00816900	-1.22411500	0.55536900
O	-0.89612800	2.86908600	-2.57768500	C	5.65822000	-1.08087700	-2.17863700	H	-6.18239900	-2.17090500	0.02639900
H	-1.15465800	3.21641600	-3.44541300	H	5.84282600	-1.48997300	-3.18288800	H	-6.70997000	-0.47049500	0.18643900
H	-0.42595800	3.60426900	-2.03921500	H	5.66103600	0.01204300	-2.30002900	H	-6.17558500	-1.41119400	1.62170900
O	0.51535100	4.33279200	-0.98502100	C	6.85617300	-1.49772700	-1.28672700	O	-1.67294000	-1.82465000	2.79203200
H	1.42682300	4.43228300	-1.34052900	H	7.00933800	-2.58144500	-1.33784800	C	-0.88506100	-1.33491500	3.67154000
O	-2.07728800	3.26912200	0.06060600	H	7.76189500	-1.02079200	-1.68592800	O	-0.00938800	-0.44683900	3.46583200
C	-2.06079200	4.24701500	0.85673500	C	6.66766400	-1.16021400	0.19165800	C	-1.02318300	-1.90274700	5.07926800
O	-0.95554900	4.67221900	1.35185500	O	6.28562300	-2.01665200	1.00046900	H	-0.56267500	-2.90403600	5.07015200
C	-3.35382200	4.92920200	1.25736100	N	6.86901400	0.13173500	0.55980600	H	-0.43030600	-1.27717900	5.75740200
H	-3.94444300	5.06350300	0.34059000	H	7.18277200	0.79582500	-0.13698000	C	-2.47923600	-2.01859100	5.55692900
H	-3.90802200	4.19495400	1.86230900	C	6.49259400	0.61932000	1.89255000	H	-3.04014700	-2.62344100	4.83352900
C	-3.18524800	6.24482300	2.01842800	H	6.89684500	-0.08070900	2.63167900	H	-2.94023400	-1.01942900	5.55070300
H	-2.64956100	6.98633500	1.41332600	H	6.98892800	1.58700300	2.03720400	C	-2.58745100	-2.62774600	6.95871700
H	-2.61417200	6.09365600	2.94113100	C	4.96918800	0.73311700	2.07838800	H	-2.16291400	-3.64154900	6.98554000
H	-4.16592600	6.66079400	2.28162900	H	4.52233500	-0.25455000	1.92693300	H	-3.63469900	-2.69671100	7.28146200
O	-0.13872700	-1.34102200	-3.20383000	H	4.76286000	1.01011800	3.12125500	H	-2.04852500	-2.02345700	7.70217300
C	-1.07228700	-0.74164700	-3.86574300	C	4.32094500	1.74539200	1.13062500	O	0.49575200	1.01091000	-1.41087300
O	-1.77796200	0.19672900	-3.42927500	H	4.71590900	1.62038500	0.10944400	H	1.26667100	1.44683100	-0.99515500
C	-1.25637200	-1.25482800	-5.29205400	H	4.55719600	2.78030100	1.41727100	H	0.23567200	1.59728700	-2.17164200
H	-0.27407600	-1.20566900	-5.78652900	C	2.80727400	1.63612500	0.99936800	O	3.33610100	4.47222300	-1.40617200
H	-1.48685400	-2.32866500	-5.21826200	O	2.20897300	0.63695900	1.44722500	H	3.41552800	5.30832700	-0.91581400
C	-2.31740300	-0.52638000	-6.11991300	O	2.24236800	2.60540300	0.33397700	H	3.18609900	3.79333400	-0.71081200
H	-2.08421600	0.54759400	-6.14609100	O	-0.18868100	-3.61546400	-1.01084000				
H	-3.29182100	-0.61445400	-5.61793500	C	-1.04997000	-4.08457200	-0.20792600				

TS4:

Ca	-2.21174500	0.98500900	-1.34737800	O	-0.89279600	2.27957300	-3.17560600	H	-2.35811000	7.19206100	-0.18128100
Mn	-0.06734600	-1.78938700	-0.90564000	H	-1.28098200	2.51280800	-4.03369900	H	-2.26155400	6.68627500	1.51195700
Mn	-1.76942900	-1.14367800	1.15990600	H	-0.40824400	3.08909000	-2.80385300	H	-3.83181100	7.14090700	0.81041500
Mn	0.20160600	0.76599000	1.41835600	O	0.69019800	3.99446300	-1.95081100	O	-0.27709300	-2.06809900	-2.83515800
Mn	0.54456700	3.43835100	-0.12014100	H	1.54566500	3.73808200	-2.33778300	C	-1.20004500	-1.58154500	-3.59695700
O	-1.79417100	-1.32551400	-0.66163900	O	-1.95626400	3.24870500	-0.64725500	O	-1.83982400	-0.52806900	-3.37100400
O	0.10769800	-1.13743600	0.93428500	C	-1.87562000	4.37512200	-0.08747200	C	-1.46008500	-2.39355200	-4.86326100
O	-1.59111500	0.65979300	1.03245000	O	-0.73628700	4.84999800	0.26982900	H	-0.49333400	-2.52130600	-5.37397100
O	0.27883500	2.58685900	1.37636900	C	-3.12500100	5.18533500	0.19295500	H	-1.74919600	-3.40534000	-4.54008800
O	-4.07326900	1.05477500	-3.02640100	H	-3.76034500	5.11969200	-0.70095600	C	-2.50414100	-1.80787000	-5.81656200
H	-4.70484000	0.64845900	-2.39682800	H	-3.66555200	4.63943500	0.98189400	H	-2.21142700	-0.78479800	-6.09249700
H	-3.69091900	0.31580400	-3.54475400	C	-2.87868200	6.63647800	0.60823100	H	-3.46561900	-1.71865100	-5.29030500

C	-2.68684200	-2.65714300	-7.07956400	H	7.08870500	1.80951900	1.34919100	H	-6.17087600	-0.75158300	1.98841100	
H	-1.74810700	-2.73732000	-7.64561800	C	5.06312000	1.04260100	1.68976300	H	-6.24525600	-1.87112800	0.62370000	
H	-3.01029900	-3.67750300	-6.83089600	H	4.59969400	0.06025900	1.82419800	H	-6.70481400	-0.16086100	0.37731500	
H	-3.44202200	-2.22122300	-7.74632500	H	4.90661800	1.59131300	2.62844800	O	-1.65542000	-1.11124200	3.14399000	
N	1.97765400	-2.13213500	-0.98868600	C	4.38705000	1.78337400	0.53297000	C	-0.82191100	-0.47583100	3.87593700	
C	2.93186200	-1.78468700	-1.92149500	H	4.75297400	1.40148700	-0.43383000	O	0.08591700	0.29848800	3.45748400	
H	2.64659800	-1.38884000	-2.88704700	H	4.62588600	2.85663400	0.53836000	C	-0.94612700	-0.70196800	5.37750100	
C	4.18563600	-2.03765300	-1.41202900	C	2.87306800	1.65158200	0.47515600	H	-0.55467500	-1.71064100	5.58662100	
N	3.95759400	-2.57307200	-0.15045300	O	2.28032200	0.80800100	1.17841500	H	-0.29040400	0.01576400	5.88479600	
H	4.68820000	-2.73263000	0.55091200	O	2.28762700	2.42525500	-0.40034100	C	-2.38985000	-0.60107900	5.89557200	
C	2.62661800	-2.59601700	0.07192700	O	-0.35391300	-3.77569200	-0.18228800	H	-3.01409400	-1.31147300	5.33920100	
H	2.15911700	-2.90601200	0.99547800	C	-1.20628900	-4.01280400	0.72511000	H	-2.78307100	0.40181600	5.67095000	
C	5.55230300	-1.79873200	-2.00556400	O	-1.85779800	-3.13932300	1.38409600	C	-2.48982500	-0.86898300	7.40086100	
H	5.69808800	-2.45012300	-2.87974700	C	-1.48620700	-5.47912300	1.04806500	H	-2.13298700	-1.87867800	7.64951800	
H	5.58355000	-0.77052400	-2.39459900	H	-0.51220900	-5.98137000	1.13095100	H	-3.52763000	-0.78717600	7.74988700	
C	6.76204800	-2.02009000	-1.06122100	H	-1.96035300	-5.90618000	0.15085100	H	-1.88673400	-0.15324100	7.97720500	
H	6.87892100	-3.08610000	-0.83654200	C	-2.34907400	-5.72319300	2.28627900	O	0.45005100	0.60993500	-1.66885500	
H	7.66979800	-1.69606100	-1.58860700	H	-2.51094500	-6.79902400	2.43425500	H	1.23522400	1.10847500	-1.35801900	
C	6.63015900	-1.30920200	0.28554100	H	-1.87105900	-5.32043300	3.18752500	H	0.22120800	0.98812500	-2.55468000	
O	6.24037400	-1.91585200	1.29296000	H	-3.32469000	-5.23425400	2.18899900	O	3.35901700	5.02069800	-1.21955600	
N	6.88800800	0.02336100	0.30877300	O	-4.32575200	0.23195500	-0.42315100	H	2.46822600	5.33762800	-1.45379400	
H	7.21637700	0.47410700	-0.53619000	C	-4.57782700	-0.52186000	0.55066200	H	3.20672200	4.08895900	-0.97589000	
C	6.57566600	0.84933400	1.48273400	O	-3.71223300	-1.09693600	1.30521300					
H	7.00254600	0.35810100	2.36401800	C	-6.02294300	-0.83318900	0.90596800					

X:

Ca	-2.39522000	0.22392000	-1.61379200	C	-1.59899400	-3.53349300	-5.30545100	H	4.30050200	3.34336700	0.00594500	
Mn	0.23482000	-1.94497900	-0.37264100	H	-1.60750800	-2.54922900	-5.79505700	C	2.57621300	2.11177300	0.18035700	
Mn	-1.67915500	-1.01626500	1.35636700	H	-2.59238300	-3.65591400	-4.85055600	O	1.99279500	1.44432400	1.06855200	
Mn	-0.03027900	1.19484100	1.15177900	C	-1.36934300	-4.63239400	-6.34907300	O	2.01212600	2.63433500	-0.85709800	
Mn	0.17555100	3.41699200	-1.01590800	H	-0.39528700	-4.51507800	-6.84439000	O	0.16340400	-3.69561900	0.77276400	
O	-1.54430800	-1.67753400	-0.35086500	H	-1.38778200	-5.63011500	-5.88870500	C	-0.69521200	-3.80872900	1.70614900	
O	0.18538300	-0.78168600	1.18354400	H	-2.14359800	-4.60970700	-7.12676100	O	-1.48057100	-2.89626500	2.10529600	
O	-1.76067500	0.67827200	0.72982100	N	2.29562300	-1.98896600	-0.36598400	C	-0.78654200	-5.16965000	2.39120000	
O	-0.22442800	2.91310400	0.64052400	C	3.20714300	-1.58937800	-1.32495700	H	0.24116700	-5.48467000	2.62061200	
O	-4.10952500	-0.44845900	-3.30250600	H	2.88983000	-1.18986000	-2.28013100	H	-1.14465700	-5.87596100	1.62637100	
H	-4.72381400	-0.78528600	-2.61830900	C	4.47923400	-1.71685900	-0.81884800	C	-1.67648000	-5.21492200	3.63328200	
H	-3.60863100	-1.22540300	-3.62481300	N	4.31351700	-2.22278500	0.46608100	H	-1.69636900	-6.22927400	4.05264600	
O	-0.57926400	0.94583300	-3.16356200	H	5.05131100	-2.22956300	1.17556600	H	-1.31058000	-4.52971100	4.40746700	
H	-0.76364900	0.62437600	-4.06253900	C	2.99117300	-2.35089800	0.70590100	H	-2.70311400	-4.91709800	3.39311700	
H	-0.34579100	1.94199800	-3.21223000	H	2.56337200	-2.68423900	1.64031900	O	-4.38314300	-0.63825500	-0.56119000	
O	0.36802500	3.34001100	-2.89542000	C	5.81280800	-1.42883700	-1.45857000	C	-4.53449000	-1.11983200	0.58974600	
H	1.27958100	3.10556400	-3.15398500	H	6.05524700	-2.21356700	-2.19067900	O	-3.60978700	-1.27980200	1.46610700	
O	-2.63427000	2.56425600	-1.73041400	H	5.71214200	-0.50296400	-2.04160200	C	-5.91053400	-1.58556300	1.03667100	
C	-2.57640100	3.79815600	-1.53772700	C	7.02147800	-1.31199200	-0.49322000	H	-6.12890500	-1.20211700	2.03962100	
O	-1.48815200	4.42391100	-1.24851900	H	7.29758800	-2.29979800	-0.10748200	H	-5.91576900	-2.68198500	1.09904200	
C	-3.84651300	4.63120300	-1.65406500	H	7.88197200	-0.93186000	-1.06065800	H	-6.67844600	-1.25825100	0.33002200	
H	-4.26302700	4.42521400	-2.65070600	C	6.73203800	-0.43798700	0.72440800	O	-1.70969300	-0.46454300	3.25562300	
H	-4.56479400	4.19918400	-0.94195800	O	6.39816200	-0.93769200	1.80691000	C	-1.04766200	0.47312000	3.82041600	
C	-3.68385900	6.13408000	-1.42641000	N	6.78883000	0.90625500	0.53513200	O	-0.25823500	1.26854200	3.23833600	
H	-2.97646400	6.56903600	-2.14258800	H	7.04057700	1.25433000	-0.38177000	C	-1.23280500	0.60466500	5.32687300	
H	-3.31133000	6.34373900	-0.41628300	C	6.26529200	1.85209400	1.52692300	H	-0.66005800	-0.21339400	5.79319800	
H	-4.64782300	6.64519500	-1.54445700	H	6.65927700	1.55963100	2.50607600	H	-0.77044500	1.54707500	5.64431000	
O	0.25324900	-2.45232300	-2.25361000	H	6.67266500	2.84063600	1.28050100	C	-2.69874300	0.52072300	5.78032800	
C	-0.68834000	-2.45497700	-3.14385600	C	4.72761200	1.87641400	1.57965100	H	-3.12763400	-0.42053200	5.41447400	
O	-1.64122400	-1.64699200	-3.18907800	H	4.36898800	0.88304000	1.86910400	H	-3.27056700	1.32982700	5.30145000	
C	-0.53644600	-3.54179600	-4.20401200	H	4.41783800	2.56365700	2.37914500	C	-2.84466800	0.61680800	7.30258900	
H	0.47267200	-3.44078100	-4.63197400	C	4.08593800	2.29429000	0.25415100	H	-2.30912400	-0.20094200	7.80565900	
H	-0.52813300	-4.50694500	-3.67444200	H	4.49803200	1.69849600	-0.57560000	H	-3.89884300	0.55957100	7.60408200	

H	-2.43895800	1.56357200	7.68633800	H	1.35270700	0.70348300	-3.20245600	H	0.48586700	5.01409800	0.84356000
O	2.30847000	0.92627000	-3.21240200	O	0.73143700	5.43724400	-0.00654500				
H	2.41193100	1.43916700	-2.38831800	H	-0.09418600	5.87374000	-0.29577400				

TS3:

Ca	-2.69570200	0.69374400	-0.85601800	H	-4.80207400	-3.08526300	-3.23550600	O	-0.39631600	-3.77677700	0.63269300
Mn	-0.33706100	-2.00449200	-0.47315700	C	-4.54862300	-4.48560600	-4.86907300	C	-0.89173200	-3.77175300	1.80709200
Mn	-1.38220700	-0.82873600	1.76936600	H	-3.90268100	-4.64792000	-5.74338900	O	-1.27396500	-2.74598200	2.44593200
Mn	0.38654100	1.08360300	0.79997800	H	-4.49468800	-5.38916000	-4.24579400	C	-1.03625200	-5.12777500	2.49268100
Mn	0.55232300	3.71186100	-1.11586400	H	-5.58061600	-4.39120000	-5.23064100	H	-0.08138600	-5.65727900	2.36570500
O	-1.93935500	-1.46044800	0.11248800	N	1.60001600	-2.45092000	-1.05287100	H	-1.76707100	-5.69755100	1.89824600
O	0.32614300	-0.89912400	0.97127800	C	2.29658600	-2.22127500	-2.22109400	C	-1.45470400	-5.07159400	3.96187500
O	-1.40917000	0.86940800	1.18365100	H	1.78439300	-1.93256700	-3.12927500	H	-1.54742900	-6.08563800	4.37217400
O	0.12809500	2.80024600	0.29691200	C	3.64022000	-2.42311000	-2.00123000	H	-0.71898600	-4.52316400	4.56231800
O	-5.00086900	0.48425100	-1.81854300	N	3.73161500	-2.80759800	-0.66988700	H	-2.41621600	-4.55936400	4.07789100
H	-5.38084900	0.21769800	-0.95555600	H	4.61260000	-2.88704200	-0.14990000	O	-4.37440000	0.18259100	0.81894700
H	-4.83345100	-0.34243000	-2.31294000	C	2.49476000	-2.79357300	-0.13374800	C	-4.27455200	-0.34528200	1.95546500
O	-0.45203200	0.51085900	-1.88986200	H	2.27182500	-2.99690300	0.90345400	O	-3.19059100	-0.76832700	2.49854900
H	-0.44164100	-0.29032600	-2.45270000	C	4.82396200	-2.25594100	-2.92141300	C	-5.52328100	-0.55134300	2.79776100
H	-0.13087700	1.29935200	-2.44360500	H	4.77126900	-2.99277600	-3.73623800	H	-6.33695000	0.08771500	2.44215600
O	1.16650400	4.76057100	-2.73547500	H	4.74673500	-1.27199900	-3.40650000	H	-5.30981700	-0.34991000	3.85259300
H	2.12967700	4.63264500	-2.81246700	C	6.22394200	-2.39173600	-2.26859600	H	-5.83522900	-1.60202600	2.71905700
O	-2.51602900	3.00427700	-1.42212500	H	6.40172000	-3.42878300	-1.96257700	O	-0.66150900	-0.31984500	3.51376800
C	-2.27234400	4.19184100	-1.08985200	H	6.97893300	-2.14095200	-3.02633300	C	0.28035700	0.52411400	3.74396900
O	-1.09902000	4.72184300	-1.10273700	C	6.40530700	-1.53477200	-1.01554400	O	0.91937600	1.17399600	2.87780400
C	-3.42374100	5.08904800	-0.65365400	O	6.25998400	-2.01720100	0.11660000	C	0.60497000	0.71948800	5.22190600
H	-4.23908300	4.93825600	-1.37459700	N	6.66759100	-0.21662100	-1.20319000	H	-0.31035300	1.10171100	5.70002600
H	-3.78929700	4.66607800	0.29550600	H	6.76308600	0.13183800	-2.14901900	H	0.76506200	-0.27848700	5.65628300
C	-3.08463700	6.57062100	-0.48775900	C	6.61258600	0.74408600	-0.09460800	C	1.79170100	1.64307500	5.50753800
H	-2.73188300	7.00522800	-1.43084900	H	7.12945400	0.29053300	0.75728300	H	1.60565700	2.62183700	5.04559600
H	-2.29393700	6.71233100	0.25729900	H	7.17960400	1.63174800	-0.40214400	H	2.68881400	1.24255500	5.01460900
H	-3.97116200	7.13017000	-0.16273700	C	5.17446300	1.11310500	0.31033800	C	2.05045900	1.80969600	7.00928700
O	-0.95105900	-2.21702100	-2.37212400	H	4.64236800	0.20509000	0.61360900	H	1.17732300	2.24022900	7.51979300
C	-2.18422100	-2.13059200	-2.79236700	H	5.22179200	1.76123000	1.19707100	H	2.90469600	2.47432700	7.19421900
O	-2.91032400	-1.13114700	-2.61611200	C	4.40098000	1.81811000	-0.80814600	H	2.26915600	0.84464600	7.48830500
C	-2.68554700	-3.34386100	-3.56217400	H	4.45431000	1.21721200	-1.73115800	O	0.01525900	2.72802700	-3.14240400
H	-1.97915000	-3.51958800	-4.38841000	H	4.83502700	2.79733200	-1.04591100	H	0.65395500	3.81283700	-3.24113900
H	-2.56936700	-4.21342100	-2.89674200	C	2.91028200	2.01471700	-0.54334700	H	-0.93228900	2.95841200	-3.18706700
C	-4.12041300	-3.24061900	-4.08417600	O	2.30351500	1.13574300	0.12482200				
H	-4.21195400	-2.34767900	-4.71817200	O	2.40418700	3.05295800	-1.09839400				

W':

Ca	-2.90970000	0.58179000	-0.24142000	O	-3.46409400	2.57572900	0.86922700	H	-3.60210600	0.79663100	-5.36466900
Mn	0.03923300	-1.26742100	-1.46775200	C	-3.07097200	3.57719500	1.50835000	H	-3.83865800	-0.90696900	-5.00311000
Mn	-1.13650100	-1.96983900	0.90150700	O	-1.91190500	4.12444500	1.38182800	C	-3.17345100	-0.52590300	-7.03056800
Mn	0.24747100	0.34619400	1.58003700	C	-4.02297000	4.23010000	2.50509500	H	-2.54636200	0.18336100	-7.58888500
Mn	-0.22477600	3.38096500	0.78943400	H	-5.00743700	4.28764100	2.02085900	H	-2.78230400	-1.53519500	-7.22123000
O	-1.61739500	-1.45033700	-0.82332500	H	-4.14088100	3.50199700	3.32286300	H	-4.18614200	-0.47634100	-7.45070100
O	0.53398000	-1.27058200	0.40808300	C	-3.58284600	5.58758500	3.05381500	N	2.01625100	-0.98092100	-1.99980800
O	-1.48635400	-0.32392200	1.52311200	H	-3.47820600	6.32748900	2.25064500	C	2.64556800	-0.03849500	-2.78731700
O	-0.28745500	2.01839100	1.92060900	H	-2.61325900	5.51179600	3.55825700	H	2.07075100	0.64650200	-3.39617500
O	-5.11946300	0.57277700	-1.42687000	H	-4.32012100	5.96638100	3.77355300	C	4.00948200	-0.15727500	-2.64031300
H	-5.41889400	-0.24560800	-0.98081600	O	-0.50888400	0.01908400	-2.90873200	N	4.18439000	-1.21674100	-1.75898100
H	-4.79599000	0.30611300	-2.30884000	C	-1.71308200	0.06107300	-3.43183500	H	5.08024100	-1.46629700	-1.32488100
O	-1.11342400	2.14861300	-1.04585400	O	-2.72961000	0.37128500	-2.78772900	C	2.97108900	-1.66860000	-1.38385500
H	-0.61211700	1.63175800	-1.71724000	C	-1.78054500	-0.26826900	-4.91549700	H	2.80304900	-2.44638600	-0.65300600
H	-1.48348100	2.97146600	-1.53797000	H	-1.09282100	0.41934500	-5.43237200	C	5.13796200	0.65116100	-3.23224100
O	-0.00742000	4.94750300	-0.24533700	H	-1.33829600	-1.26858900	-5.04463400	H	5.18102900	0.49311300	-4.31979900
H	0.90097600	4.95957500	-0.59451000	C	-3.17981300	-0.20376200	-5.53215400	H	4.90276100	1.71682600	-3.09748600

C	6.55533500	0.36696000	-2.66909800	O	1.70140300	3.07277900	0.41711500	O	-0.46832700	-2.60508900	2.62633400
H	6.90378600	-0.61938300	-2.99495400	O	0.23978100	-3.28796200	-1.82344500	C	0.26778700	-1.96127700	3.45870100
H	7.24468300	1.11213100	-3.08922400	C	-0.18987300	-4.12366900	-0.95706300	O	0.73499900	-0.80434000	3.29009400
C	6.61894300	0.36330200	-1.14132200	O	-0.67214000	-3.83145600	0.17533300	C	0.55844600	-2.70358200	4.75838800
O	6.59245800	-0.69934700	-0.50391600	C	-0.10785500	-5.59802300	-1.34066700	H	-0.39523600	-2.75748000	5.30776800
N	6.62958200	1.56983300	-0.52156600	H	0.90108700	-5.77335400	-1.73991600	H	0.80582100	-3.74256900	4.49841600
H	6.63007400	2.40809300	-1.08960100	H	-0.78786400	-5.73226500	-2.19611900	C	1.64557900	-2.07286600	5.63279800
C	6.39444800	1.69580200	0.92336600	C	-0.44512100	-6.57879200	-0.21766200	H	1.37036600	-1.03361500	5.85463500
H	7.03663000	0.96688200	1.42853200	H	-0.37550600	-7.61273200	-0.57976200	H	2.58444100	-2.02212700	5.06269300
H	6.72402000	2.69959700	1.21899800	H	0.24281100	-6.46346600	0.62854500	C	1.86767700	-2.85045000	6.93499300
C	4.92537000	1.45076100	1.31373100	H	-1.45896800	-6.40960700	0.16149600	H	0.95034500	-2.88660100	7.53960000
H	4.64897200	0.42866400	1.03419900	O	-4.34559100	-1.20773500	0.50753300	H	2.65103500	-2.38436200	7.54701900
H	4.84314800	1.50533100	2.40802700	C	-4.06610500	-2.29247600	1.07622800	H	2.17263100	-3.88779200	6.73647600
C	3.96382400	2.44790700	0.66496900	O	-2.88417300	-2.71894400	1.34043700	O	-1.85527400	4.43711500	-2.01104300
H	4.15260100	2.51111300	-0.41828500	C	-5.18651400	-3.23525000	1.48341400	H	-1.13539700	4.82920300	-1.40977300
H	4.11204500	3.46529400	1.05354900	H	-6.13075000	-2.69038400	1.57616400	H	-2.68669500	4.66367800	-1.55808200
C	2.47683100	2.12984200	0.79701800	H	-4.94033500	-3.74165500	2.42206000				
O	2.12949700	0.98864400	1.20671900	H	-5.29876600	-4.00685700	0.70889300				

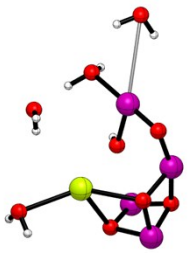
Y:

Ca	-2.39522000	0.22392000	-1.61379200	C	-1.36934300	-4.63239400	-6.34907300	O	-1.48057100	-2.89626500	2.10529600
Mn	0.23482000	-1.94497900	-0.37264100	H	-0.39528700	-4.51507800	-6.84439000	C	-0.78654200	-5.16965000	2.39120000
Mn	-1.67915500	-1.01626500	1.35636700	H	-1.38778200	-5.63011500	-5.88870500	H	0.24116700	-5.48467000	2.62061200
Mn	-0.03027900	1.19484100	1.15177900	H	-2.14359800	-4.60970700	-7.12676100	H	-1.14465700	-5.87596100	1.62637100
Mn	0.17555100	3.41699200	-1.01590800	N	2.29562300	-1.98896600	-0.36598400	C	-1.67648000	-5.21492200	3.63328200
O	-1.54430800	-1.67753400	-0.35086500	C	3.20714300	-1.58937800	-1.32495700	H	-1.69636900	-6.22927400	4.05264600
O	0.18538300	-0.78168600	1.18354400	H	2.88983000	-1.18986000	-2.28013100	H	-1.31058000	-4.52971100	4.40746700
O	-1.76067500	0.67827200	0.72982100	C	4.47923400	-1.71685900	-0.81884800	H	-2.70311400	-4.91709800	3.39311700
O	-0.22442800	2.91310400	0.64052400	N	4.31351700	-2.22278500	0.46608100	O	-4.38314300	-0.63825500	-0.56119000
O	-4.10952500	-0.44845900	-3.30250600	H	5.05131100	-2.22956300	1.17556600	C	-4.53449000	-1.11983200	0.58974600
H	-4.72381400	-0.78528600	-2.61830900	C	2.99117300	-2.35089800	0.70590100	O	-3.60978700	-1.27980200	1.46610700
H	-3.60863100	-1.22540300	-3.62481300	H	2.56337200	-2.68423900	1.64031900	C	-5.91053400	-1.58556300	1.03667100
O	-0.57926400	0.94583300	-3.16356200	C	5.81280800	-1.42883700	-1.45857000	H	-6.12890500	-1.20211700	2.03962100
H	-0.76364900	0.62437600	-4.06253900	H	6.05524700	-2.21356700	-2.19067900	H	-5.91576900	-2.68198500	1.09904200
H	-0.34579100	1.94199800	-3.21223000	H	5.71214200	-0.50296400	-2.04160200	H	-6.67844600	-1.25825100	0.33002200
O	0.36802500	3.34001100	-2.89542000	C	7.02147800	-1.31199200	-0.49322000	O	-1.70969300	-0.46454300	3.25562300
H	1.27958100	3.10556400	-3.15398500	H	7.29758800	-2.29979800	-0.10748200	C	-1.04766200	0.47312000	3.82041600
O	-2.63427000	2.56425600	-1.73041400	H	7.88197200	-0.93186000	-1.06065800	O	-0.25823500	1.26854200	3.23833600
C	-2.57640100	3.79815600	-1.53772700	C	6.73203800	-0.43798700	0.72440800	C	-1.23280500	0.60466500	5.32687300
O	-1.48815200	4.42391100	-1.24851900	O	6.39816200	-0.93769200	1.80691000	H	-0.66005800	-0.21339400	5.79319800
C	-3.84651300	4.63120300	-1.65406500	N	6.78883000	0.90625500	0.53513200	H	-0.77044500	1.54707500	5.64431000
H	-4.26302700	4.42521400	-2.65070600	H	7.04057700	1.25433000	-0.38177000	C	-2.69874300	0.52072300	5.78032800
H	-4.56479400	4.19918400	-0.94195800	C	6.26529200	1.85209400	1.52692300	H	-3.12763400	-0.42053200	5.41447400
C	-3.68385900	6.13408000	-1.42641000	H	6.65927700	1.55963100	2.50607600	H	-3.27056700	1.32982700	5.30145000
H	-2.97646400	6.56903600	-2.14258800	H	6.67266500	2.84063600	1.28050100	C	-2.84466800	0.61680800	7.30258900
H	-3.31133000	6.34373900	-0.41628300	C	4.72761200	1.87641400	1.57965100	H	-2.30912400	-0.20094200	7.80565900
H	-4.64782300	6.64519500	-1.54445700	H	4.36898800	0.88304000	1.86910400	H	-3.89884300	0.55957100	7.60408200
O	0.25324900	-2.45232300	-2.25361000	H	4.41783800	2.56365700	2.37914500	H	-2.43895800	1.56357200	7.68633800
C	-0.68834000	-2.45497700	-3.14385600	C	4.08593800	2.29429000	0.25415100	O	2.30847000	0.92627000	-3.21240200
O	-1.64122400	-1.64699200	-3.18907800	H	4.49803200	1.69849600	-0.57560000	H	2.41193100	1.43916700	-2.38831800
C	-0.53644600	-3.54179600	-4.20401200	H	4.30050200	3.34336700	0.00594500	H	1.35270700	0.70348300	-3.20245600
H	0.47267200	-3.44078100	-4.63197400	C	2.57621300	2.11177300	0.18035700	O	0.73143700	5.43724400	-0.00654500
H	-0.52813300	-4.50694500	-3.67444200	O	1.99279500	1.44432400	1.06855200	H	-0.09418600	5.87374000	-0.29577400
C	-1.59899400	-3.53349300	-5.30545100	O	2.01212600	2.63433500	-0.85709800	H	0.48586700	5.01409800	0.84356000
H	-1.60750800	-2.54922900	-5.79505700	O	0.16340400	-3.69561900	0.77276400				
H	-2.59238300	-3.65591400	-4.85055600	C	-0.69521200	-3.80872900	1.70614900				

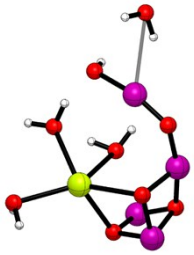
TS5*:

Ca	-2.39672200	-0.14397900	-1.62603400	C	-1.10562100	-5.45528400	-5.71456000	O	-1.27328900	-2.64495000	2.48161300
Mn	0.40622200	-1.96587800	-0.12228800	H	-0.14038400	-5.35581100	-6.23068500	C	-0.48913600	-4.82982600	3.06879100
Mn	-1.55935700	-0.91052800	1.47254200	H	-1.08304300	-6.39852200	-5.15112100	H	0.55041500	-5.07180600	3.33075400
Mn	-0.03701100	1.33542600	0.94809700	H	-1.88616700	-5.54349900	-6.48128900	H	-0.82228800	-5.64651700	2.40992000
Mn	-0.14865900	3.31607600	-1.43143800	N	2.45982400	-1.91696000	-0.04522200	C	-1.37350700	-4.73920600	4.31245900
O	-1.39014000	-1.78559200	-0.12750600	C	3.39738000	-1.80924700	-1.05165200	H	-1.35410900	-5.68726800	4.86577200
O	0.28898700	-0.59783400	1.25464400	H	3.08976300	-1.76072100	-2.08624200	H	-1.03174700	-3.94223800	4.98397100
O	-1.73782000	0.67288800	0.61479000	C	4.64866700	-1.70104700	-0.49334200	H	-2.41127500	-4.51465800	4.04225000
O	-0.37039000	2.98429000	0.29438000	N	4.44264500	-1.76813700	0.88199800	O	-4.30330500	-1.01251300	-0.44491600
O	-4.01508400	-1.22607600	-3.19032200	H	5.14739000	-1.52302300	1.58182000	C	-4.41157700	-1.31243200	0.77115100
H	-4.59883200	-1.52609400	-2.46392100	C	3.11651400	-1.87565700	1.10829800	O	-3.47463100	-1.25666400	1.64630500
H	-3.41719000	-1.97651500	-3.38942100	H	2.65689200	-1.89181500	2.08599700	C	-5.74522200	-1.80666700	1.30759600
O	-0.90715200	0.62360600	-3.46500900	C	5.99683500	-1.54661000	-1.14818800	H	-5.97628300	-1.31133400	2.25705900
H	-1.10127800	0.27686500	-4.35149000	H	6.31114800	-2.49977400	-1.59932500	H	-5.67183500	-2.88357800	1.51082100
H	-0.67675200	1.61730500	-3.54697500	H	5.88453900	-0.84564500	-1.98723700	H	-6.54397000	-1.62953800	0.58166600
O	-0.05225900	3.07449100	-3.31321400	C	7.15061500	-1.07351000	-0.22672300	O	-1.61077500	-0.09185200	3.28062100
H	0.88178700	3.02110000	-3.58362400	H	7.45566100	-1.88246900	0.44641900	C	-0.97052100	0.92903000	3.70668200
O	-2.86259600	2.15495600	-1.90953400	H	8.01801100	-0.82915400	-0.85534900	O	-0.21160700	1.66391700	3.01289700
C	-2.93550700	3.39828400	-1.80469600	C	6.77296300	0.10505600	0.66881900	C	-1.14089200	1.25440500	5.18553800
O	-1.90762900	4.15578300	-1.63082900	O	6.45774100	-0.06670500	1.85362700	H	-0.53680200	0.52329100	5.74707900
C	-4.29596500	4.07791800	-1.88744600	N	6.73941400	1.33075500	0.08413800	H	-0.70525800	2.24420900	5.36789700
H	-4.76811700	3.72109200	-2.81395200	H	6.98845800	1.40998500	-0.89392400	C	-2.59781700	1.18723200	5.66960700
H	-4.89938500	3.65624000	-1.06997600	C	6.19679700	2.50627500	0.77389000	H	-3.00050800	0.19329000	5.43799200
C	-4.28437600	5.60543200	-1.82687400	H	6.64579500	2.54378000	1.77262500	H	-3.20087700	1.90801700	5.09710500
H	-3.69106600	6.03039700	-2.64553600	H	6.53399400	3.39095900	0.21924600	C	-2.72915900	1.47977400	7.16793000
H	-3.85575600	5.96063300	-0.88200200	C	4.66460000	2.48369500	0.90734200	H	-2.16174200	0.75261700	7.76618400
H	-5.30583900	5.99901600	-1.90513800	H	4.37212600	1.60930400	1.49737100	H	-3.77739000	1.43096900	7.49097800
O	0.44463500	-2.82182300	-1.86690300	H	4.35950300	3.36836600	1.48432700	H	-2.34975800	2.48095800	7.41688000
C	-0.47804600	-2.92344000	-2.76777000	C	3.93620400	2.46570800	-0.44014500	O	1.78541500	0.11985700	-2.85762800
O	-1.43612500	-2.13279700	-2.91608300	H	4.30226000	1.62634500	-1.05355700	H	1.88559300	1.01639300	-2.48964700
C	-0.29767600	-4.11407500	-3.70598200	H	4.12001000	3.37987200	-1.01971800	H	0.84062400	0.09784000	-3.12531000
H	0.70298100	-4.02215600	-4.15574000	C	2.42937000	2.26944400	-0.34242600	O	0.30891900	5.47775500	-0.72175400
H	-0.24901900	-5.01617800	-3.07745100	O	1.95768400	1.67374100	0.65735700	H	-0.57775600	5.80446900	-0.97310300
C	-1.36758100	-4.26087100	-4.79020700	O	1.75061300	2.68487300	-1.35941400	H	0.18591400	5.14996900	0.19430900
H	-1.41613300	-3.33483400	-5.38043500	O	0.39939200	-3.55159600	1.26045800				
H	-2.35291500	-4.37155200	-4.31439100	C	-0.45112900	-3.57238500	2.20372800				

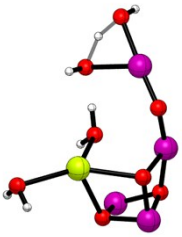
3D images for TSs:



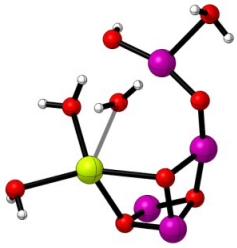
TS1*



TS4

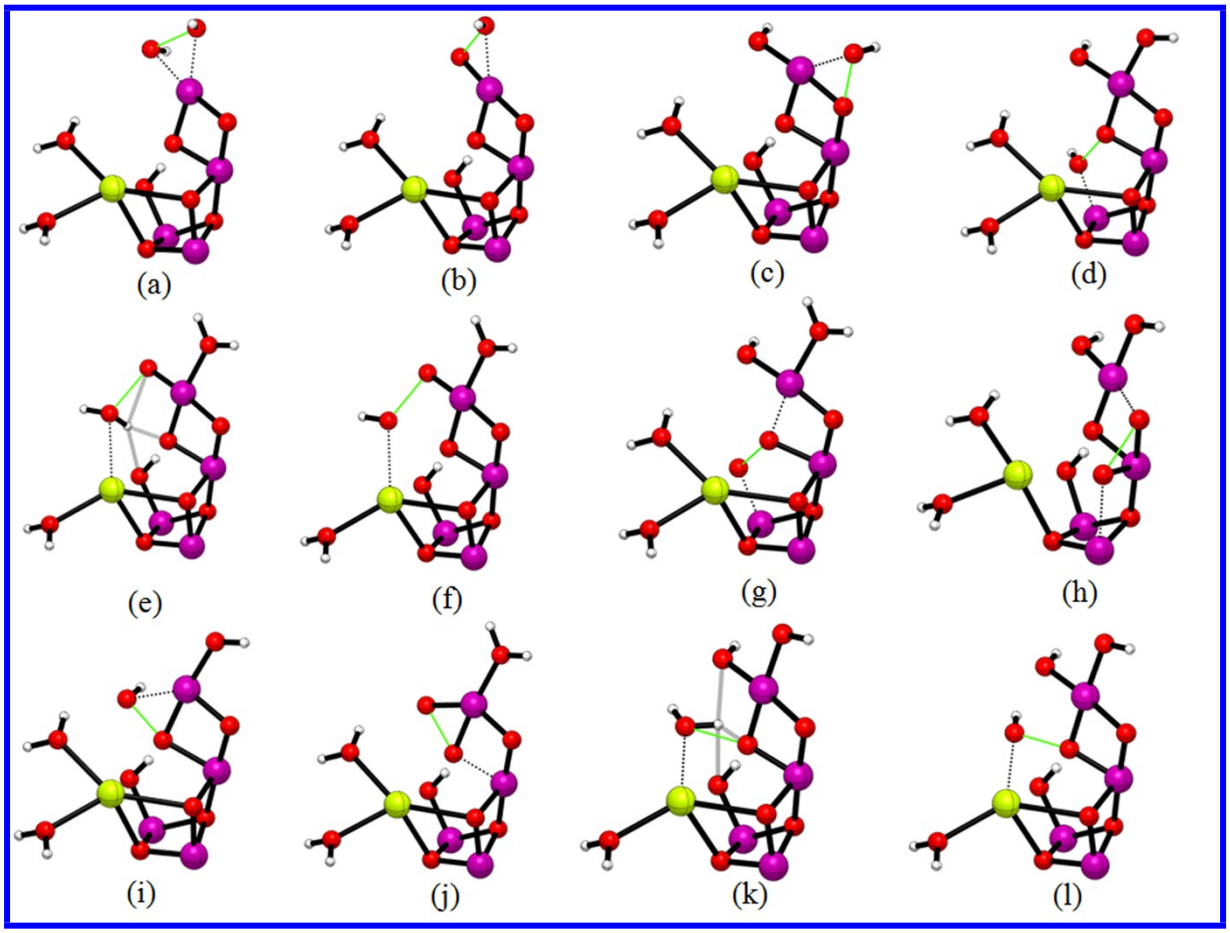


TS3



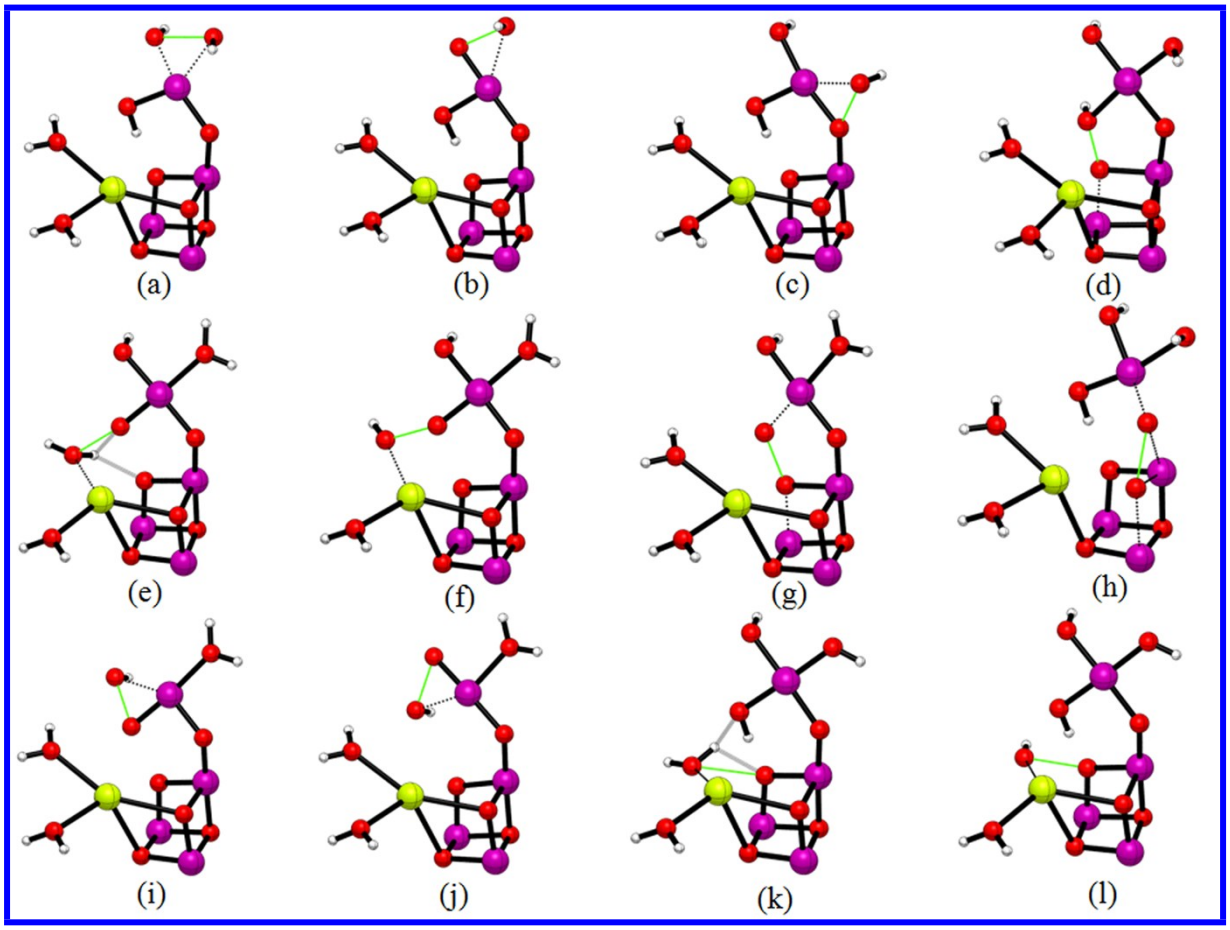
TS5*:

VII. Implications for O-O bond formation



Scheme S8. (a) W1 (hydroxyl)-W2 (hydroxyl) coupling; (b) W1 (hydroxyl) nucleophilic attack W2 (Mn4-oxo); (c) W1 (hydroxyl) nucleophilic attack O4; (d) Wx (hydroxyl) nucleophilic attack O5; (e) W3 (water) nucleophilic attack W2 (Mn4-oxo); (f) W3 (hydroxyl) nucleophilic attack W2

(Mn4-oxo); (g) oxo-oxyl coupling; (h) O2-O4 coupling; (i) W2 (hydroxyl) nucleophilic attack O5; (j) W2 (Mn4-oxo)-O5 coupling; (k) W3 (water) nucleophilic attack O5; (l) W3 (hydroxyl) nucleophilic attack O5.



Scheme S9. (a) W1 (hydroxyl)-W2 (hydroxyl) coupling; (b) W1 (hydroxyl) nucleophilic attack W2 (Mn4-oxo); (c) W1 (hydroxyl) nucleophilic attack O4; (d) Wx(hydroxyl) nucleophilic attack O5; (e) W3 (water) nucleophilic attack Wx (Mn4-oxo); (f) W3 (hydroxyl) nucleophilic attack Wx (Mn4-oxo); (g) oxo-oxyl coupling; (h) O2-O4 coupling; (i) W2 (hydroxyl) nucleophilic attack Wx (Mn4-oxo); (j) Wx (hydroxyl) nucleophilic attack W2 (Mn4-oxo); (k) W3 (water) nucleophilic attack O5; (l) W3 (hydroxyl) nucleophilic attack O5.

Notes and references

1 Ames, W.; Pantazis, D. A.; Krewald, V.; Cox, N.; Messinger, J.; Lubitz, W.; Neese, F. *J. Am. Chem. Soc.* **2011,** 133, 19743-19757.

2 Krewald, V.; Neese, F.; Pantazis, D. A. *Isr. J. Chem.* **2015,** 55, 1-15.

3 Kolling, D. R. J.; Cox, N.; Ananyev, G. M.; Pace, R. J.; Dismukes, G. C. *Biophys. J.* **2012,** 103, 313-322.

4 Rivalta, I.; Amin, M.; Luber, S.; Vassiliev, S.; Pokhrel, R.; Umena, Y.; Kawakami, K.; Shen, J.-R.; Kamiya, N.; Bruce, D.; Brudvig, G. W.; Gunner, M. R.; Batista, V. S. *Biochemistry* **2011,** 50, 6312-6315.

5 Retegan, M.; Krewald, V.; Mamedov, F.; Neese, F.; Lubitz, W.; Cox, N.; Pantazis, D. A. *Chem. Sci.* **2015,** 7, 72-84.

6 Siegbahn, P. E. M. *ChemPhysChem* **2011,** 12, 3274-3280.

7 Umena, Y.; Kawakami, K.; Shen, J.-R.; Kamiya, N. *Nature* **2011,** 473, 55-60.

8 Suga, M.; Akita, F.; Hirata, K.; Ueno, G.; Murakami, H.; Nakajima, Y.; Shimizu, T.; Yamashita, K.; Yamamoto, M.; Ago, H.; Shen, J.-R. *Nature* **2015,** 517, 99-103.

9 Retegan, M.; Neese, F.; Pantazis, D. A. *J. Chem. Theory Comput.* **2013,** 9, 3832-3842.

10 Bacskay, G. B. *Chem. Phys.* **1981,** 61, 285-404.

11 Klein, J. H.; Schmidt, D.; Steiner, U. E.; Lambert, C. *J. Am. Chem. Soc.* **2015,** 137, 11011-11021.

12 Marian, C. M. *WIREs. Comput. Mol. Sci.* **2012,** 2, 187-203.

13 Harvey, J. N. *WIREs Comput. Mol. Sci.* **2014,** 4, 1-14.

14 Harvey, J. N.; Aschi, M.; Schwarz, H.; Koch, W. *Theor. Chem. Acc.* **1998,** 99, 95-99.

15 Poli, R.; Harvey, J. N. *Chem. Soc. Rev.* **2003,** 32, 1-8.

16 Harvey, J. N. *Phys. Chem. Chem. Phys.* **2007,** 9, 331-343.

17 CYLview 1.0b; Legault, C. Y., Université de Sherbrooke, 2009.

18 Askerka, M.; Vinyard, D. J.; Brudvig, G. W.; Batista, V. S. *Biochemistry* **2015,** 54, 5783-5786.

19 Askerka, M.; Wang, J.; Vinyard, D. J.; Brudvig, G. W.; Batista, V. S. *Biochemistry* **2016,** 18, 181-185.

20 Boussac, A.; Sugiura, M.; Inoue, Y.; Rutherford, A. W. *Biochemistry* **2000,** 39, 13788-13799.

21 Retegan, M.; Pantazis, D. A. *Chem. Sci.* **2016,** 7, 6463-6476.

22 Siegbahn, P. E. M. *Chem. Eur. J.* **2006,** 12, 9217-9227.

23 Siegbahn, P. E. M. *Acc. Chem. Res.* **2009,** 42, 1871-1880.

24 Schweitzer, C.; Schmidt, R. *Chem. Rev.* **2003,** 103, 1685-1758.

25 Krewald, V.; Retegan, M.; Neese, F.; Lubitz, W.; Pantazis, D. A.; Cox, N. *Inorg. Chem.* **2016,** 55, 488-501.

26 Pal, R.; A., C. F.; Negre, L. V.; Pokhrel, R.; Ertem, M. Z.; Brudvig, G. W.; Batista, V. S. *Biochemistry* **2013,** 52, 7703-7706.