

Electronic Supplementary Information for

The elusive reaction mechanism of Mn(II)-mediated benzylic oxidations of
alkylarene by H₂O₂: A *gem*-diol one or a dual hydrogen abstraction one?

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Part I Conversion of the Mn^{III}-OOH species **1** to a Mn^{III}-peracetate species **3** via a Mn^{IV}(O)(AcO[•]) species **2**.

Table S1. Various SCF and Gibbs free energies of the conversion of the Mn^{III}-OOH species **1** to a cyclic Mn^{III}-peracetate complex **3** via the high-valent metal-oxo species **2**. Calculations were done at the UB3LYP-D3(BJ)/B2//B1 level in solvent.

	OPT/B1+ZPE	ΔE	SPE/B2+ZPE	ΔE	G	ΔG
1	-2763.302959 ^a	37.1	-2763.691505	36.3	-2763.371872	38.2
3 1	-2763.342761	12.1	-2763.730944	11.5	-2763.413376	12.2
5 1	-2763.362020	0.0	-2763.749324	0.0	-2763.432784	0.0
3 TS 12	-2763.332883	18.3	-2763.720383	18.2	-2763.401743	19.5
5 TS 12	-2763.321193	25.6	-2763.708047	25.9	-2763.392229	25.4
1 2	-2763.330826	19.6	-2763.723238	16.4	-2763.401502	19.6
3 2	-2763.357951	2.6	-2763.746994	1.5	-2763.429288	2.2
5 2	-2763.333140	18.1	-2763.720721	17.9	-2763.403385	18.4
3 TS 23	-2763.337702	15.3	-2763.726768	14.2	-2763.408919	15.0
5 TS 23	-2763.325909	22.7	-2763.713561	22.4	-2763.395741	23.2
1 3	-2763.297441	40.5	-2763.686947	39.1	-2763.366835	41.4
3 3	-2763.343361	11.7	-2763.733197	10.1	-2763.413418	12.2
5 3	-2763.356164	3.7	-2763.744896	2.8	-2763.428282	2.8

a. Absolute energies are in au units and the relative ones are in kcal mol⁻¹ units

Mn-O1 = 1.862/1.877
Mn-O2 = 2.136/2.229
O1-O3 = 1.447/1.438
O3-H1 = 1.639/1.689

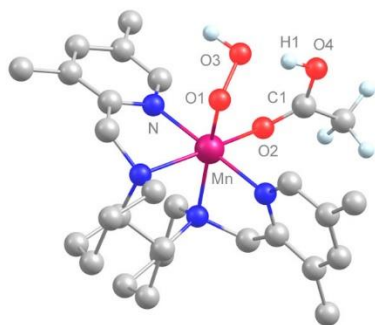
$\overline{\text{Mn-N}} = 2.125/2.131$
 $\angle \text{Mn-O1-O3} = 114.9/113.5$

O1-O3 = 1.745/1.796
O3-H1 = 1.418/1.509
O4-H1 = 1.064/1.037
Mn-O1 = 1.716/1.755
Mn-O2 = 2.003/2.075

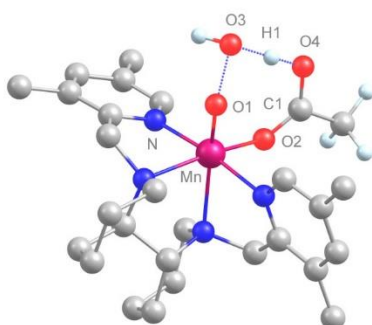
$\overline{\text{Mn-N}} = 2.149/2.132$
 $\angle \text{Mn-O1-O3} = 119.9/142.5$
 $\angle \text{O3-H1-O4} = 176.8/170.6$
 $\nu_{\text{img}} = i 715.5/807.4$

O3-H1 = 0.971/0.997
O1-O4 = 2.247/3.329
Mn-O1 = 1.685/1.797
Mn-O2 = 1.887/1.872

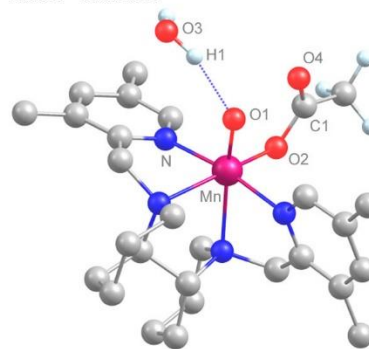
$\overline{\text{Mn-N}} = 2.169/2.157$
 $\text{H1-O1/O4} = 1.910/1.642$
 $\angle \text{O1-Mn-O2-O4} = 4.4/10.8$



3/51



3/5TS₁₂



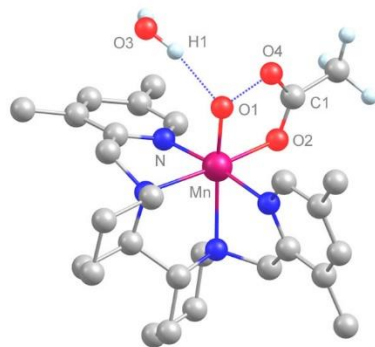
3/52

O1-O4 = 1.659/2.589
Mn-O1 = 1.774/1.810
Mn-O2 = 2.034/1.867
H1-O1/O4 = 1.914/1.733

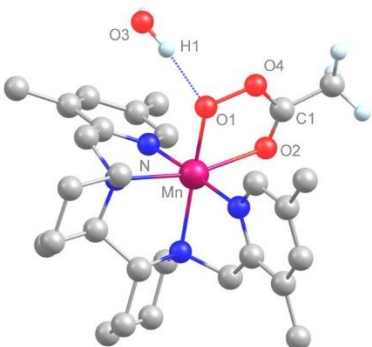
$\overline{\text{Mn-N}} = 2.159/2.162$
 $\angle \text{O1-Mn-O2-O4} = 2.4/-3.7$
 $\nu_{\text{img}} = i 574.3/29.0$

O1-O4 = 1.489/1.443
O1-H1 = 1.878/1.878
Mn-O1 = 1.876/1.932
Mn-O2 = 1.981/2.260

$\overline{\text{Mn-N}} = 2.049/2.111$



3/5TS₂₃



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Figure S1. Optimized structures of the conversion of the Mn^{III}-OOH species **1** to a cyclic Mn^{III}-peracetate complex **3** via the high-valent metal-oxo species **2**. Calculations were done at the UB3LYP-D3(BJ)/B1 level in solvent. Hydrogen atoms of *rac*-L are omitted for clarity. Lengths are in Å units, angles are in degree units and imaginary frequencies are in cm⁻¹ units.

Table S2. Mulliken charges and spin densities of the conversion of the Mn^{III}-OOH species **1** to a cyclic Mn^{III}-peracetate complex **3** *via* the high-valent metal-oxo species **2**. Calculations were done at the UB3LYP-D3(BJ)/B1 level in solvent.

	Mulliken charge						spin densities					
	Mn	O1	<i>rac</i> -L	OH	H	OAc	Mn	O1	<i>rac</i> -L	OH	H	OAc
³1	0.65	-0.32	1.48	0.01	0.37	-0.19	2.14	0.02	-0.16	0.02	0.00	-0.01
⁵1	0.78	-0.32	1.40	0.02	0.37	-0.24	4.04	-0.05	-0.03	0.01	0.00	0.03
³TS₁₂	0.58	-0.30	1.64	-0.12	0.34	-0.14	2.41	0.07	-0.18	-0.31	0.00	-0.01
⁵TS₁₂	0.63	-0.43	1.69	-0.08	0.35	-0.17	3.41	0.28	-0.21	0.52	-0.01	0.00
³2	0.52	-0.32	1.87	-0.35	0.33	-0.05	3.00	-0.41	-0.29	0.01	0.00	-0.30
⁵2	0.55	-0.30	1.85	-0.14	0.35	-0.31	3.08	0.86	-0.27	0.30	-0.01	0.04
³TS₂₃	0.57	-0.33	1.63	-0.34	0.34	0.13	2.29	0.03	-0.18	0.00	0.00	-0.13
⁵TS₂₃	0.53	-0.26	1.87	-0.22	0.36	-0.27	3.09	0.96	-0.26	0.19	-0.01	0.03
³3	0.48	-0.36	1.69	-0.36	0.35	0.21	2.13	0.02	-0.14	0.00	0.00	-0.02
⁵3	0.76	-0.40	1.54	-0.36	0.35	0.11	4.01	0.00	-0.07	0.00	0.00	0.06

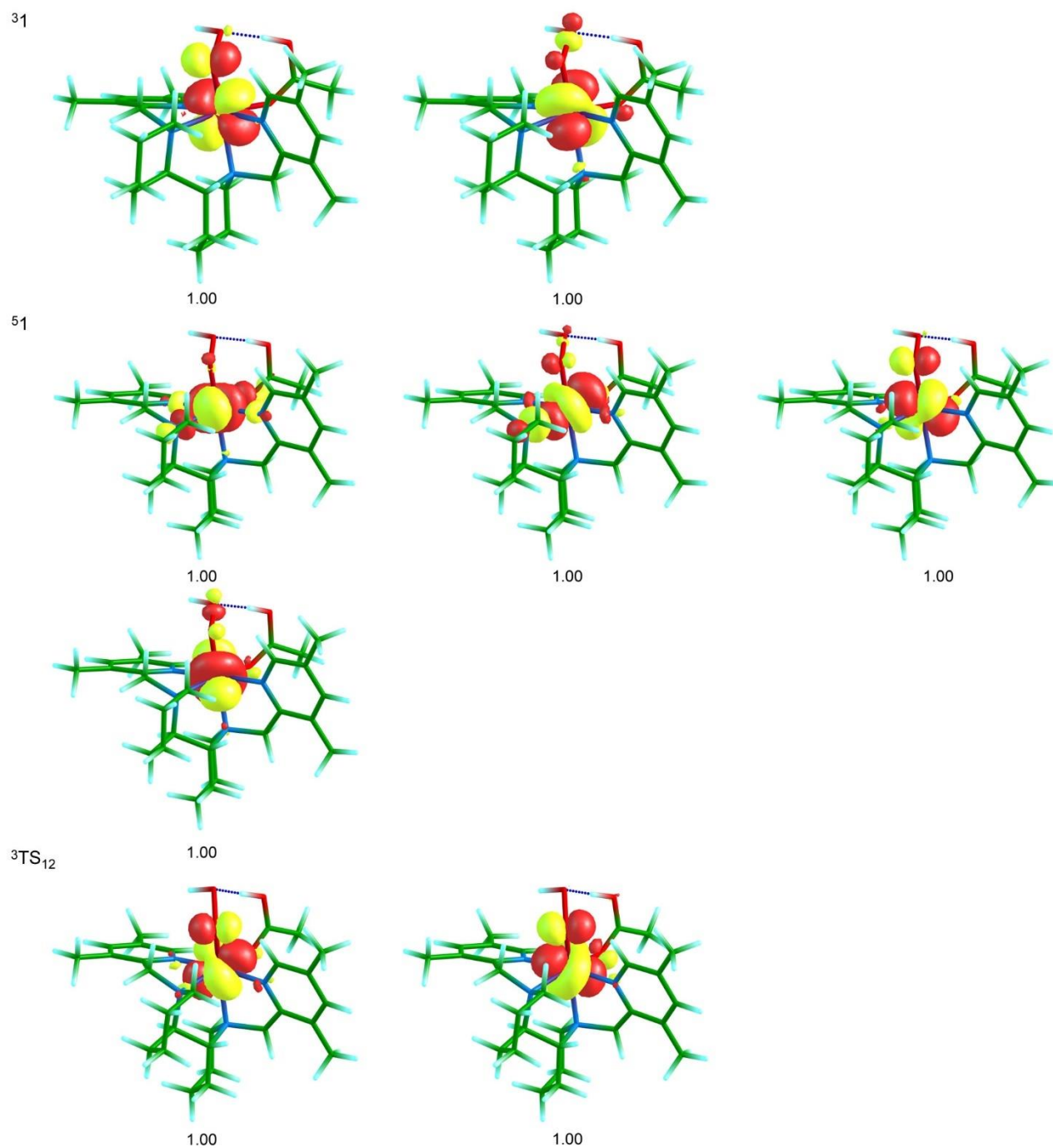
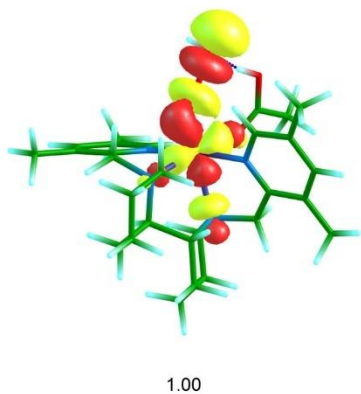
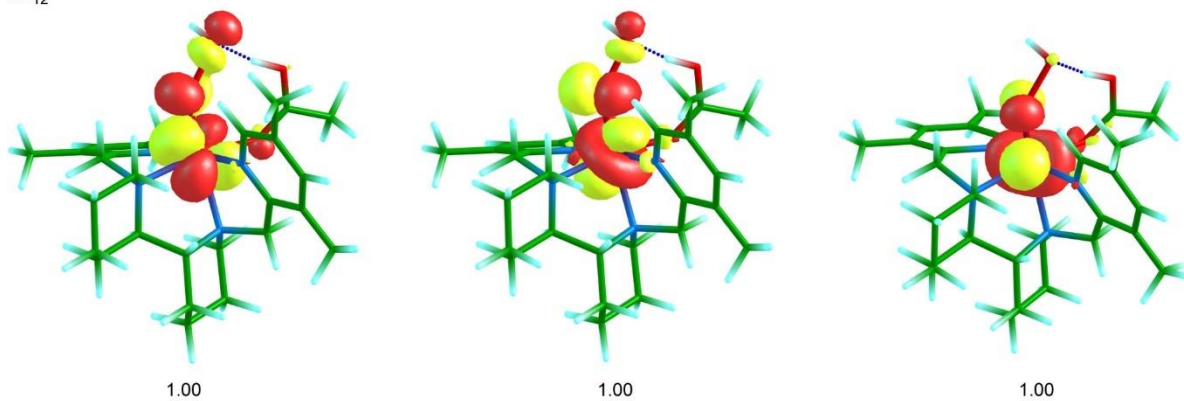


Figure S2. Singly-occupied natural orbitals (SNOs) of the conversion of the $\text{Mn}^{\text{III}}\text{-OOH}$ species **1** to a cyclic Mn^{III} -peracetate complex **3** *via* the high-valent metal-oxo species **2**. Calculations were done at the UB3LYP-D3(BJ)/B1 level in solvent. Positive values represent alpha-electron occupations and netative ones represent beta occupations. (To be continued)

$^5\text{TS}_{12}$



$^3\text{2}$

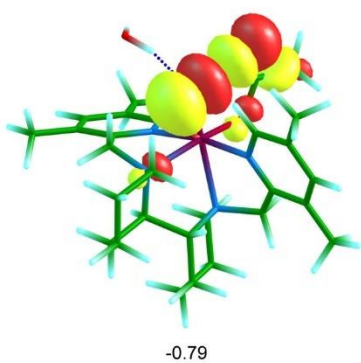
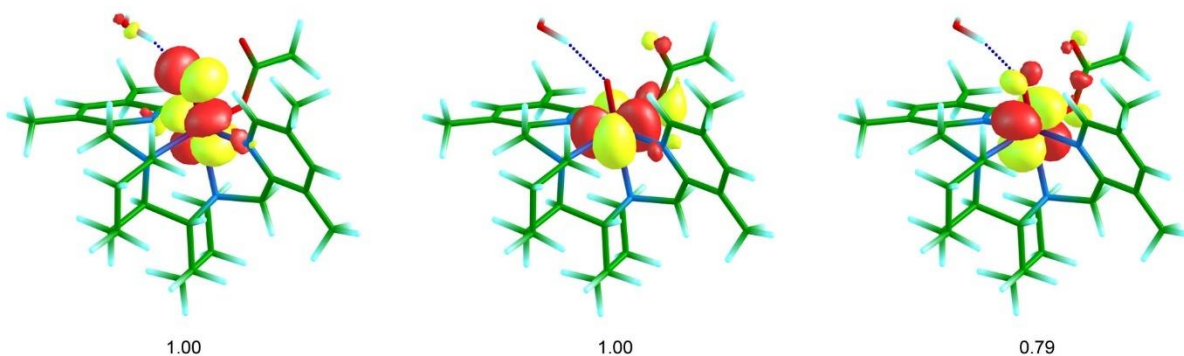


Figure S2. Singly-occupied natural orbitals (SNOs) of the conversion of the $\text{Mn}^{\text{III}}\text{-OOH}$ species **1** to a cyclic Mn^{III} -peracetate complex **3** *via* the high-valent metal-oxo species **2**. Calculations were done at the UB3LYP-D3(BJ)/B1 level in solvent. Positive values represent alpha-electron occupations and netative ones represent beta occupations. (To be continued)

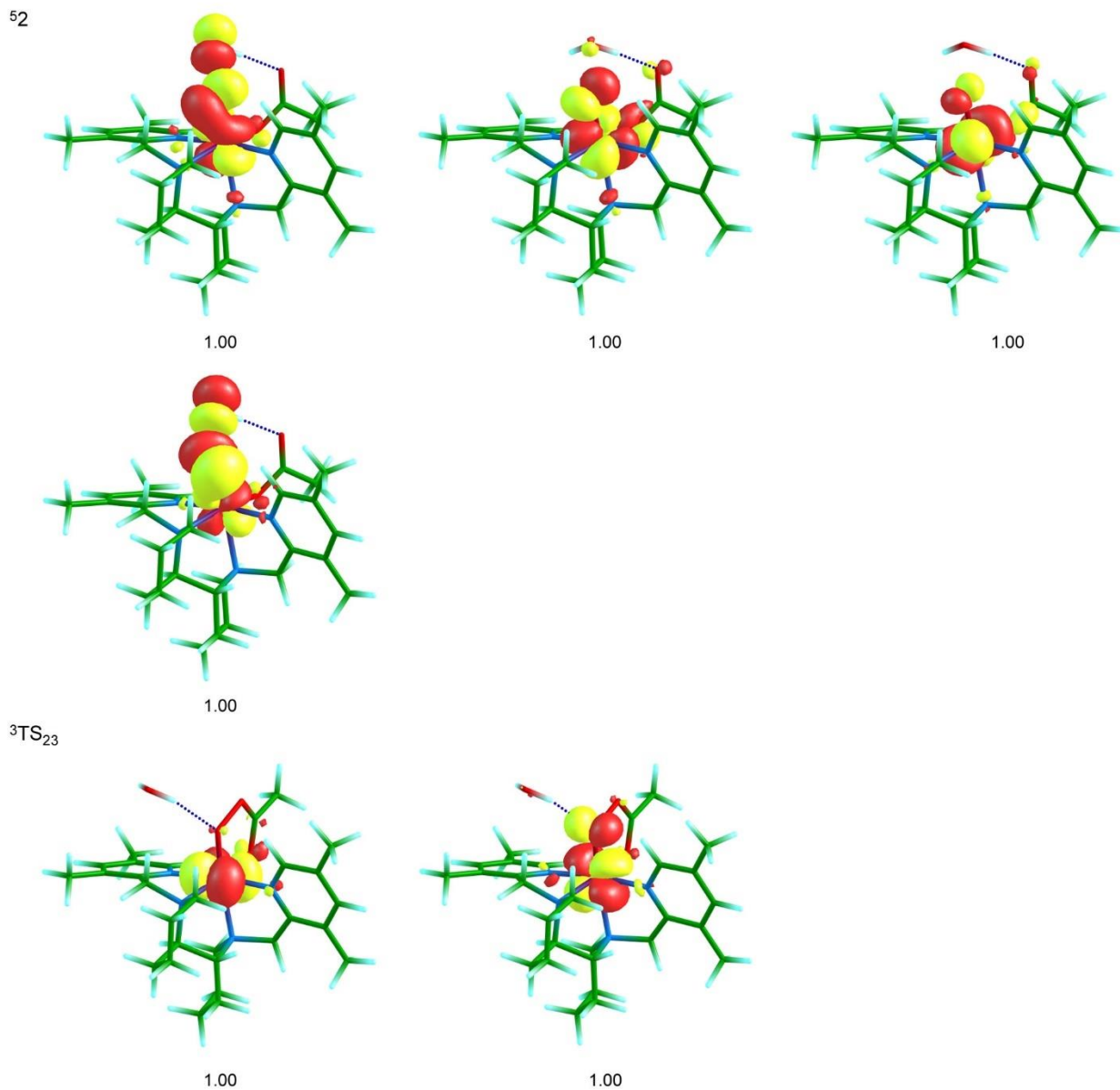
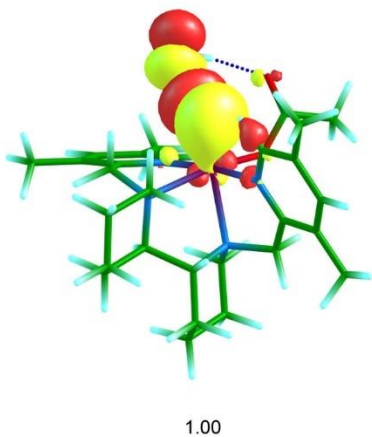
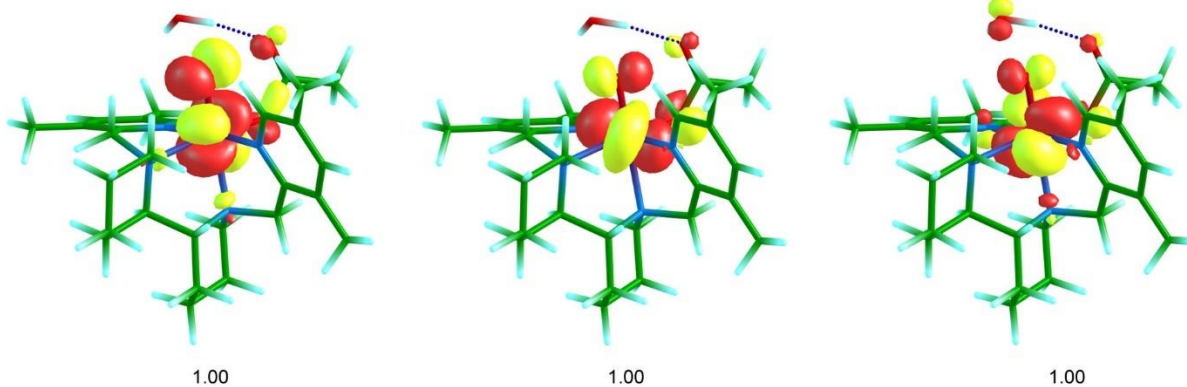


Figure S2. Singly-occupied natural orbitals (SNOs) of the conversion of the $\text{Mn}^{\text{III}}\text{-OOH}$ species **1** to a cyclic Mn^{III} -peracetate complex **3** *via* the high-valent metal-oxo species **2**. Calculations were done at the UB3LYP-D3(BJ)/B1 level in solvent. Positive values represent alpha-electron occupations. (To be continued)

$^5\text{TS}_{23}$



33

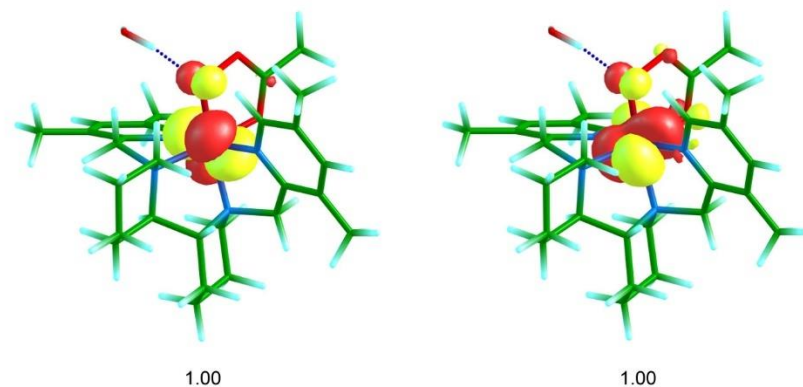


Figure S2. Singly-occupied natural orbitals (SNOs) of the conversion of the $\text{Mn}^{\text{III}}\text{-OOH}$ species **1** to a cyclic Mn^{III} -peracetate complex **3** via the high-valent metal-oxo species **2**. Calculations were done at the UB3LYP-D3(BJ)/B1 level in solvent. Positive values represent alpha-electron occupations. (To be continued)

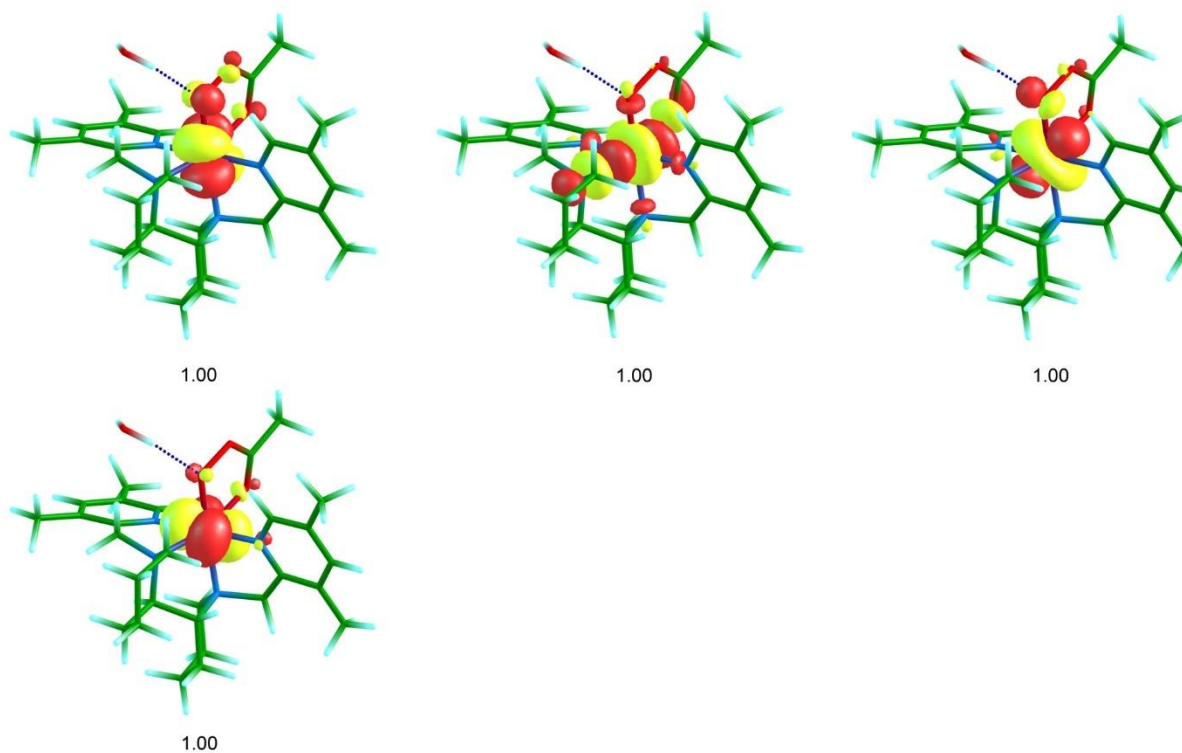


Figure S2. Singly-occupied natural orbitals (SNOs) of the conversion of the Mn^{III} -OOH species **1** to a cyclic Mn^{III} -peracetate complex **3** via the high-valent metal-oxo species **2**. Calculations were done at the UB3LYP-D3(BJ)/B1 level in solvent. Positive values represent alpha-electron occupations.

Part II Hydroxylation of PBA to 4-OH-PBA by the proximal and distal oxygen of the $\text{Mn}^{\text{III}}(\text{OOH})$ species 1.

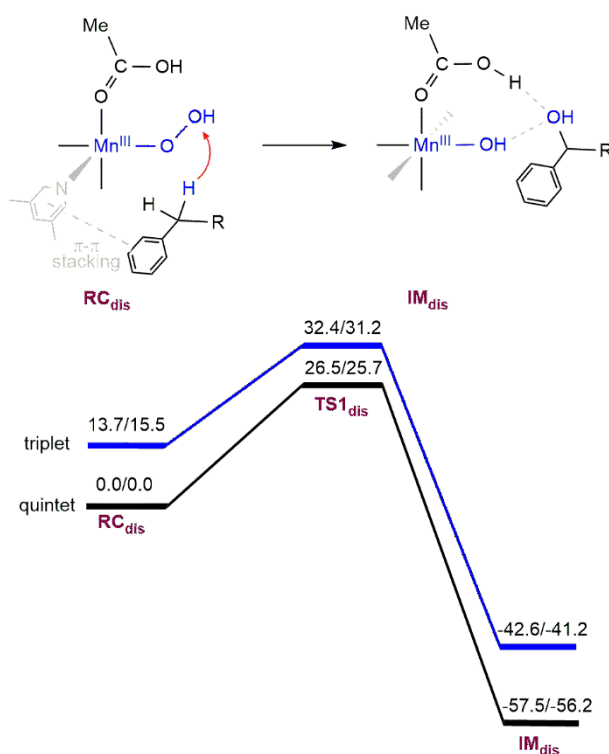


Figure S3. The energy profile (in kcal mol⁻¹) for the hydroxylation of PBA by the distal oxygen of the $\text{Mn}^{\text{III}}\text{-OOH}$ species **1**. Values before slashes are the SCF energies calculated at the UB3LYP-D3(BJ)/B2//B1 level including ZPE/B1 corrections and those after slashes are Gibbs free energies calculated at the UB3LYP-D3(BJ)/B1 level, respectively.

Table S3. Various SCF and Gibbs free energies of the hydroxylation of PBA by the distal oxygen of the Mn^{III}-OOH species **1**. Calculations were done at the UB3LYP-D3(BJ)/B2//B1 level in solvent.

	OPT/B1+ZPE	ΔE	SPE/B2+ZPE	ΔE	G	ΔG
³RC	-3302.046030	14.1	-3302.575136	13.7	-3302.134250	15.5
⁵RC	-3302.068435	0.0	-3302.596908	0.0	-3302.158912	0.0
³TS_{dis}	-3302.019226	30.9	-3302.545253	32.4	-3302.109117	31.2
⁵TS_{dis}	-3302.028792	24.9	-3302.554681	26.5	-3302.117936	25.7
³IM_{dis}	-3302.136347	-42.6	-3302.664814	-42.6	-3302.224546	-41.2
⁵IM_{dis}	-3302.160572	-57.8	-3302.688477	-57.5	-3302.248510	-56.2

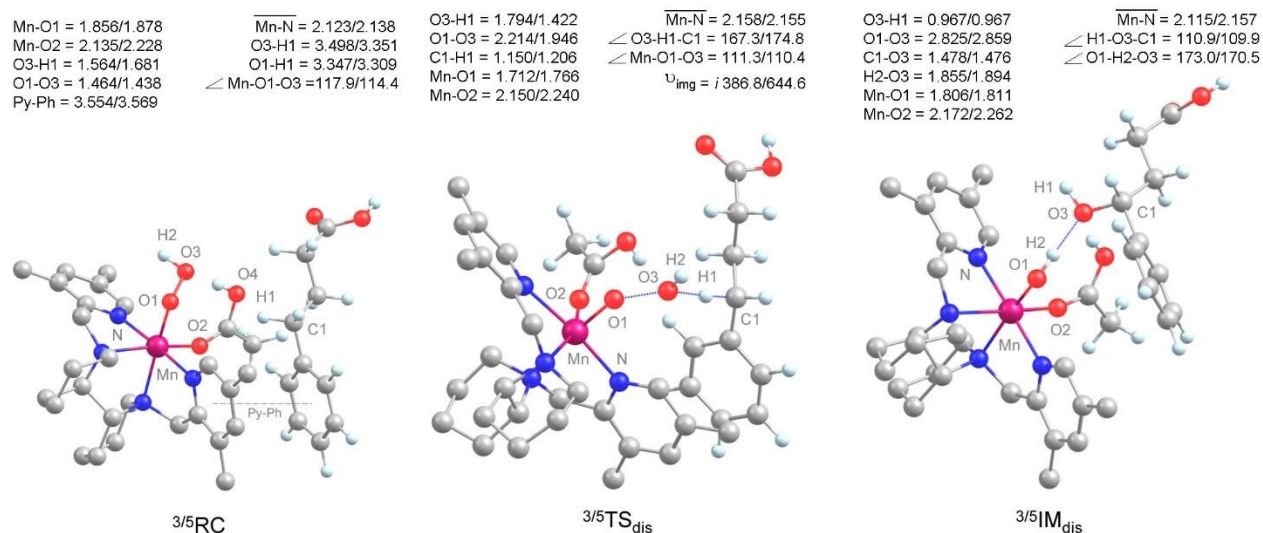
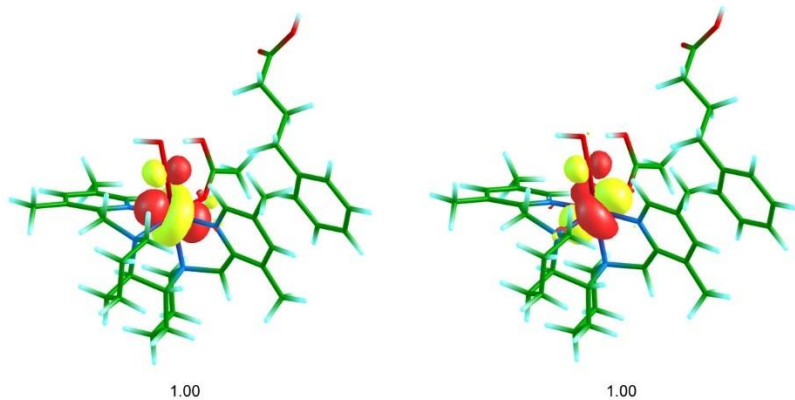


Figure S4. Optimized structures of key intermediates of the hydroxylation of PBA by the distal oxygen of the Mn^{III} -OOH species **1**. Calculations were done at the UB3LYP-D3(BJ)/B1 level in solvent. Hydrogen atoms of *rac*-L are omitted for clarity. Lengths are in Å units, angles are in degree units and imaginary frequency is in cm^{-1} units.

Table S4. Mulliken charges and spin densities of key intermediates of the hydroxylation of PBA by the distal oxygen of the Mn^{III}-OOH species **1**. Calculations were done at the UB3LYP-D3(BJ)/B1 level in solvent.

	Mulliken charge								spin densities							
	Mn	O1	<i>rac</i> -L	OH	H1	OAc	H2	Sub-H2	Mn	O1	<i>rac</i> -L	OH	H1	OAc	H2	Sub-H2
³RC	0.64	-0.33	1.49	0.00	0.36	-0.19	0.12	-0.09	2.14	0.03	-0.15	-0.01	0.00	-0.01	0.00	0.00
⁵RC	0.79	-0.32	1.36	0.02	0.36	-0.24	0.12	-0.09	4.05	-0.05	-0.04	0.01	0.00	0.03	0.00	0.00
³TS_{dis}	0.75	-0.29	1.38	-0.21	0.35	-0.26	0.19	0.09	3.75	-0.82	-0.06	-0.61	0.01	0.03	0.00	-0.29
⁵TS_{dis}	0.79	-0.38	1.28	-0.18	0.36	-0.26	0.21	0.17	3.89	-0.55	-0.02	0.25	0.00	0.03	0.01	0.39
³IM_{dis}	0.67	-0.65	1.39	-0.22	0.39	-0.25	0.37	0.30	2.05	0.10	-0.15	0.01	0.00	-0.01	0.00	0.00
⁵IM_{dis}	0.80	-0.65	1.28	-0.21	0.37	-0.27	0.37	0.30	3.97	0.03	-0.02	0.01	0.00	0.02	0.00	0.00

3RC



5RC

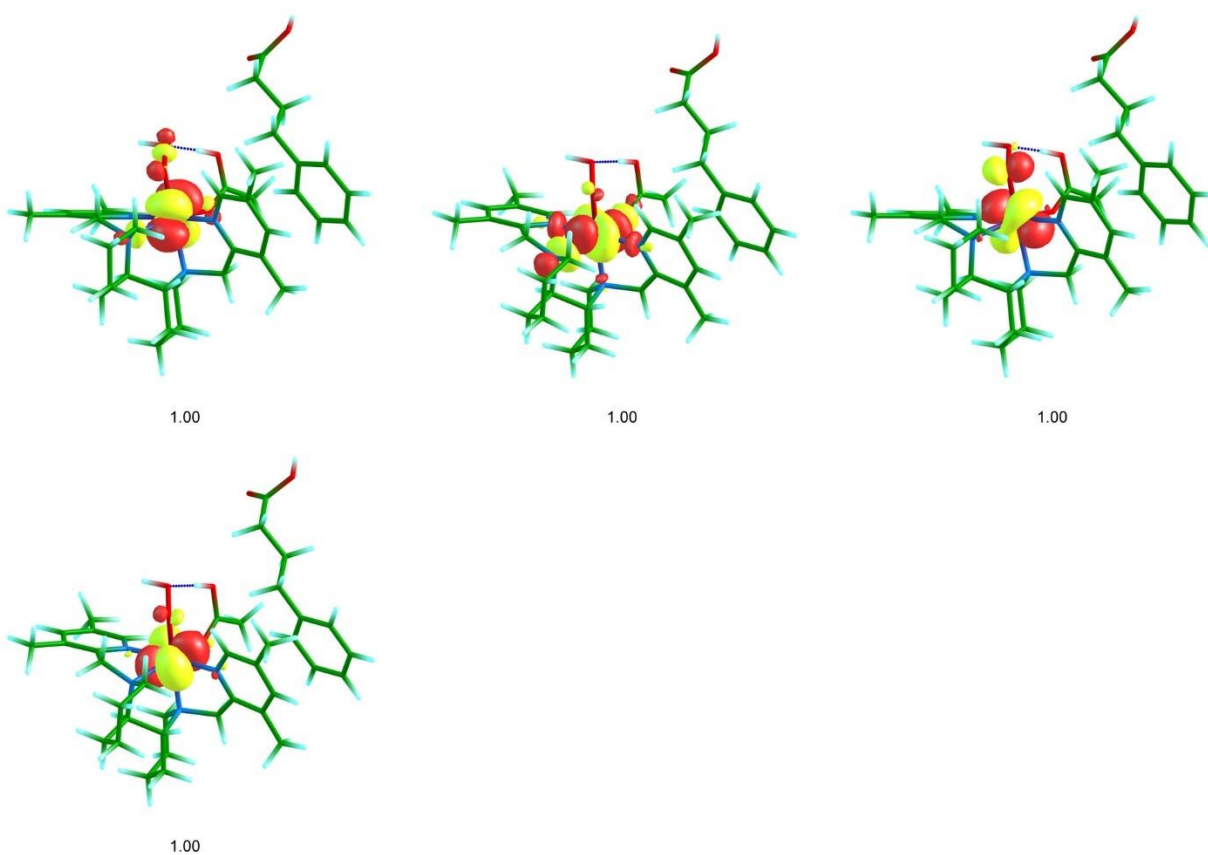
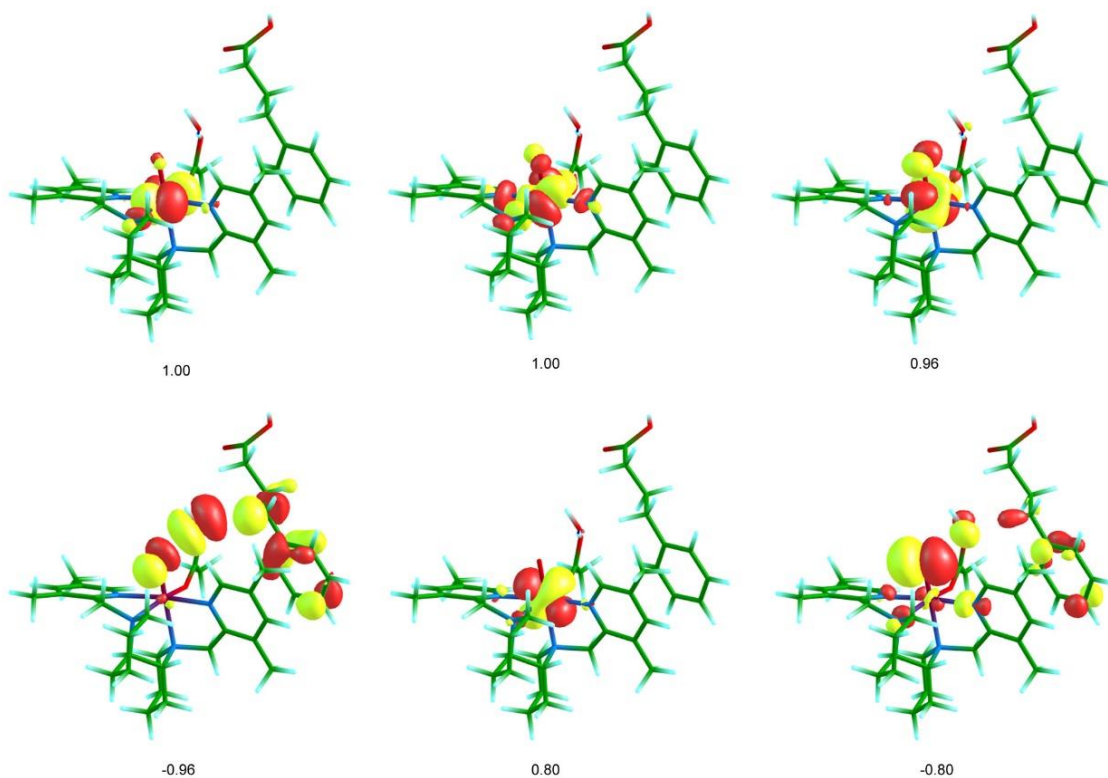


Figure S5. Singly-occupied natural orbitals (SNOs) of key intermediates of the hydroxylation of PBA by the distal oxygen of the Mn^{III} -OOH species **1**. Calculations were done at the UB3LYP-D3(BJ)/B1 level in solvent. Positive values represent alpha-electron occupations and negative ones represent beta occupations. (To be continued)

$^3\text{TS}_{\text{dis}}$



$^5\text{TS}_{\text{dis}}$

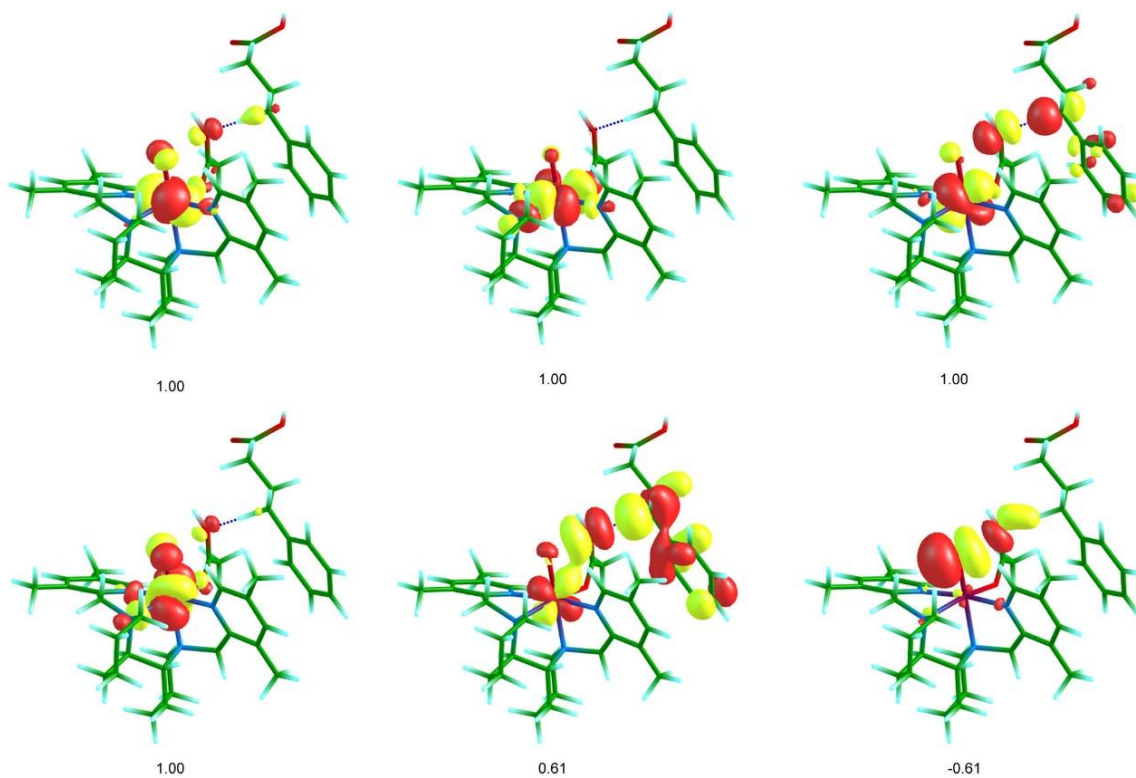


Figure S5. Singly-occupied natural orbitals (SNOs) of key intermediates of the hydroxylation of PBA by the distal oxygen of the $\text{Mn}^{\text{III}}\text{-OOH}$ species **1**. Calculations were done at the UB3LYP-D3(BJ)/B1 level in solvent. Positive values represent alpha-electron occupations and negative ones represent beta occupations. (To be continued)

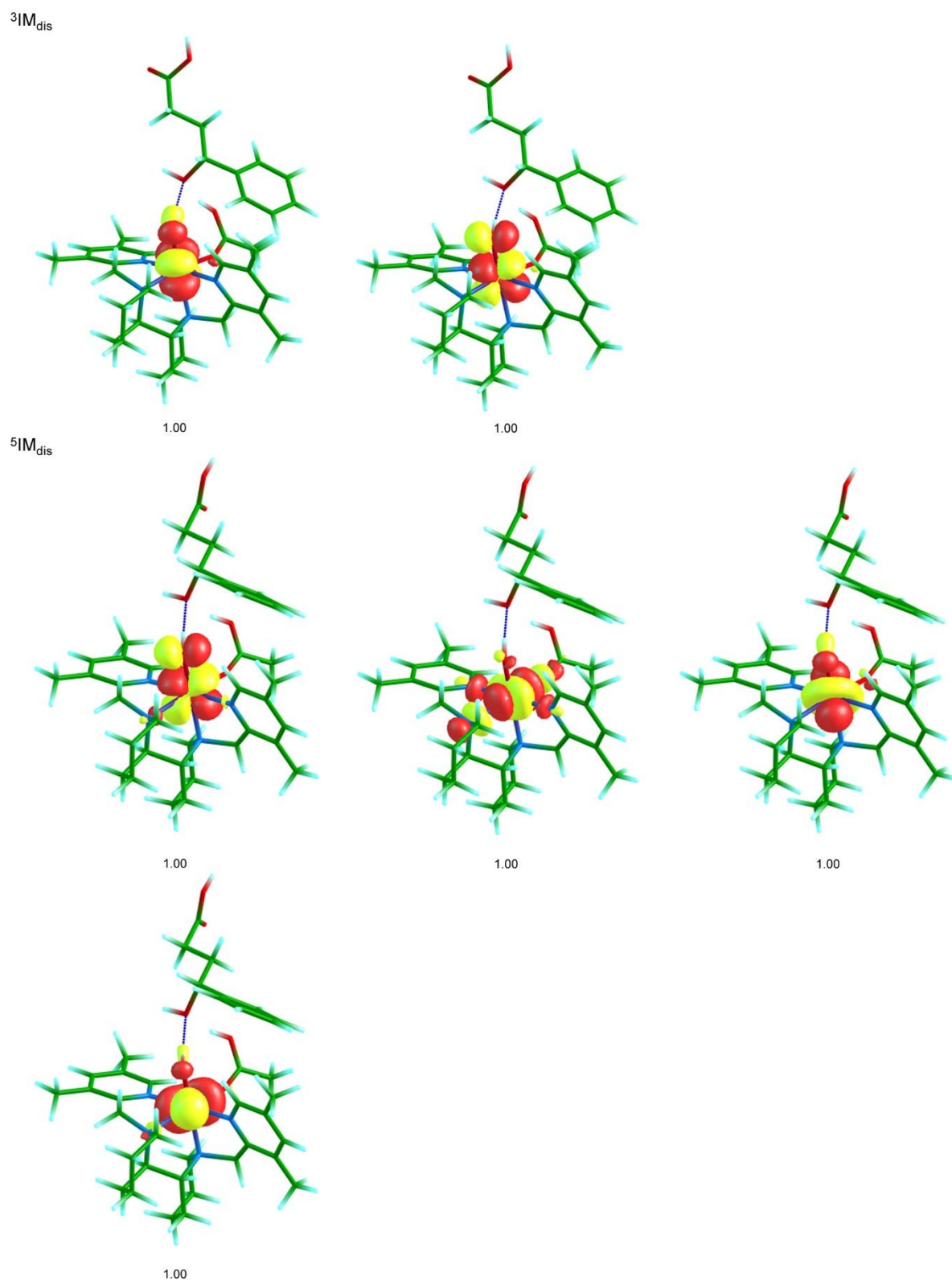


Figure S5. Singly-occupied natural orbitals (SNOs) of key intermediates of the hydroxylation of PBA by the distal oxygen of the $\text{Mn}^{\text{III}}\text{-OOH}$ species **1**. Calculations were done at the UB3LYP-D3(BJ)/B1 level in solvent. Positive values represent alpha-electron occupations and negative ones represent beta occupations.

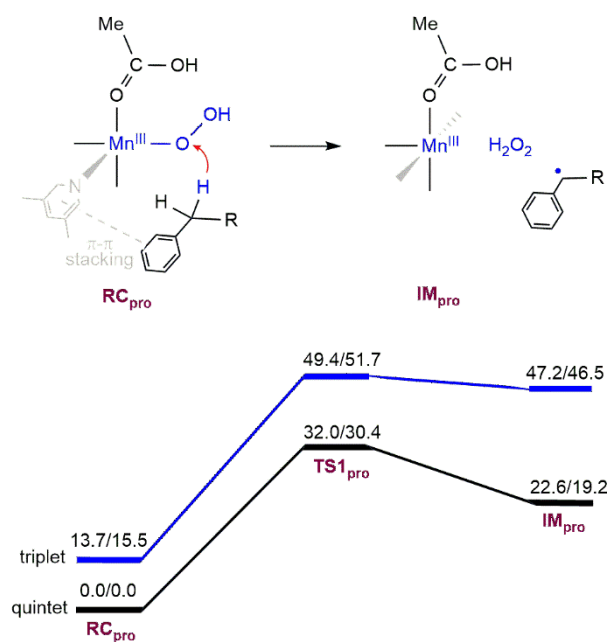


Figure S6. The energy profile (in kcal mol⁻¹) for the hydroxylation of PBA by the proximal oxygen of the Mn^{III}-OOH species **1**. Values before slashes are the SCF energies calculated at the UB3LYP-D3(BJ)/B2//B1 level including ZPE/B1 corrections and those after slashes are Gibbs free energies calculated at the UB3LYP-D3(BJ)/B1 level, respectively.

Table S5. Various SCF and Gibbs free energies of the hydroxylation of PBA by the proximal oxygen of the Mn^{III}-OOH species **1**. Calculations were done at the UB3LYP-D3(BJ)/B2//B1 level in solvent.

	OPT/B1+ZPE	ΔE	SPE/B2+ZPE	ΔE	G	ΔG
³RC	-3302.046030	14.1	-3302.575136	13.7	-3302.134250	15.5
⁵RC	-3302.068435	0.0	-3302.596908	0.0	-3302.158912	0.0
³TS_{pro}	-3301.990287	49.0	-3302.518107	49.4	-3302.076536	51.7
⁵TS_{pro}	-3302.020975	29.8	-3302.545889	32.0	-3302.110428	30.4
³IM_{pro}	-3301.992427	47.7	-3302.521724	47.2	-3302.084786	46.5
⁵IM_{pro}	-3302.033662	21.8	-3302.560822	22.6	-3302.128365	19.2

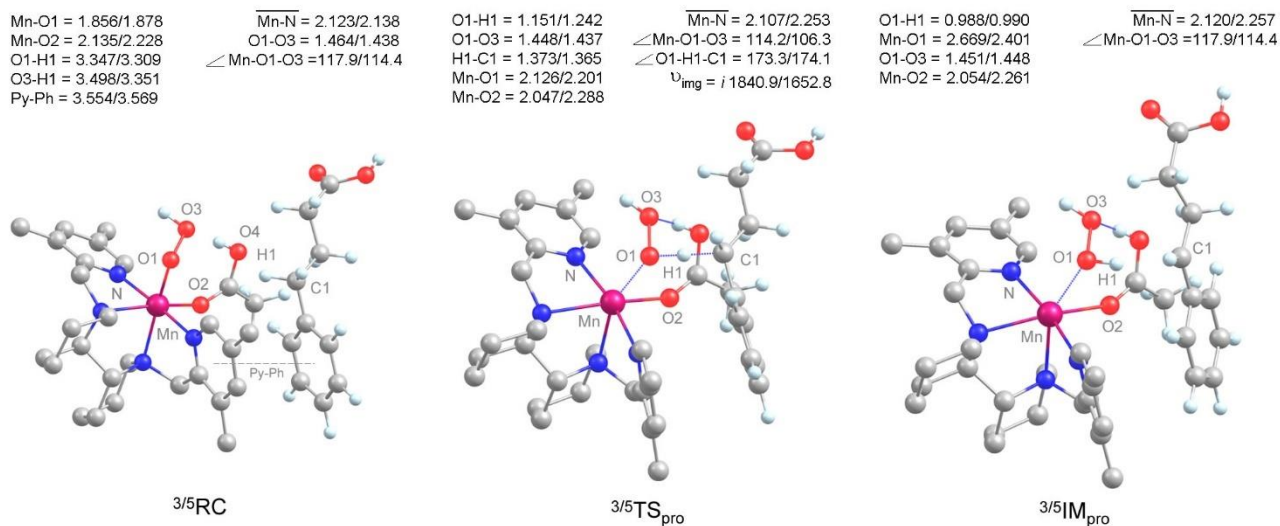
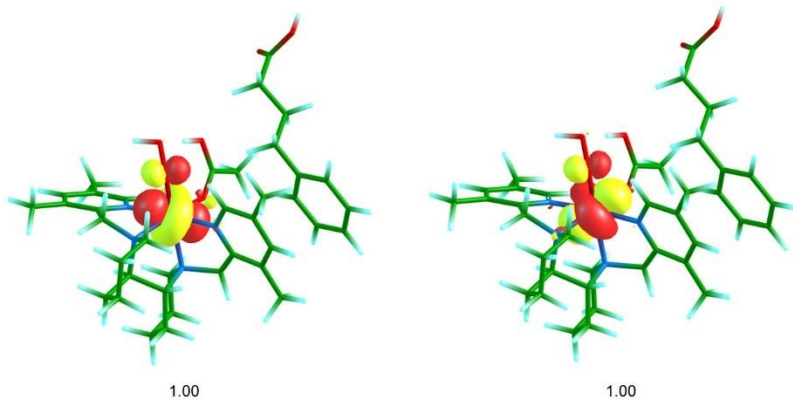


Figure S7. Optimized structures of key intermediates of the hydroxylation of PBA by the proximal oxygen of the Mn^{III} -OOH species **1**. Calculations were done at the UB3LYP-D3(BJ)/B1 level in solvent. Hydrogen atoms of *rac-L* are omitted for clarity. Lengths are in Å units, angles are in degree units and imaginary frequency is in cm^{-1} units.

Table S6. Mulliken charges and spin densities of key intermediates of the hydroxylation of PBA by the proximal oxygen of the Mn^{III}-OOH species **1**. Calculations were done at the UB3LYP-D3(BJ)/B1 level in solvent.

	Mulliken charge								spin densities							
	Mn	O1	<i>rac</i> -L	OH	H1	OAc	H2	Sub-H2	Mn	O1	<i>rac</i> -L	OH	H1	OAc	H2	Sub-H2
³RC	0.64	-0.33	1.49	0.00	0.36	-0.19	0.12	-0.09	2.14	0.03	-0.15	-0.01	0.00	-0.01	0.00	0.00
⁵RC	0.79	-0.32	1.36	0.02	0.36	-0.24	0.12	-0.09	4.05	-0.05	-0.04	0.01	0.00	0.03	0.00	0.00
³TS_{pro}	0.76	-0.36	1.19	0.04	0.37	-0.18	0.24	-0.04	2.72	-0.14	-0.13	0.01	0.00	-0.01	-0.02	-0.43
⁵TS_{pro}	1.08	-0.37	0.75	0.01	0.38	-0.27	0.25	0.17	4.78	-0.19	0.08	-0.01	0.00	0.01	-0.04	-0.63
³IM_{pro}	0.84	-0.33	0.95	0.01	0.36	-0.23	0.31	0.09	3.07	-0.01	-0.07	0.00	0.00	-0.01	-0.03	-0.95
⁵IM_{pro}	1.09	-0.33	0.71	0.02	0.37	-0.27	0.32	0.09	4.86	0.00	0.11	0.01	0.00	0.01	-0.04	-0.95

3RC



5RC

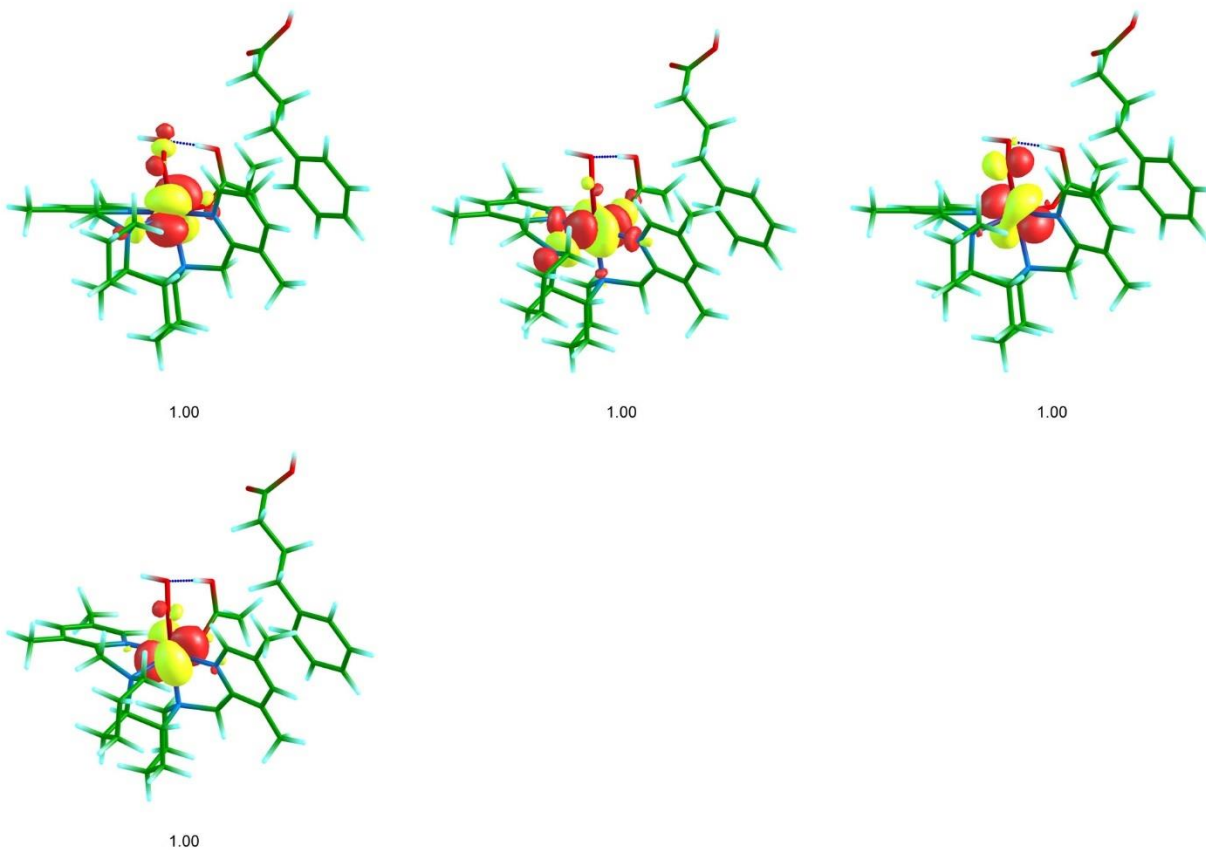


Figure S8. Singly-occupied natural orbitals (SNOs) of key intermediates of the hydroxylation of PBA by the proximal oxygen of the Mn^{III} -OOH species **1**. Calculations were done at the UB3LYP-D3(BJ)/B1 level in solvent. Positive values represent alpha-electron occupations and netative ones represent beta occupations. (To be continued)

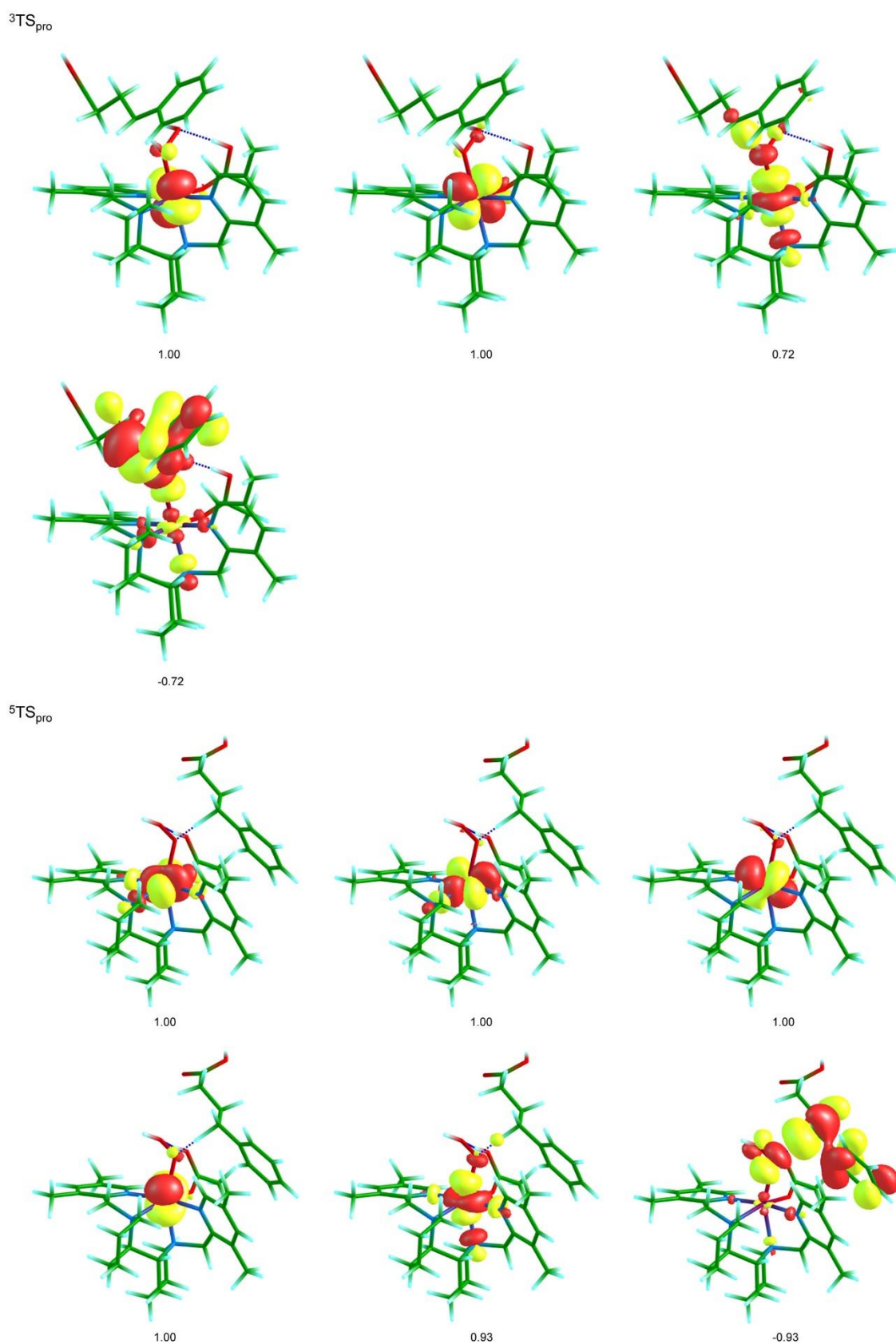


Figure S8. Singly-occupied natural orbitals (SNOs) of key intermediates of the hydroxylation of PBA by the proximal oxygen of the $\text{Mn}^{\text{III}}\text{-OOH}$ species **1**. Calculations were done at the UB3LYP-D3(BJ)/B1 level in solvent. Positive values represent alpha-electron occupations and negative ones represent beta occupations. (To be continued)

$^3\text{IM}_{\text{pro}}$

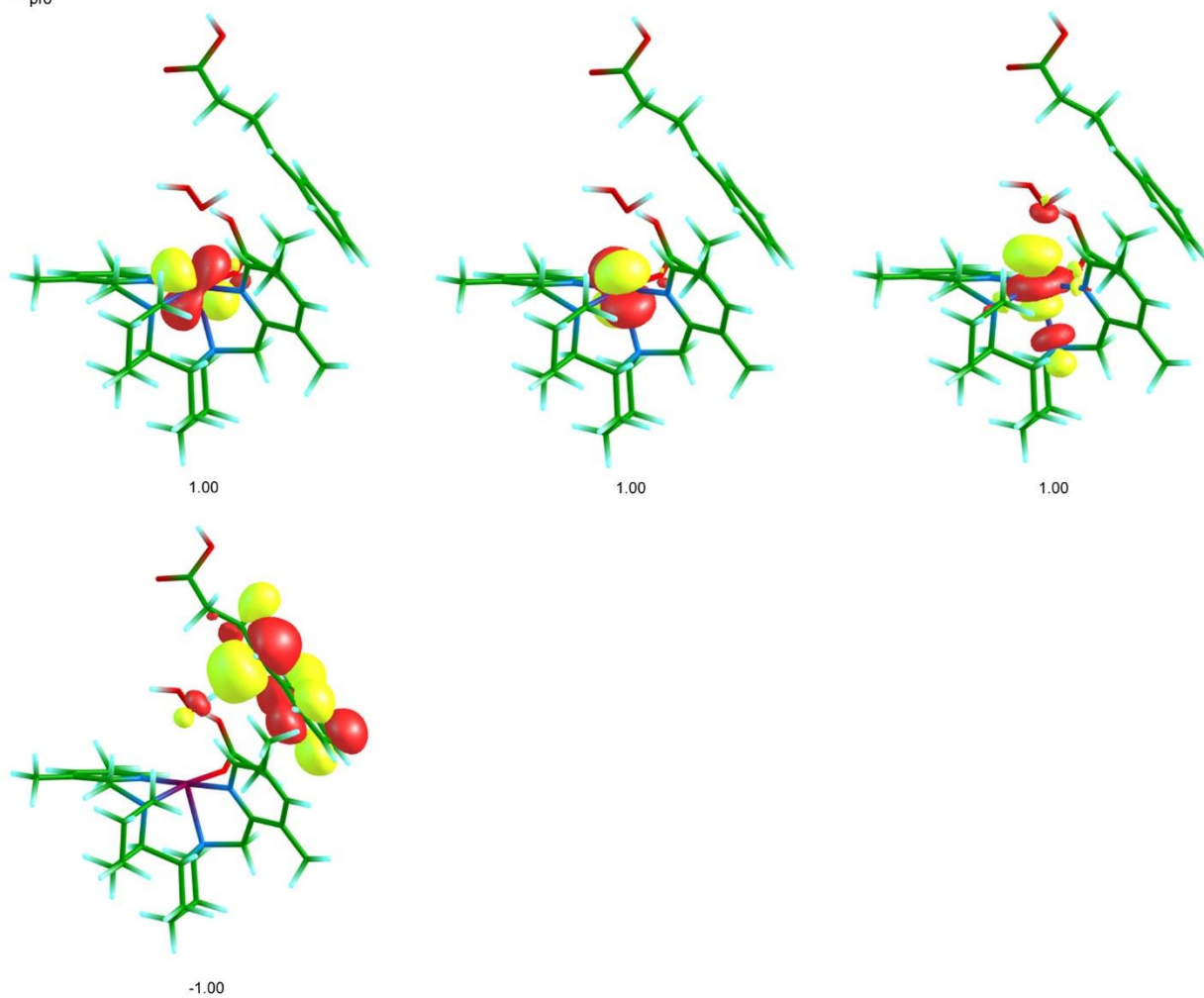


Figure S8. Singly-occupied natural orbitals (SNOs) of key intermediates of the hydroxylation of PBA by the proximal oxygen of the Mn^{III} -OOH species **1**. Calculations were done at the UB3LYP-D3(BJ)/B1 level in solvent. Positive values represent alpha-electron occupations and netative ones represent beta occupations. (To be continued)

$^5M_{pro}$

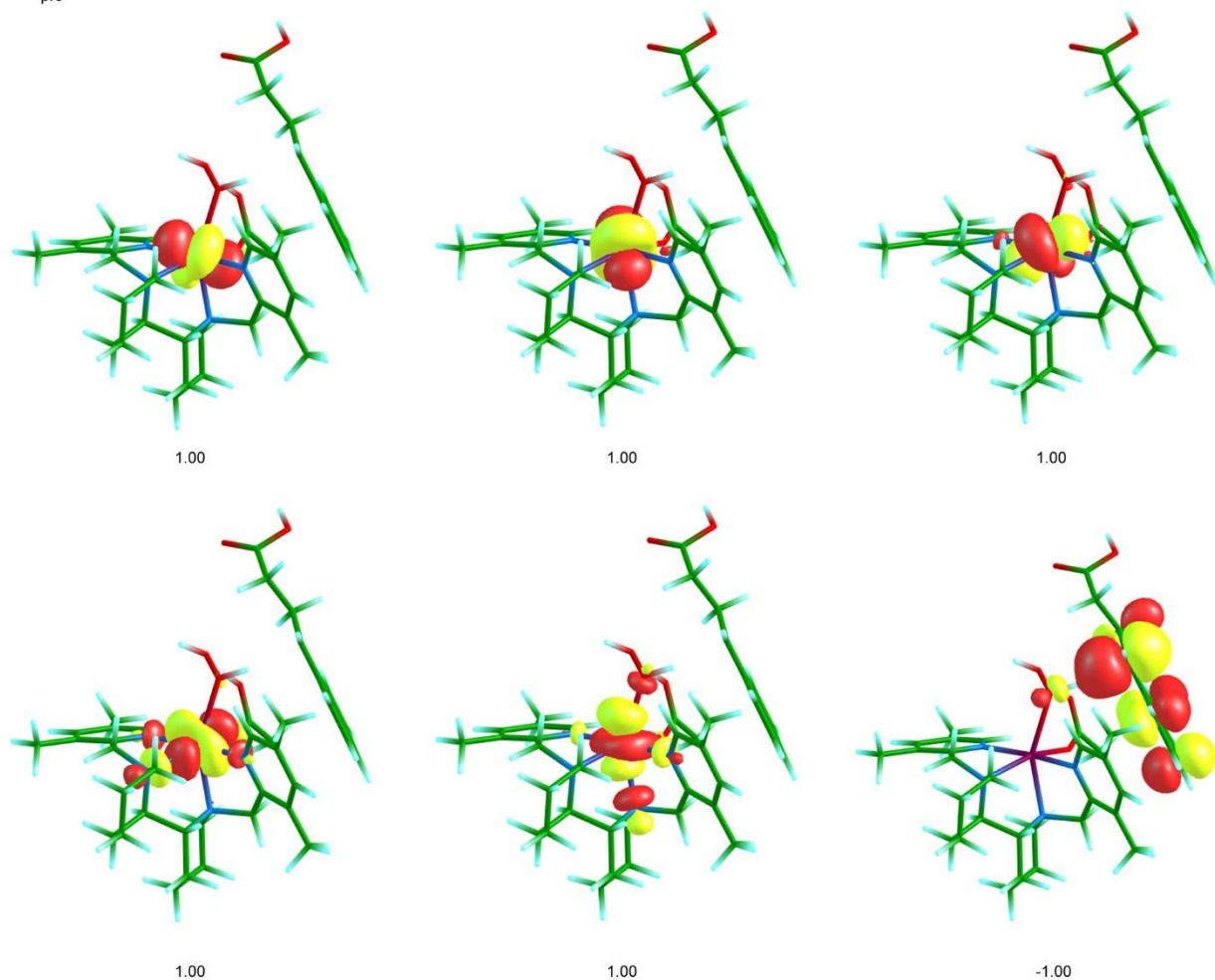


Figure S8. Singly-occupied natural orbitals (SNOs) of key intermediates of the hydroxylation of PBA by the proximal oxygen of the Mn^{III} -OOH species **1**. Calculations were done at the UB3LYP-D3(BJ)/B1 level in solvent. Positive values represent alpha-electron occupations and netative ones represent beta occupations.

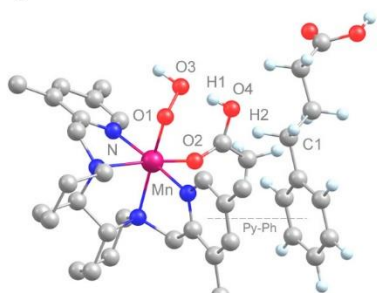
Part III Hydroxylation of PBA to 4-OH-PBA by the Mn^{IV}(O)(AcO[•]) species 2 generated from the Mn^{III}-OOH species 1.

Table S7. Various SCF and Gibbs free energies of the hydroxylation of PBA by the high-valent Mn-oxo species 2 generated from the Mn^{III}-OOH species 1. Calculations were done at the UB3LYP-D3(BJ)/B2//B1 level in solvent.

	OPT/B1+ZPE	ΔE	SPE/B2+ZPE	ΔE	G	ΔG
³ RC	-3302.046030	14.1	-3302.575136	13.7	-3302.134250	15.5
⁵ RC	-3302.068435	0.0	-3302.596908	0.0	-3302.158912	0.0
³ TS1	-3302.039249	18.3	-3302.567879	18.2	-3302.128022	19.4
⁵ TS1	-3302.023681	28.1	-3302.551095	28.7	-3302.113539	28.5
³ IM1	-3302.067290	0.7	-3302.596887	0.0	-3302.157976	0.6
⁵ IM1	-3302.039694	18.0	-3302.568248	18.0	-3302.132223	16.7
³ TS2	-3302.063018	3.4	-3302.590385	4.1	-3302.147404	7.2
⁵ TS2	-3302.033582	21.9	-3302.568112	18.1	-3302.119675	24.6
³ IM2	-3302.117477	-30.8	-3302.644156	-29.6	-3302.204443	-28.6
⁵ IM2	-3302.134953	-41.7	-3302.660117	-39.7	-3302.224128	-40.9
³ TS3	-3302.111578	-27.1	-3302.637165	-25.3	-3302.194782	-22.5
⁵ TS3	-3302.130050	-38.7	-3302.654573	-36.2	-3302.213569	-34.3
³ PC	-3302.137244	-43.2	-3302.666140	-43.4	-3302.222632	-40.0
⁵ PC	-3302.166907	-61.8	-3302.695061	-61.6	-3302.253274	-59.2

Mn-O1 = 1.856/1.878
 Mn-O2 = 2.135/2.228
 O3-H1 = 1.564/1.681
 O1-O3 = 1.464/1.438
 Py-Ph = 3.554/3.569

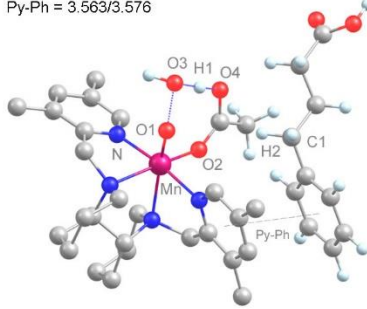
Mn-N = 2.123/2.138
 O3-H2 = 3.498/3.351
 O1-H2 = 3.347/3.309
 \angle Mn-O1-O3 = 117.9/114.4



3/5RC

O3-H1 = 1.396/1.669
 O1-O3 = 1.742/2.038
 H1-O4 = 1.071/0.999
 Mn-O1 = 1.718/1.777
 Mn-O2 = 2.011/2.235
 Py-Ph = 3.563/3.576

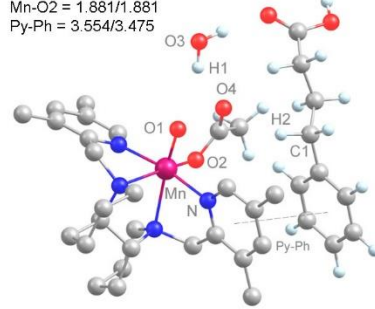
Mn-N = 2.148/2.137
 \angle Mn-O1-O3 = 120.4/117.0
 \angle O3-H1-O4 = 176.4/170.8
 $\nu_{\text{img}} = i 726.0/366.2$



3/5TS1

O1-O4 = 2.342/3.314
 H1-O4 = 2.107/1.631
 O1-H1 = 3.720/3.250
 C1-O1 = 4.698/4.318
 Mn-O1 = 1.678/1.799
 Mn-O2 = 1.881/1.881
 Py-Ph = 3.554/3.475

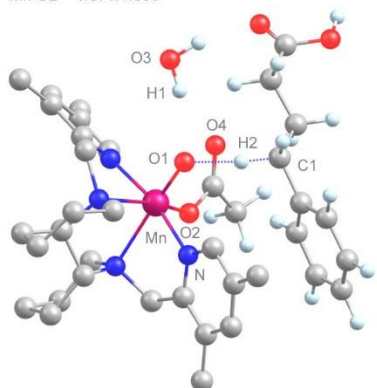
Mn-N = 2.169/2.157
 \angle O1-Mn-O2-O4 = 5.8/-7.8



3/5IM

H2-O1 = 1.675/1.966
 H2-C1 = 1.153/1.105
 O1-O4 = 3.233/3.199
 Mn-O1 = 1.686/1.814
 Mn-O2 = 1.871/1.886

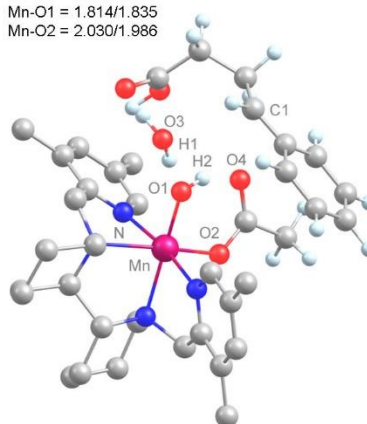
Mn-N = 2.163/2.158
 \angle O1-H2-C1 = 168.3/172.7
 \angle O1-Mn-O2-O4 = -37.4/-30.5
 $\nu_{\text{img}} = i 28.7/15.1$



3/5TS2

H2-O1 = 0.984/0.984
 O1-O4 = 3.345/2.707
 O1-C1 = 3.267/3.236
 Mn-O1 = 1.814/1.835
 Mn-O2 = 2.030/1.986

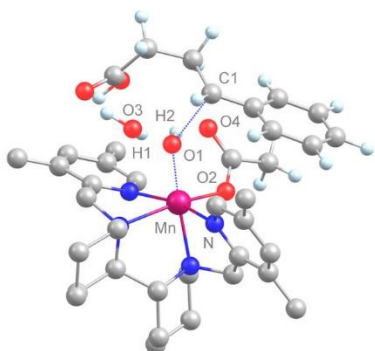
Mn-N = 2.149/2.195
 \angle O1-Mn-O2-O4 = -28.7/-21.5



3/5IM2

O1-C1 = 2.481/2.195
 H2-O1 = 0.988/0.986
 Mn-O1 = 1.841/1.929
 Mn-O2 = 2.008/1.941

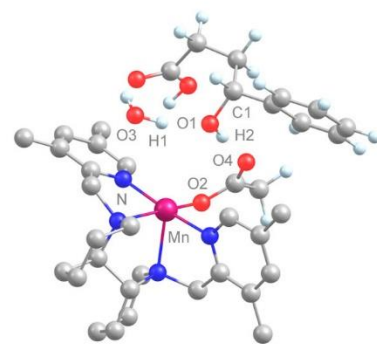
Mn-N = 2.156/2.211
 \angle Mn-O1-C1 = 119.7/137.2
 \angle O1-Mn-O2-O4 = -41.1/-32.6
 $\nu_{\text{img}} = i 60.7/150.7$



3/5TS3

O1-C1 = 1.443/1.442
 H2-O1 = 0.982/0.981
 Mn-O1 = 3.634/3.616
 Mn-O2 = 1.884/1.893

Mn-N = 2.032/2.097
 \angle O1-Mn-O2-O4 = 17.0/16.4



3/5PC

Figure S9. Optimized structures of the hydroxylation of PBA by the high-valent Mn-oxo species **2** generated from the Mn^{III}-OOH species **1**. Calculations were done at the UB3LYP-D3(BJ)/B1 level in solvent. Hydrogen atoms of *rac*-L are omitted for clarity. Lengths are in Å units, angles are in degree units and imaginary frequencies are in cm⁻¹ units.

Table S8. Mulliken charges and spin densities of the hydroxylation of PBA by the high-valent Mn-oxo species **2** generated from the Mn^{III}-OOH species **1**. Calculations were done at the UB3LYP-D3(BJ)/B1 level.

	Mulliken charge								spin densities							
	Mn	O1	<i>rac</i> -L	OH	H1	OAc	H2	Sub-H2	Mn	O1	<i>rac</i> -L	OH	H1	OAc	H2	Sub-H2
³RC	0.64	-0.33	1.49	0.00	0.36	-0.19	0.12	-0.09	2.14	0.03	-0.15	-0.01	0.00	-0.01	0.00	0.00
⁵RC	0.79	-0.32	1.36	0.02	0.36	-0.24	0.12	-0.09	4.05	-0.05	-0.04	0.01	0.00	0.03	0.00	0.00
³TS1	0.58	-0.30	1.62	-0.11	0.34	-0.15	0.11	-0.08	2.42	0.07	-0.18	-0.30	0.00	-0.01	0.00	0.00
⁵TS1	0.75	-0.34	1.45	0.00	0.35	-0.24	0.12	-0.09	3.87	-0.57	-0.07	0.74	-0.01	0.03	0.00	0.00
³IM1	0.49	-0.25	1.87	-0.39	0.35	-0.13	0.12	-0.05	2.98	-0.46	-0.29	0.00	0.00	-0.22	0.00	0.00
⁵IM1	0.56	-0.30	1.82	-0.14	0.35	-0.31	0.12	-0.10	3.10	0.86	-0.28	0.30	-0.01	0.03	0.00	0.00
³TS2	0.56	-0.38	1.76	-0.38	0.34	-0.33	0.18	0.26	2.90	-0.21	-0.26	0.00	0.00	0.01	-0.02	-0.42
⁵TS2	0.56	-0.30	1.84	-0.17	0.34	-0.31	0.16	-0.13	3.13	0.89	-0.29	0.25	-0.01	0.02	0.00	0.01
³IM2	0.71	-0.68	1.25	-0.37	0.36	-0.57	0.37	0.95	2.07	0.08	-0.13	0.00	0.00	-0.02	0.01	0.00
⁵IM2	0.87	-0.73	1.11	-0.38	0.37	-0.50	0.33	0.93	3.96	0.01	0.00	0.00	0.00	0.03	0.01	0.00
³TS3	0.73	-0.68	1.27	-0.35	0.36	-0.54	0.37	0.85	2.09	0.04	-0.13	0.00	0.00	-0.02	0.01	0.01
⁵TS3	0.91	-0.72	1.15	-0.33	0.34	-0.45	0.35	0.75	4.02	-0.02	-0.03	0.00	0.00	0.00	0.00	0.01
³PC	0.77	-0.57	1.65	-0.38	0.38	-0.41	0.36	0.20	2.17	0.00	-0.20	0.00	0.00	0.04	0.00	0.00
⁵PC	0.92	-0.58	1.48	-0.38	0.38	-0.40	0.36	0.21	4.05	0.00	-0.05	0.00	0.00	0.00	0.00	0.00

Table S9. The spin density variation of key moieties by the approach of oxo to the benzylic C-H group of PBA. d_{OH} denotes the distance between the oxo and the benzylic hydrogen, Lengths are in Å units. Calculations were done at the UB3LYP-D3(BJ)/B1 level.

d_{OH}	spin densities							
	Mn	O1	<i>rac</i> -L	OH	H1	OAc	H2	Sub-H
1.83	2.88	-0.26	-0.27	0.00	0.00	0.00	-0.01	-0.34
1.81	2.89	-0.25	-0.27	0.00	0.00	0.01	-0.01	-0.36
1.79	2.89	-0.25	-0.27	0.00	0.00	0.01	-0.01	-0.37
1.77	2.89	-0.24	-0.27	0.00	0.00	0.01	-0.01	-0.38
1.75	2.89	-0.23	-0.26	0.00	0.00	0.01	-0.01	-0.38
1.73	2.89	-0.23	-0.26	0.00	0.00	0.01	-0.02	-0.39
1.71	2.90	-0.22	-0.26	0.00	0.00	0.01	-0.02	-0.40
1.69	2.90	-0.22	-0.26	0.00	0.00	0.01	-0.02	-0.41
1.67	2.90	-0.21	-0.26	0.00	0.00	0.01	-0.02	-0.42
1.65	2.87	-0.10	-0.23	0.00	0.00	0.01	-0.03	-0.52
1.63	2.87	-0.10	-0.23	0.00	0.00	0.01	-0.03	-0.52
1.61	2.87	-0.09	-0.23	0.00	0.00	0.01	-0.03	-0.53
1.59	2.88	-0.09	-0.23	0.00	0.00	0.01	-0.04	-0.54
1.57	2.88	-0.08	-0.23	0.00	0.00	0.01	-0.04	-0.54
1.55	2.88	-0.08	-0.23	0.00	0.00	0.01	-0.04	-0.55
1.53	2.88	-0.07	-0.23	0.00	0.00	0.01	-0.04	-0.56
1.51	2.89	-0.07	-0.23	0.00	0.00	0.01	-0.04	-0.56
1.49	2.89	-0.06	-0.23	0.00	0.00	0.01	-0.04	-0.57
1.47	2.89	-0.06	-0.23	0.00	0.00	0.01	-0.04	-0.58
1.45	2.90	-0.05	-0.23	0.00	0.00	0.01	-0.04	-0.59
1.43	2.90	-0.04	-0.23	0.00	0.00	0.01	-0.04	-0.60
1.33	2.91	0.00	-0.23	0.00	0.00	0.01	-0.05	-0.65
1.23	2.95	0.06	-0.24	0.00	0.00	0.02	-0.06	-0.73
1.13	3.01	0.09	-0.27	0.00	0.00	0.02	-0.05	-0.80
1.03	3.10	0.10	-0.30	0.00	0.00	0.02	-0.03	-0.89
0.98	2.07	0.08	-0.13	0.00	0.00	-0.02	0.01	0.00

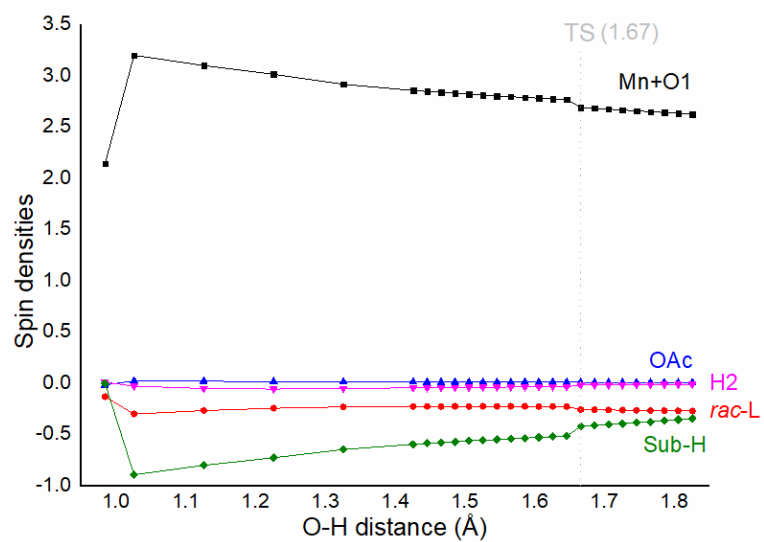


Figure S10. The plot of spin density variation of key moieties by the approach of oxo to the benzylic C-H group of PBA. Calculations were done at the UB3LYP-D3(BJ)/B1 level.

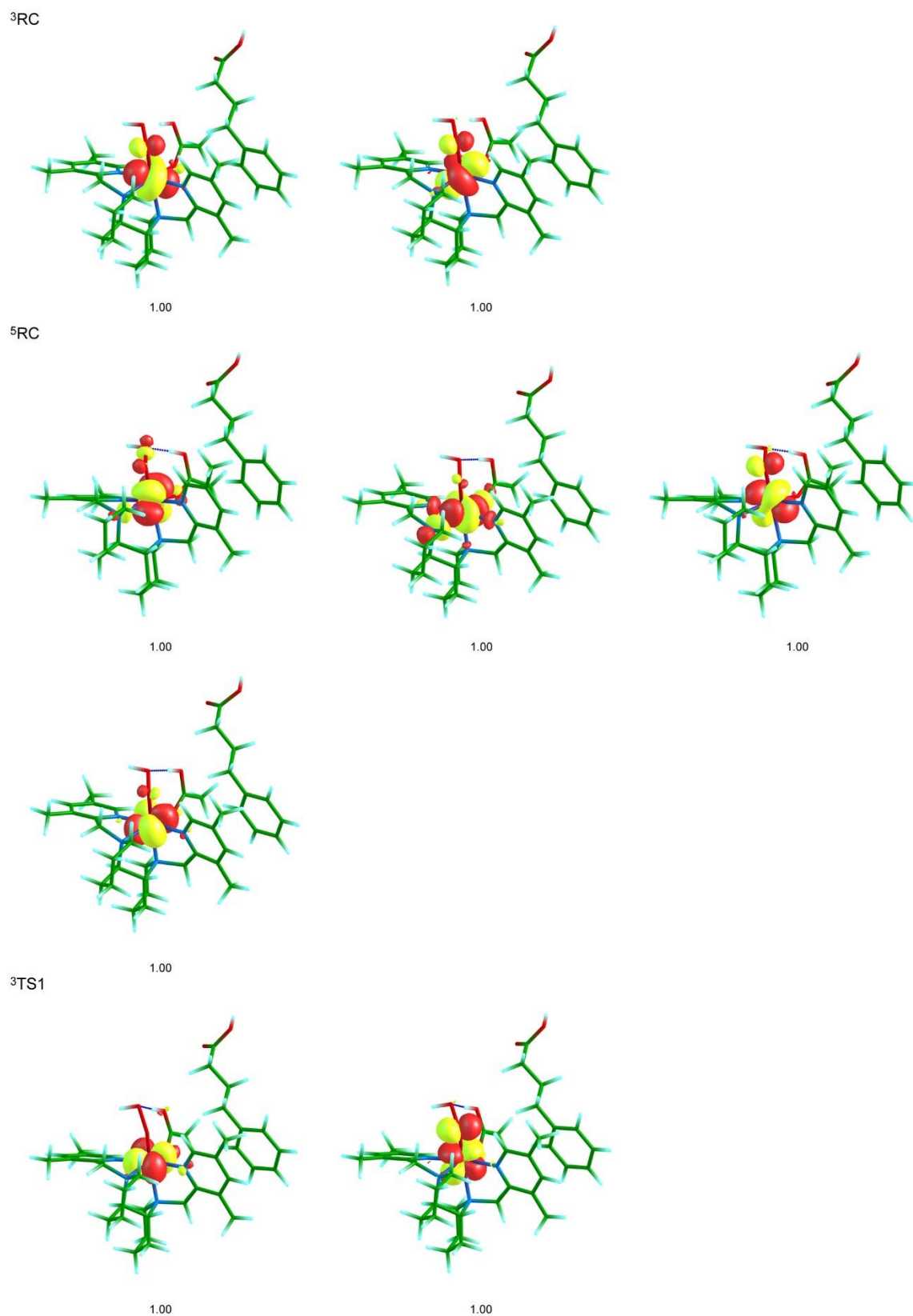
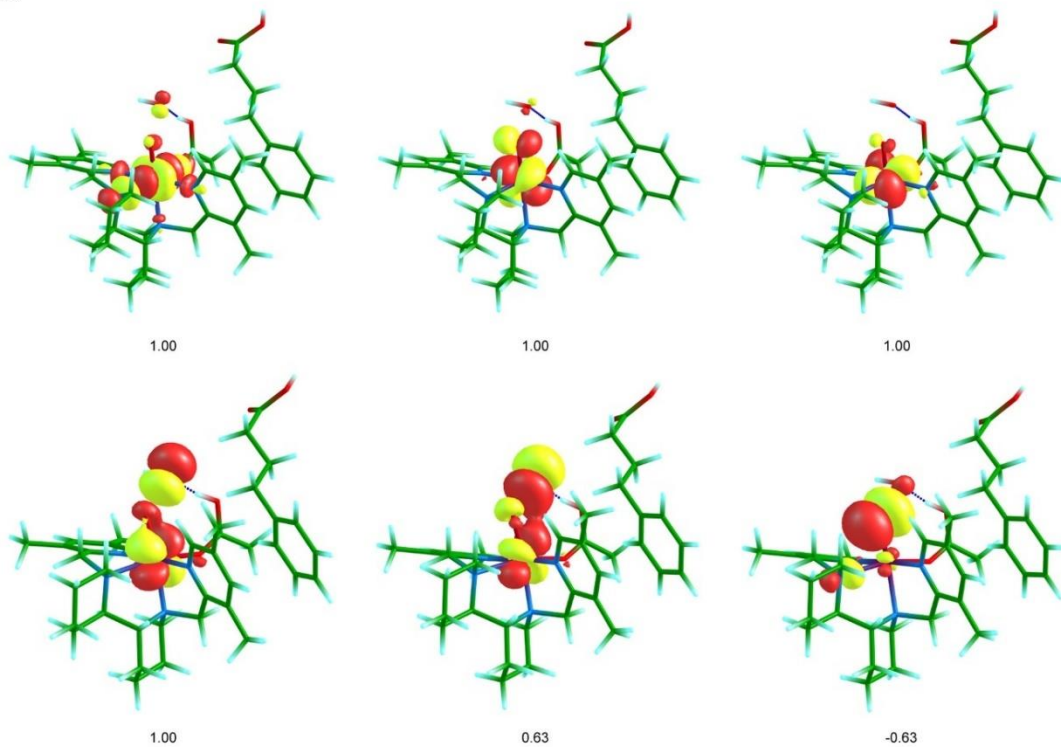


Figure S11. Singly-occupied natural orbitals (SNOs) of the hydroxylation of PBA by the high-valent Mn-oxo species **2** generated from the $\text{Mn}^{\text{III}}\text{-OOH}$ species **1**. Calculations were done at the UB3LYP-D3(BJ)/B1 level in solvent. Positive values represent alpha-electron occupations. (To be continued)

⁵TS1



³IM1

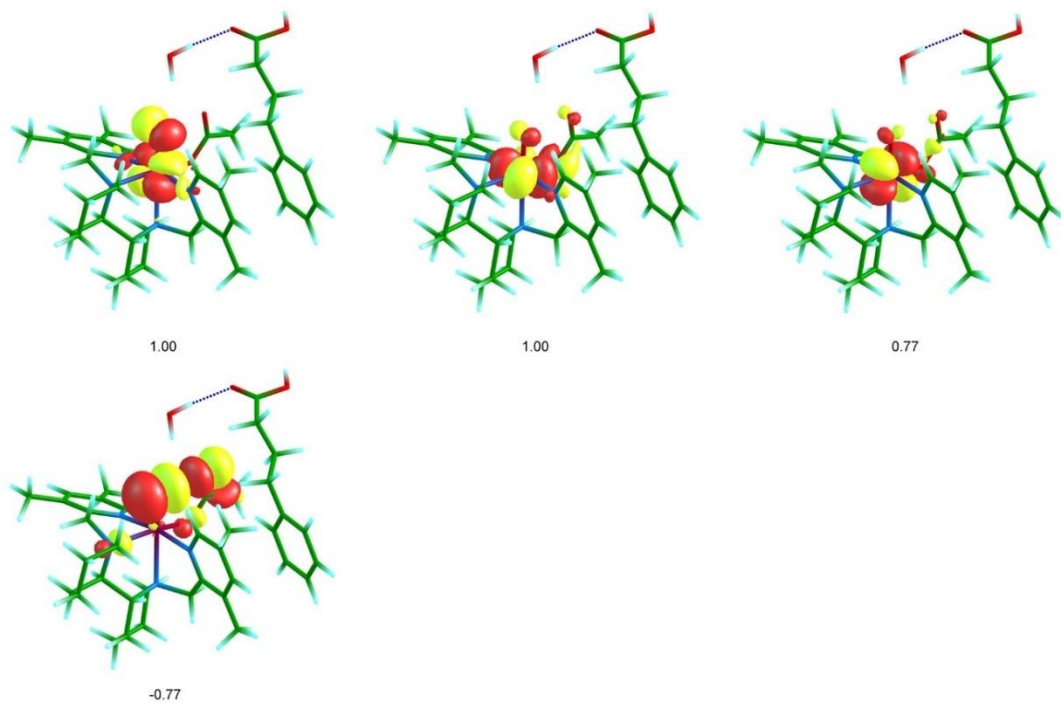


Figure S11. Singly-occupied natural orbitals (SNOs) of the hydroxylation of PBA by the high-valent Mn-oxo species **2** generated from the Mn^{III}-OOH species **1**. Calculations were done at the UB3LYP-D3(BJ)/B1 level in solvent. Positive values represent alpha-electron occupations and negative ones represent beta occupations. (To be continued)

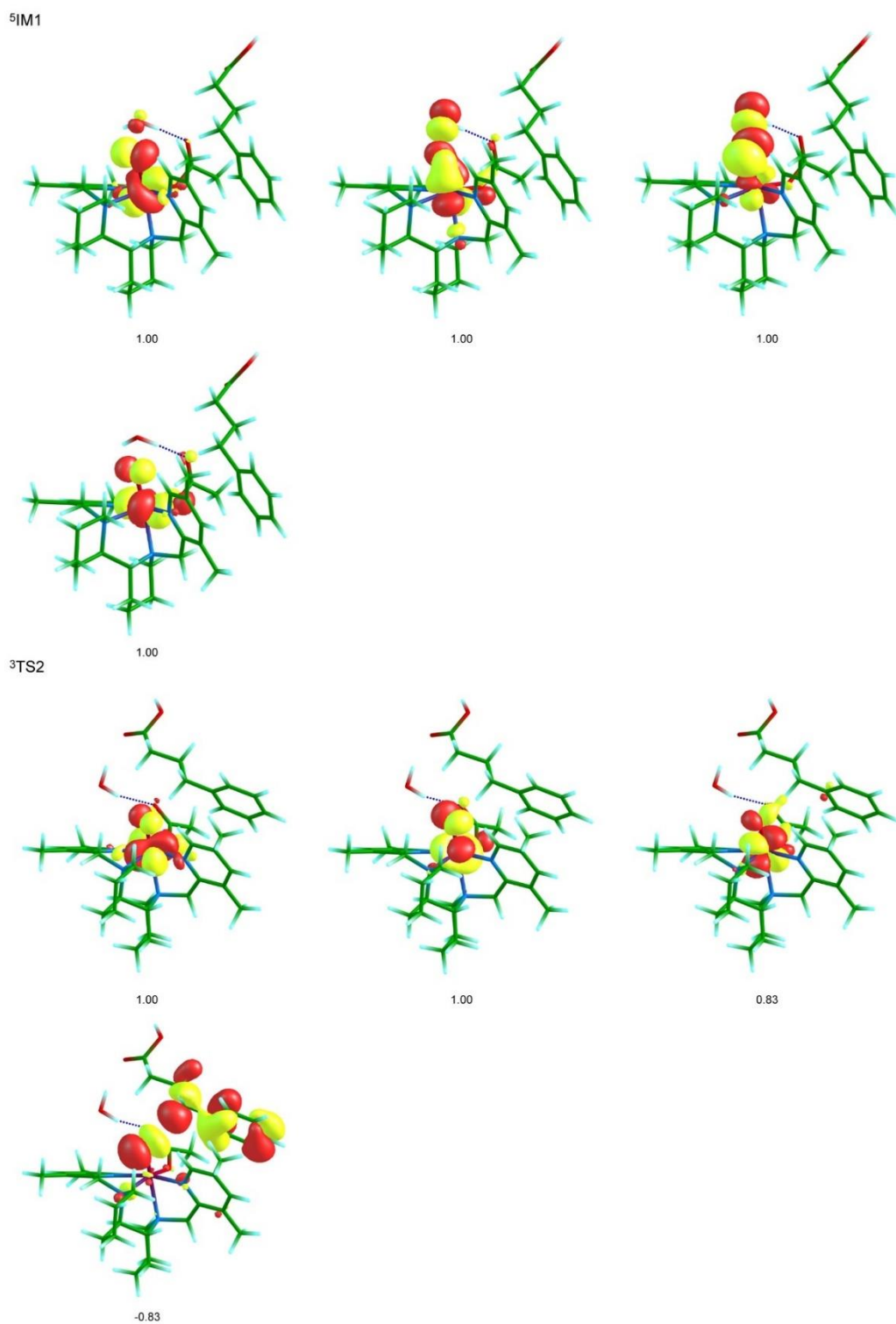
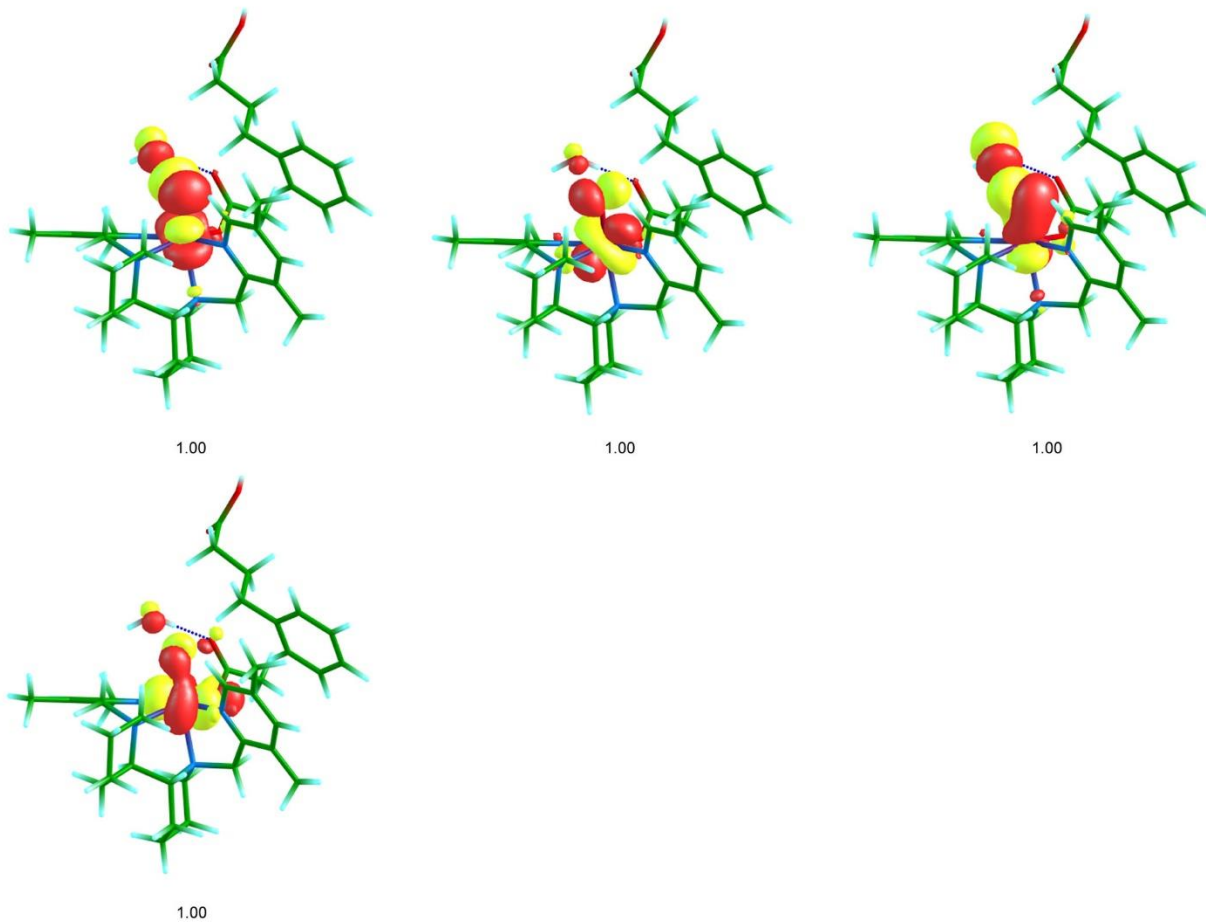


Figure S11. Singly-occupied natural orbitals (SNOs) of the hydroxylation of PBA by the high-valent Mn-oxo species **2** generated from the Mn^{III}-OOH species **1**. Calculations were done at the UB3LYP-D3(BJ)/B1 level in solvent. Positive values represent alpha-electron occupations and negative ones represent beta occupations. (To be continued)

$^5\text{TS2}$



$^3\text{IM2}$

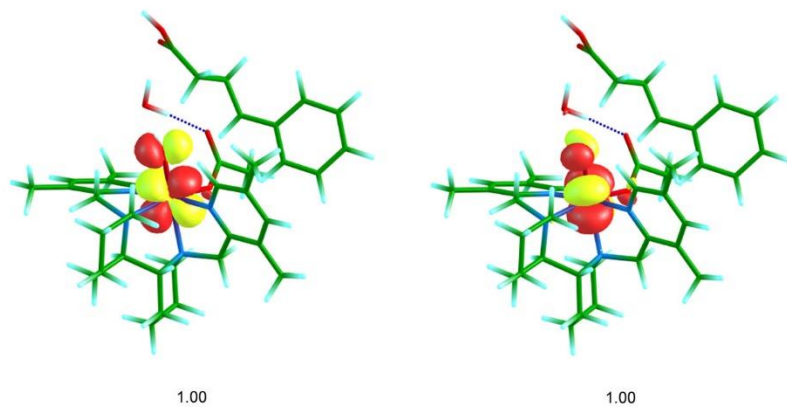
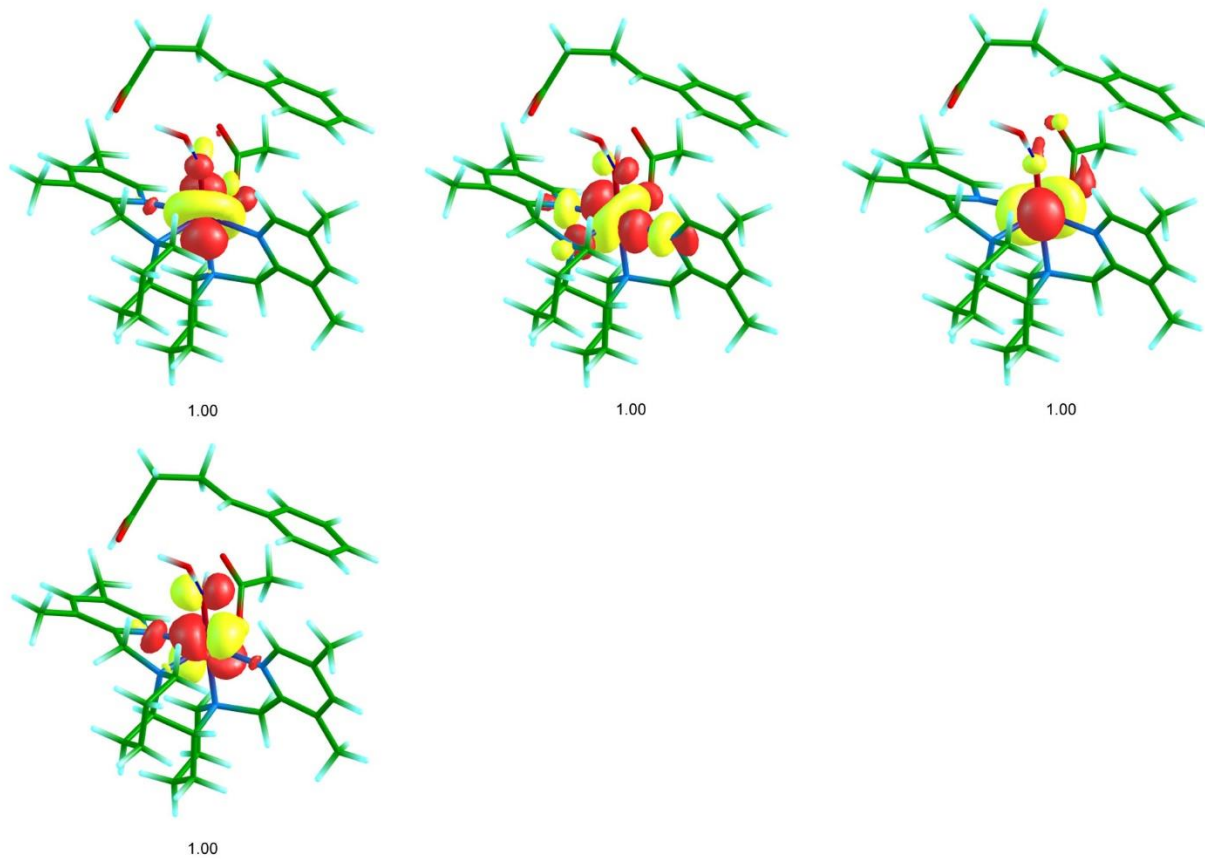


Figure S11. Singly-occupied natural orbitals (SNOs) of the hydroxylation of PBA by the high-valent Mn-oxo species **2** generated from the Mn^{III} -OOH species **1**. Calculations were done at the UB3LYP-D3(BJ)/B1 level in solvent. Positive values represent alpha-electron occupations. (To be continued)

5M2



3TS3

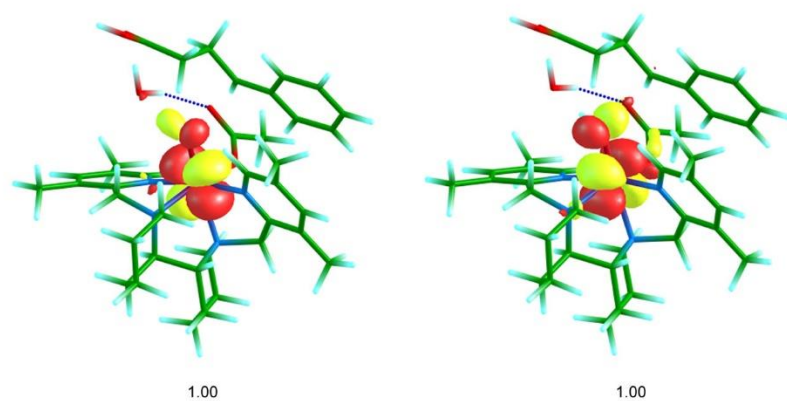
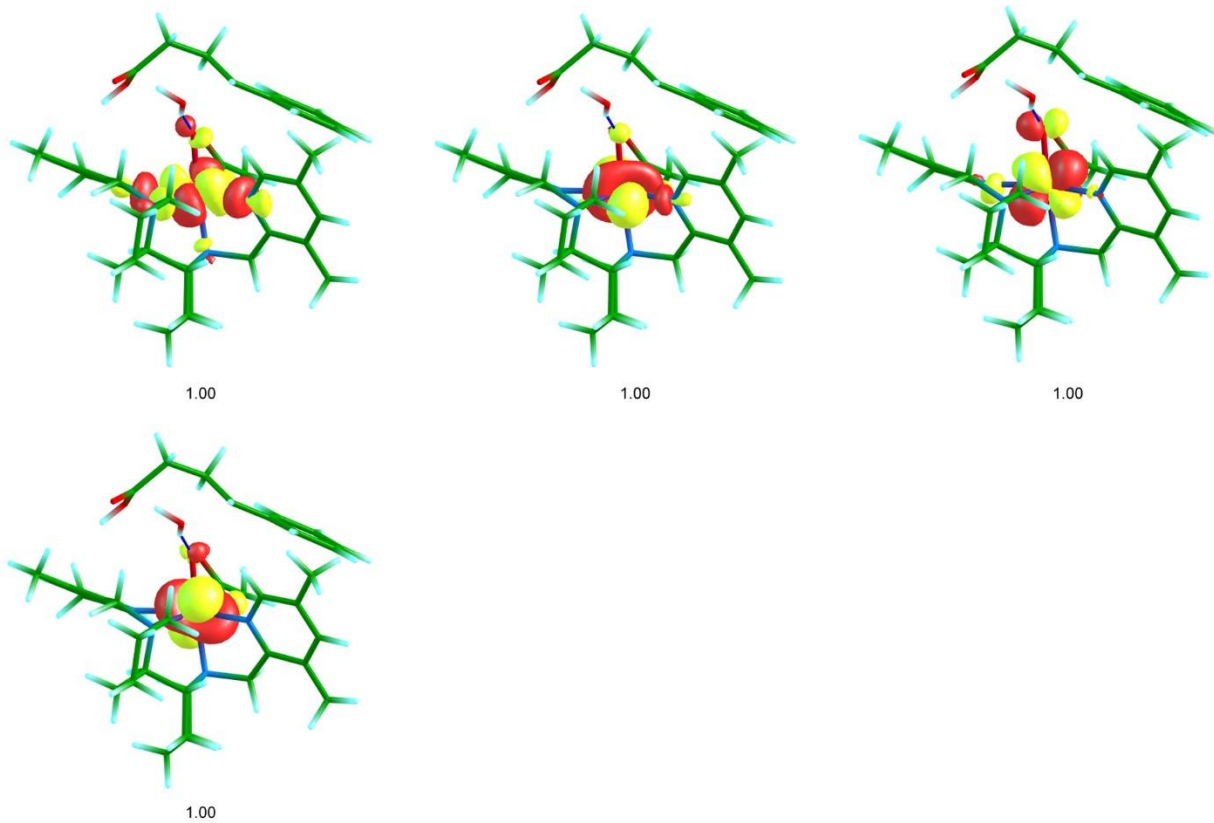


Figure S11. Singly-occupied natural orbitals (SNOs) of the hydroxylation of PBA by the high-valent Mn-oxo species **2** generated from the Mn^{III} -OOH species **1**. Calculations were done at the UB3LYP-D3(BJ)/B1 level in solvent. Positive values represent alpha-electron occupations. (To be continued)

⁵TS3



³PC

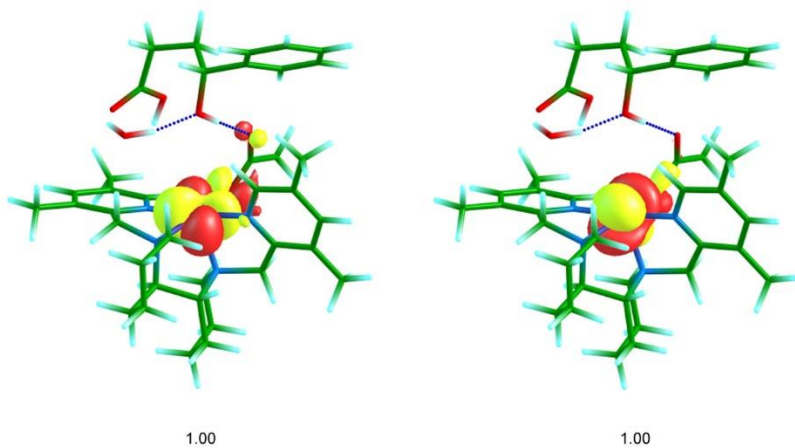


Figure S11. Singly-occupied natural orbitals (SNOs) of the hydroxylation of PBA by the high-valent Mn-oxo species **2** generated from the Mn^{III}-OOH species **1**. Calculations were done at the UB3LYP-D3(BJ)/B1 level in solvent. Positive values represent alpha-electron occupations. (To be continued)

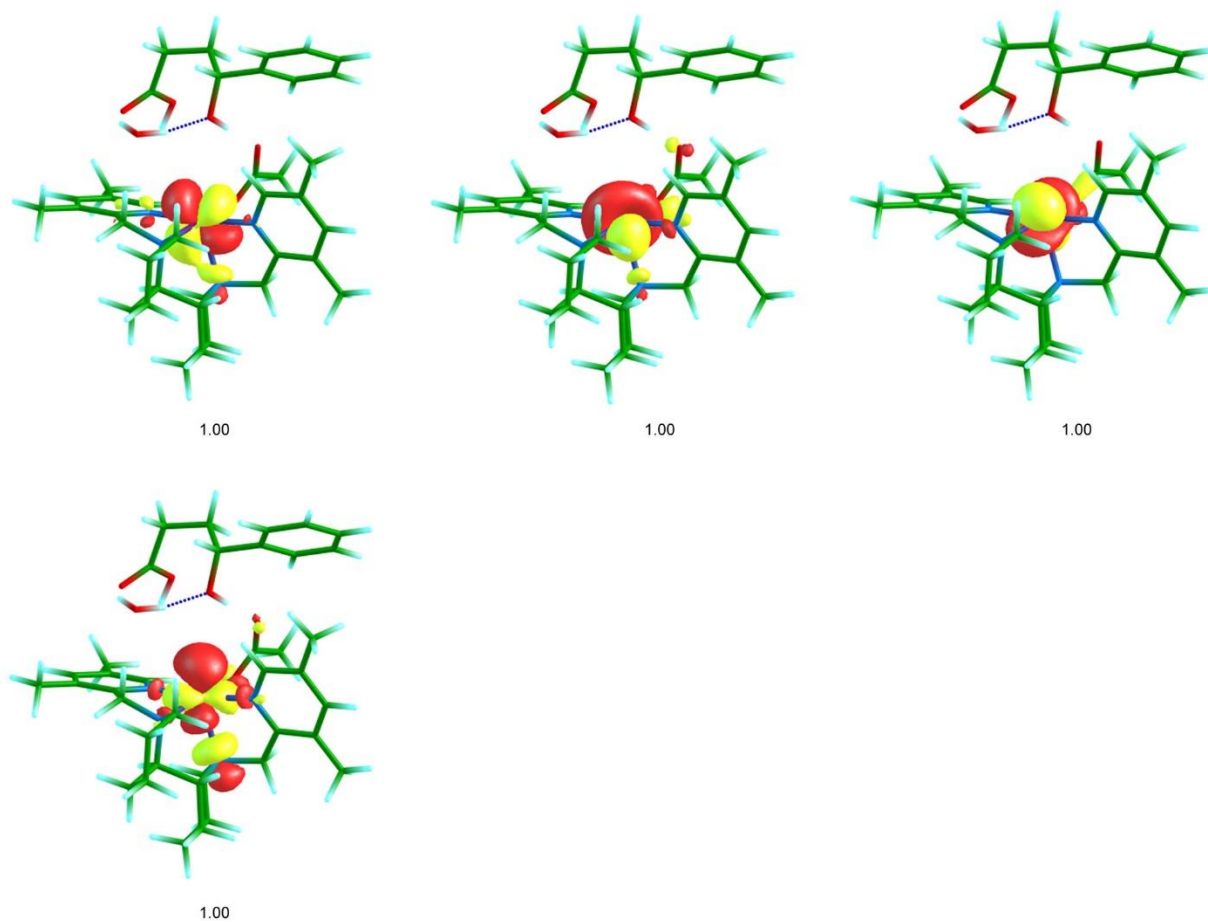


Figure S11. Singly-occupied natural orbitals (SNOs) of the hydroxylation of PBA by the high-valent Mn-oxo species **2** generated from the Mn^{III}-OOH species **1**. Calculations were done at the UB3LYP-D3(BJ)/B1 level in solvent. Positive values represent alpha-electron occupations.

Part IV Alcohol oxidation of 4-OH-PBA by the Mn^{IV}(O)(AcO[•]) species **2 via the *gem*-diol mechanism.**

Table S10. Various SCF and Gibbs free energies of alcohol oxidation of 4-OH-PBA by **2** via the *gem*-diol mechanism. Calculations were done at the UB3LYP-D3(BJ)/B2//B1 level in solvent.

	OPT/B1+ZPE	ΔE	SPE/B2+ZPE	ΔE	G	ΔG
³RC	-3300.863742	0.0	-3301.392463	0.0	-3300.949328	0.0
⁵RC	-3300.857928	3.6	-3301.379967	7.8	-3300.939823	6.0
³TS1	-3300.862878	0.5	-3301.389706	1.7	-3300.944997	2.7
⁵TS1	-3300.845133	11.7	-3301.371437	13.2	-3300.929341	12.5
³IM1	-3300.932137	-42.9	-3301.458993	-41.7	-3301.015303	-41.4
⁵IM1	-3300.952417	-55.6	-3301.478231	-53.8	-3301.039626	-56.7
³TS2_{diol}	-3300.927375	-39.9	-3301.453349	-38.2	-3301.008789	-37.3
⁵TS2_{diol}	-3300.948727	-53.3	-3301.473666	-51.0	-3301.033785	-53.0
³IM2_{diol}	-3300.938713	-47.0	-3301.463377	-44.5	-3301.020528	-44.7
⁵IM2_{diol}	-3300.962970	-62.3	-3301.486665	-59.1	-3301.049922	-63.1
³TS3	-3300.901737	-23.8	-3301.425913	-21.0	-3300.982946	-21.1
⁵TS3	-3300.922845	-37.1	-3301.446166	-33.7	-3301.006091	-35.6
³PC	-3300.956424	-58.2	-3301.483630	-57.2	-3301.040678	-57.3
⁵PC	-3300.986079	-76.8	-3301.511402	-74.6	-3301.074082	-78.3

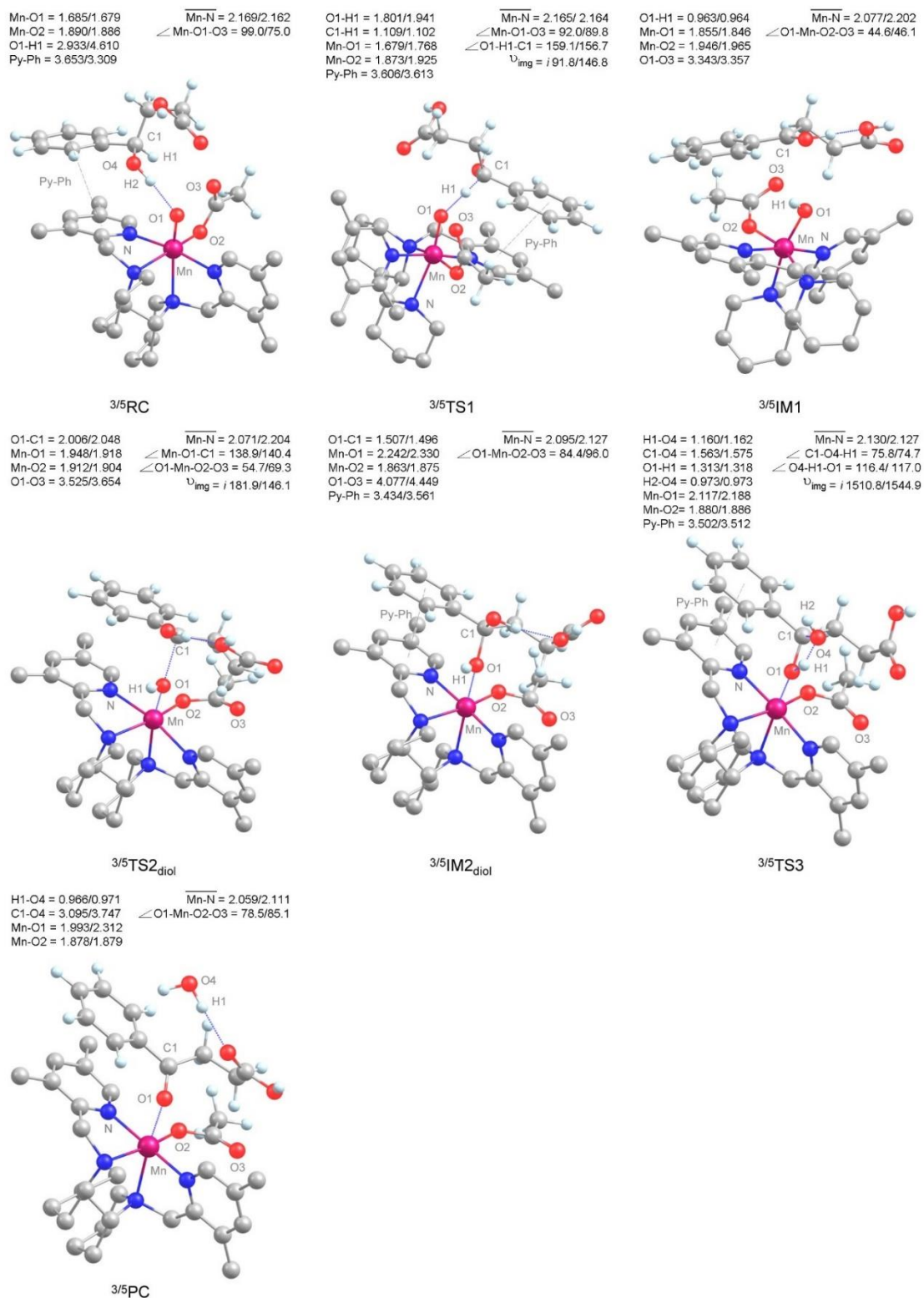


Figure S12. Optimized structures of the intermediates of alcohol oxidation of 4-OH-PBA by **2** via the *gem*-diol mechanism. Calculations were done at the UB3LYP-D3(BJ)/B1 level in solvent. Hydrogen atoms of *rac*-L are omitted for clarity. Lengths are in Å units, angles are in degree units and imaginary frequencies are in cm^{-1} units.

Table S11. Mulliken charges and spin densities of the intermediates of alcohol oxidation of 4-OH-PBA by **2** via the *gem*-diol mechanism. Calculations were done at the UB3LYP-D3(BJ)/B1 level.

	Mulliken charge						spin densities					
	Mn	O1	<i>rac</i> -L	OAc	H1	Sub-H1	Mn	O1	<i>rac</i> -L	OAc	H1	Sub-H1
³RC	0.49	-0.25	1.81	-0.09	0.14	-0.10	2.95	-0.41	-0.28	-0.27	0.00	0.00
⁵RC	0.63	-0.57	1.77	-0.37	0.14	0.40	2.71	0.44	0.23	-0.01	0.00	0.63
³TS1	0.51	-0.27	1.81	-0.19	0.12	0.01	2.97	-0.45	-0.28	-0.12	0.00	-0.12
⁵TS1	0.54	-0.32	1.75	-0.13	0.13	0.03	3.04	0.81	-0.26	0.26	0.00	0.16
³IM1	0.66	-0.70	1.29	-0.55	0.32	0.97	2.09	0.05	-0.15	-0.01	0.01	0.00
⁵IM1	0.91	-0.69	1.04	-0.56	0.32	0.97	3.97	0.00	0.00	0.02	0.01	0.00
³TS2_{diol}	0.67	-0.62	1.43	-0.49	0.32	0.69	2.13	0.00	-0.16	0.01	0.00	0.02
⁵TS2_{diol}	0.95	-0.70	1.13	-0.48	0.34	0.75	3.99	0.01	-0.02	0.01	0.00	0.01
³IM2_{diol}	0.71	-0.50	1.55	-0.43	0.35	0.31	2.14	-0.01	-0.18	0.05	0.00	0.00
⁵IM2_{diol}	0.85	-0.52	1.45	-0.44	0.35	0.31	4.02	0.01	-0.06	0.02	0.00	0.01
³TS3	0.74	-0.56	1.44	-0.45	0.42	0.41	2.15	-0.01	-0.18	0.04	0.00	0.00
⁵TS3	0.86	-0.59	1.38	-0.46	0.42	0.39	4.01	0.03	-0.07	0.01	0.00	0.01
³PC	0.60	-0.38	1.56	-0.45	0.35	0.32	2.13	0.00	-0.16	0.04	0.00	-0.01
⁵PC	0.79	-0.44	1.48	-0.43	0.34	0.25	4.01	-0.01	-0.06	0.02	0.00	0.04

Table S12. The spin density variation of key moieties by the approach of the oxo to the benzylic C-H group of 4-OH-PBA. d_{OH} denotes the distance between the oxo and the benzylic hydrogen, Lengths are in Å units.

d_{OH}	spin densities					
	Mn	O1	<i>rac</i> -L	OAc	H1	Sub-H1
1.98	2.96	-0.42	-0.28	-0.27	0.00	0.00
1.93	2.97	-0.42	-0.28	-0.26	0.00	0.00
1.88	2.97	-0.43	-0.28	-0.25	0.00	-0.02
1.87	2.97	-0.43	-0.28	-0.24	0.00	-0.02
1.86	2.97	-0.43	-0.28	-0.24	0.00	-0.02
1.85	2.97	-0.44	-0.28	-0.23	0.00	-0.03
1.84	2.98	-0.44	-0.28	-0.22	0.00	-0.04
1.83	2.98	-0.44	-0.28	-0.21	0.00	-0.04
1.82	2.98	-0.44	-0.28	-0.21	0.00	-0.05
1.81	2.97	-0.45	-0.28	-0.17	0.00	-0.08
1.80	2.86	-0.18	-0.22	0.00	-0.04	-0.42
1.79	2.86	-0.18	-0.22	0.00	-0.04	-0.42
1.78	2.86	-0.17	-0.22	0.00	-0.04	-0.43
1.77	2.86	-0.17	-0.22	0.00	-0.04	-0.43
1.76	2.86	-0.17	-0.22	0.00	-0.04	-0.44
1.75	2.86	-0.16	-0.21	0.00	-0.04	-0.44
1.74	2.86	-0.16	-0.21	0.00	-0.04	-0.45
1.73	2.86	-0.16	-0.21	0.00	-0.04	-0.45
1.72	2.86	-0.15	-0.21	0.00	-0.04	-0.46
1.71	2.86	-0.15	-0.21	0.00	-0.04	-0.46
1.70	2.87	-0.14	-0.21	0.00	-0.04	-0.47
1.69	2.87	-0.14	-0.21	0.00	-0.04	-0.47
1.68	2.87	-0.14	-0.21	0.00	-0.04	-0.47
1.67	2.87	-0.14	-0.21	0.00	-0.05	-0.48
1.62	2.87	-0.12	-0.21	0.00	-0.05	-0.50
1.57	2.84	-0.12	-0.19	0.01	-0.05	-0.49
1.52	2.84	-0.10	-0.19	0.01	-0.05	-0.52
1.47	2.84	-0.07	-0.19	0.01	-0.05	-0.54
1.42	2.84	-0.04	-0.19	0.01	-0.06	-0.56
1.37	2.84	-0.01	-0.19	0.01	-0.06	-0.59
1.32	2.84	0.02	-0.19	0.01	-0.07	-0.62
1.27	2.84	0.06	-0.19	0.01	-0.07	-0.65
1.22	2.83	0.09	-0.19	0.01	-0.07	-0.67
1.17	2.80	0.11	-0.19	0.01	-0.07	-0.66
1.12	2.10	0.04	-0.15	0.01	0.01	0.00
1.07	2.10	0.04	-0.15	0.01	0.01	0.00
1.02	2.10	0.04	-0.15	0.01	0.01	0.00

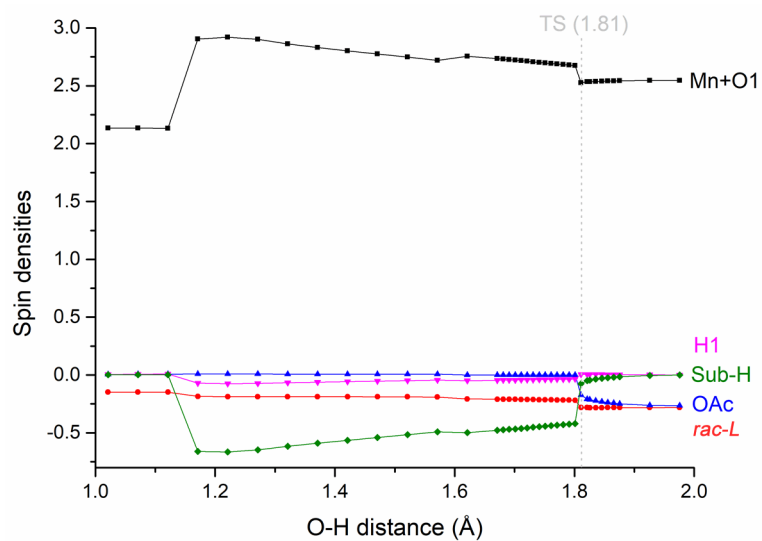


Figure S13. The plot of the spin density variation of key moieties by the approach of the oxo to the benzylic C-H group of 4-OH-PBA. Calculations were done at the UB3LYP-D3(BJ)/B1 level.

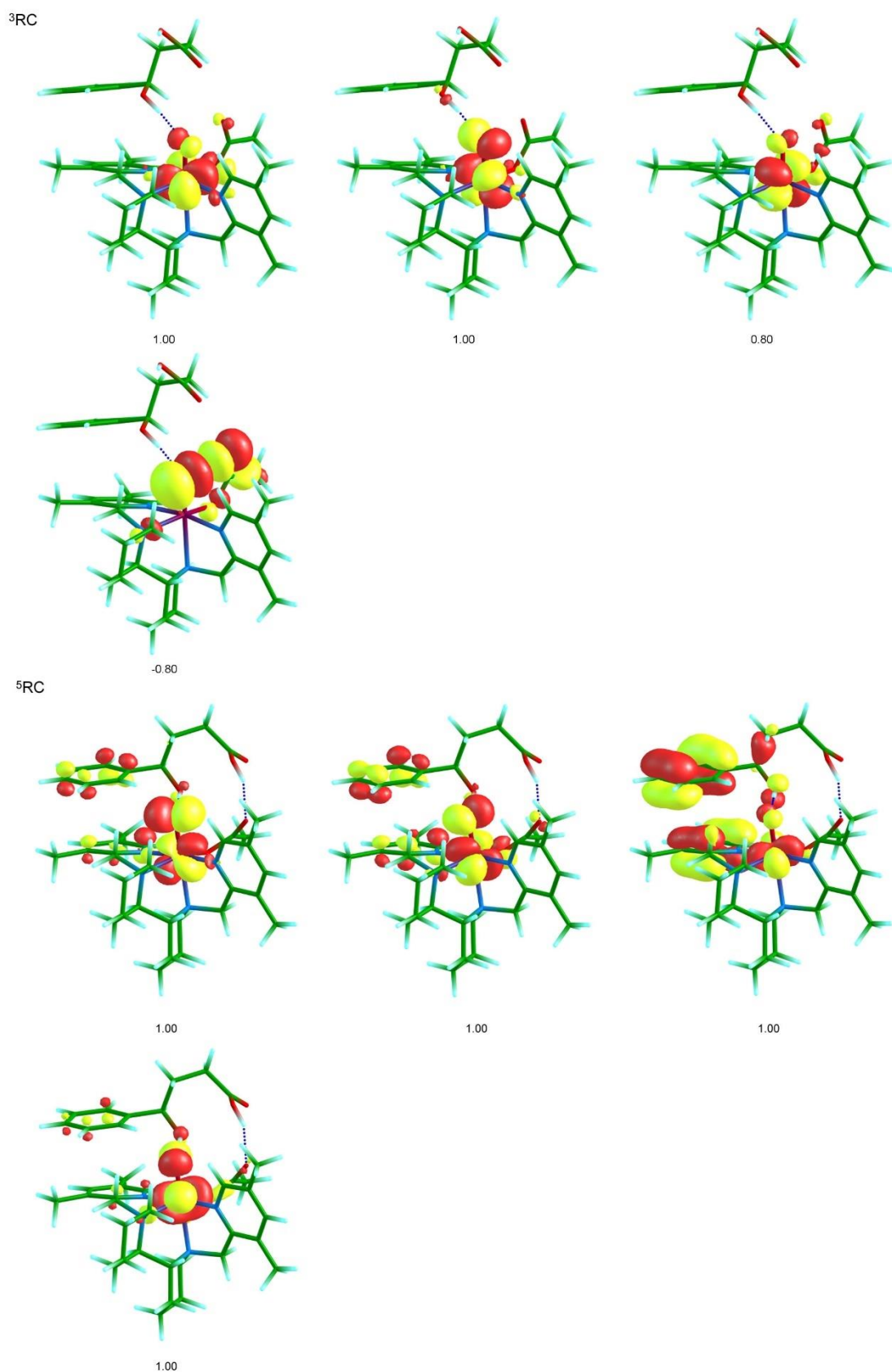
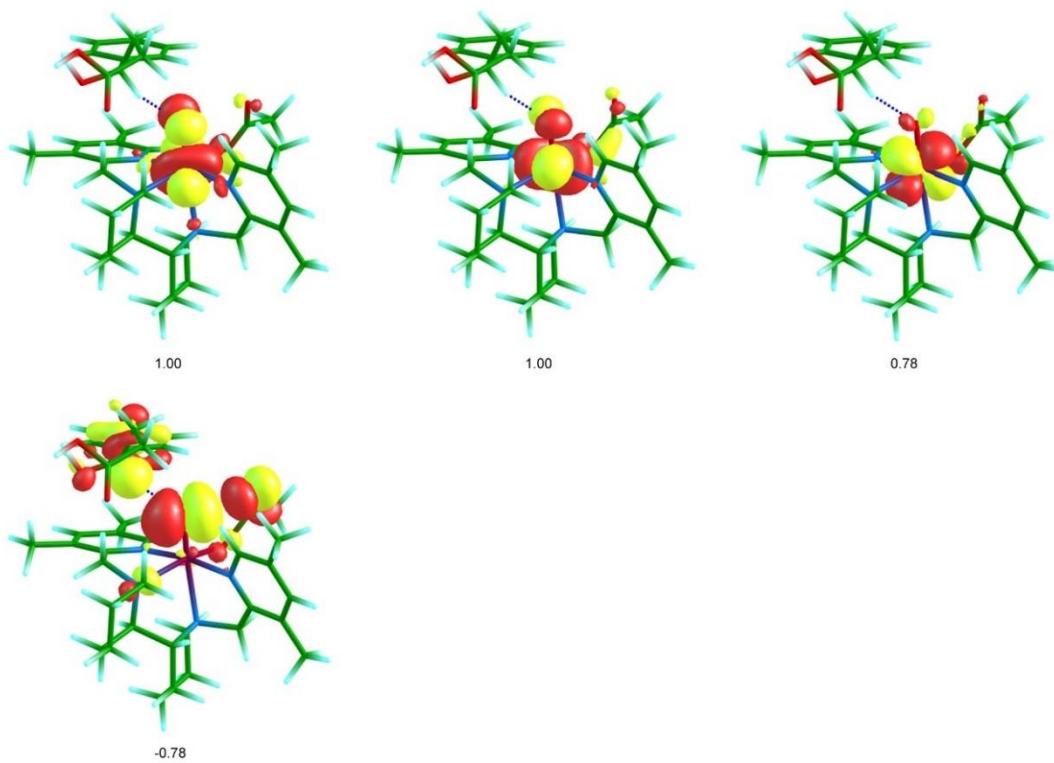


Figure S14. Singly-occupied natural orbitals (SNOs) of key moieties by the approach of the oxo to the benzylic C-H group of 4-OH-PBA. Calculations were done at the UB3LYP-D3(BJ)/B1 level in solvent. Positive values represent alpha-electron occupations and netative ones represent beta occupations. (To be continued)

³TS1



⁵TS1

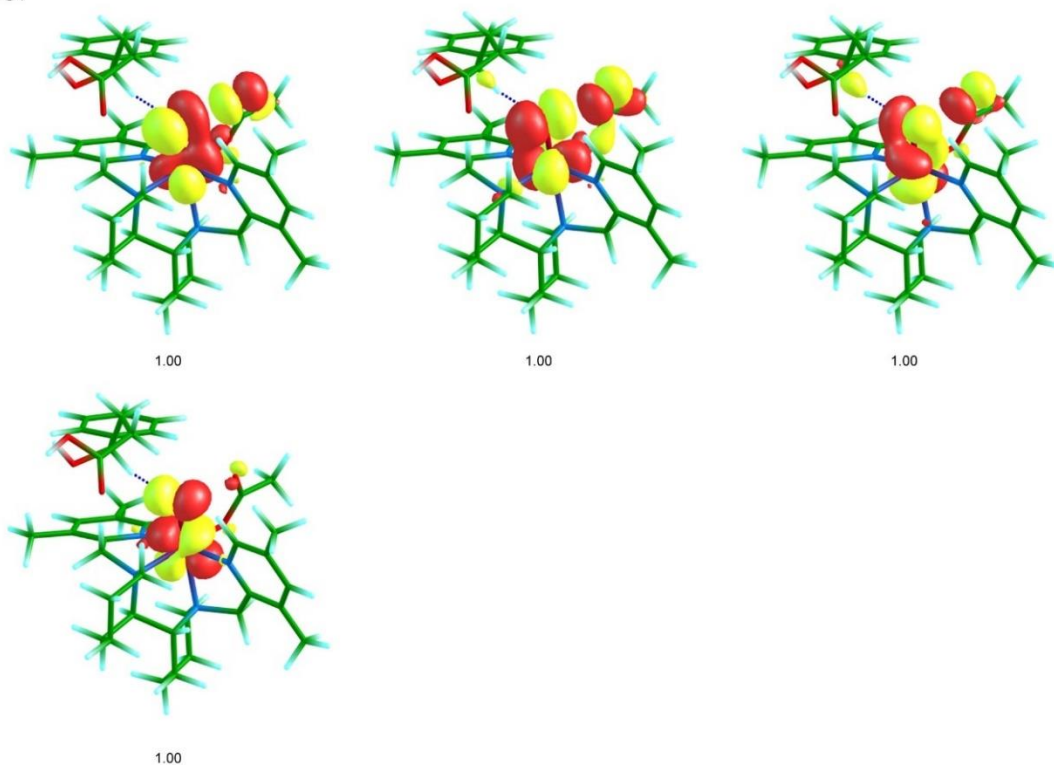
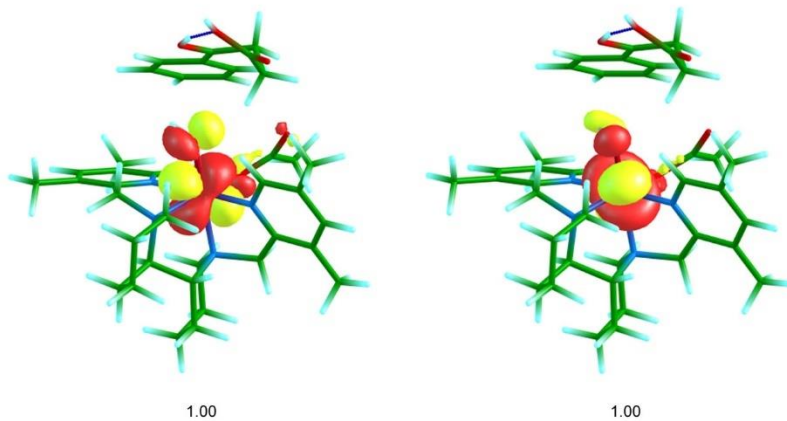


Figure S14. Singly-occupied natural orbitals (SNOs) of key moieties by the approach of the oxo to the benzylic C-H group of 4-OH-PBA. Calculations were done at the UB3LYP-D3(BJ)/B1 level in solvent. Positive and negative values represent alpha and netative ones represent beta occupations. (To be continued)

3IM1



5IM1

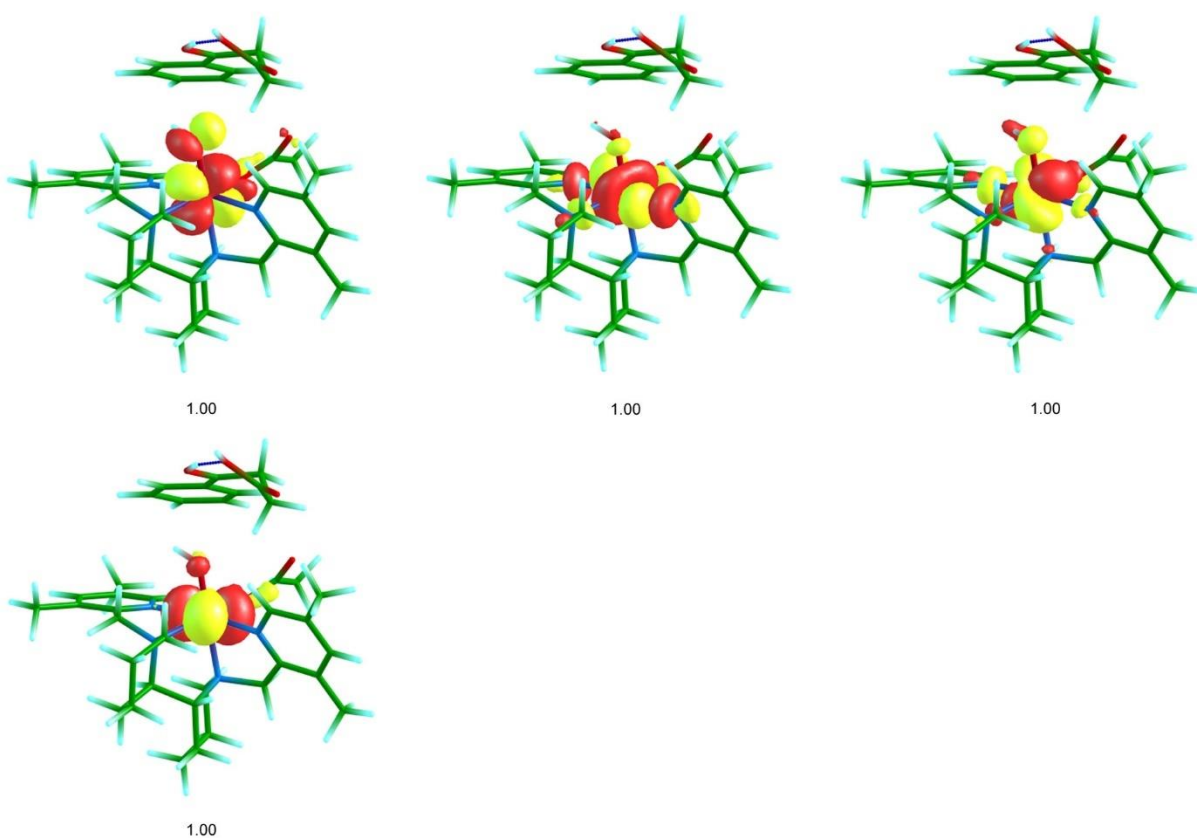
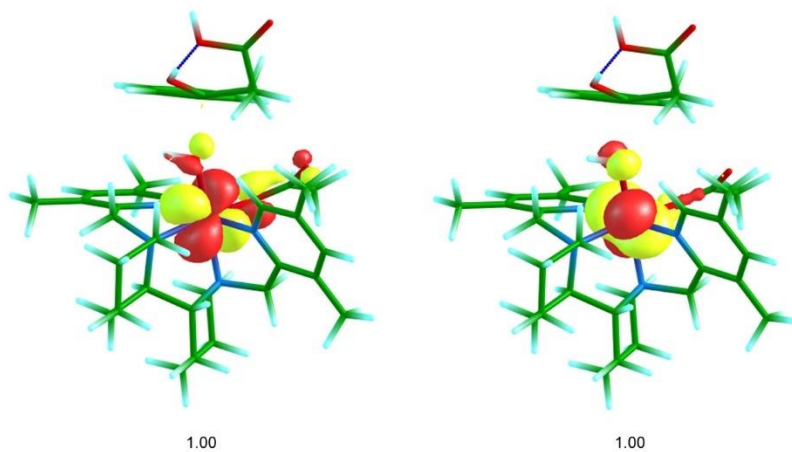


Figure S14. Singly-occupied natural orbitals (SNOs) of key moieties by the approach of the oxo to the benzylic C-H group of 4-OH-PBA. Calculations were done at the UB3LYP-D3(BJ)/B1 level in solvent. Positive values represent alpha-electron occupations. (To be continued)

${}^3\text{TS2}_{\text{diol}}$



${}^5\text{TS2}_{\text{diol}}$

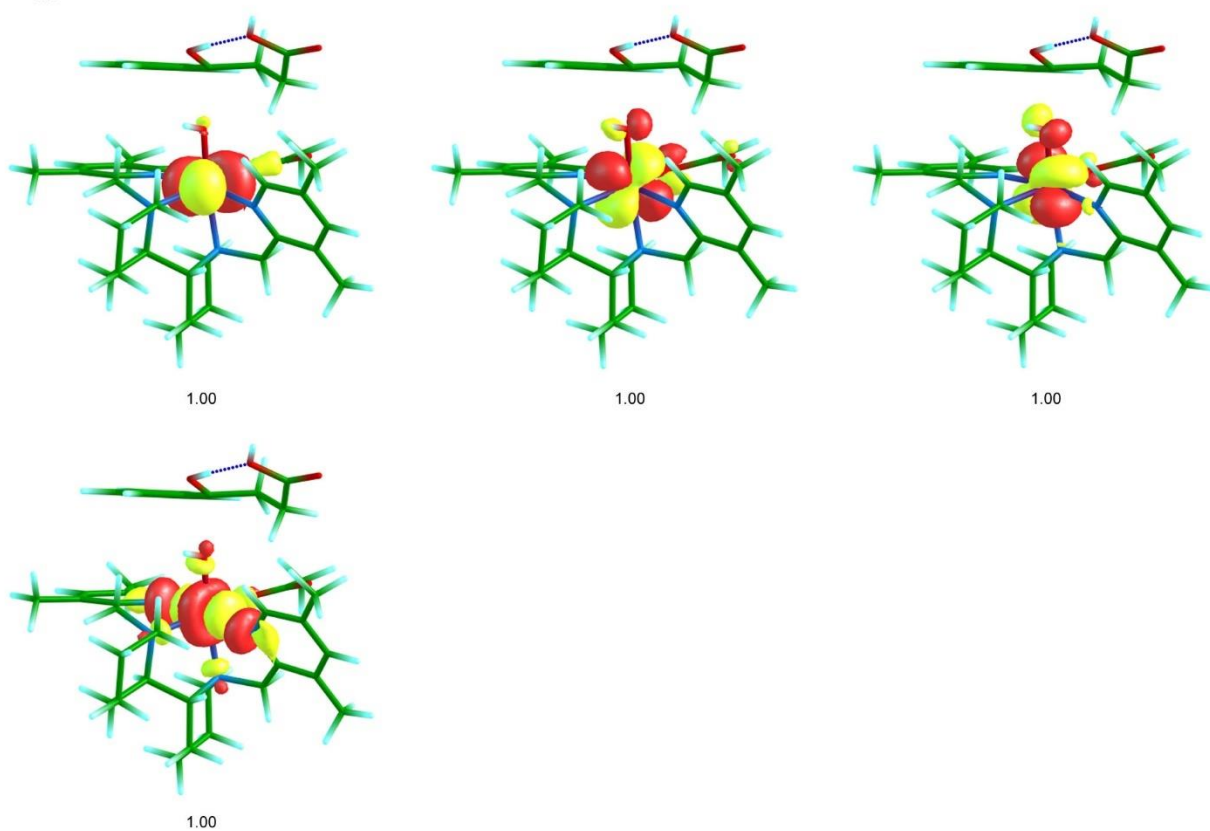
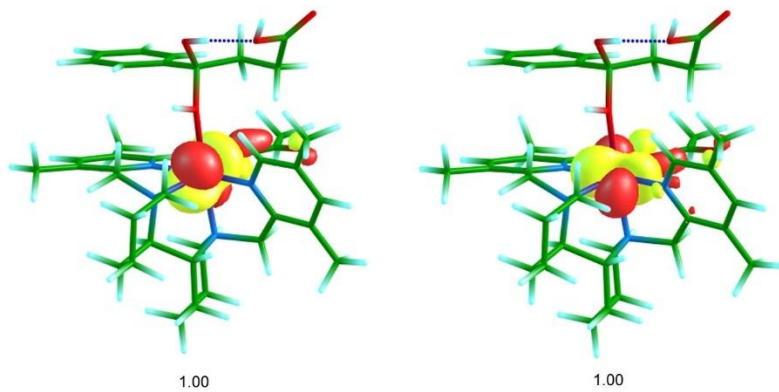


Figure S14. Singly-occupied natural orbitals (SNOs) of key moieties by the approach of the oxo to the benzylic C-H group of 4-OH-PBA. Calculations were done at the UB3LYP-D3(BJ)/B1 level in solvent. Positive values represent alpha-electron occupations. (To be continued)

${}^3\text{IM2}_{\text{diol}}$



${}^5\text{IM2}_{\text{diol}}$

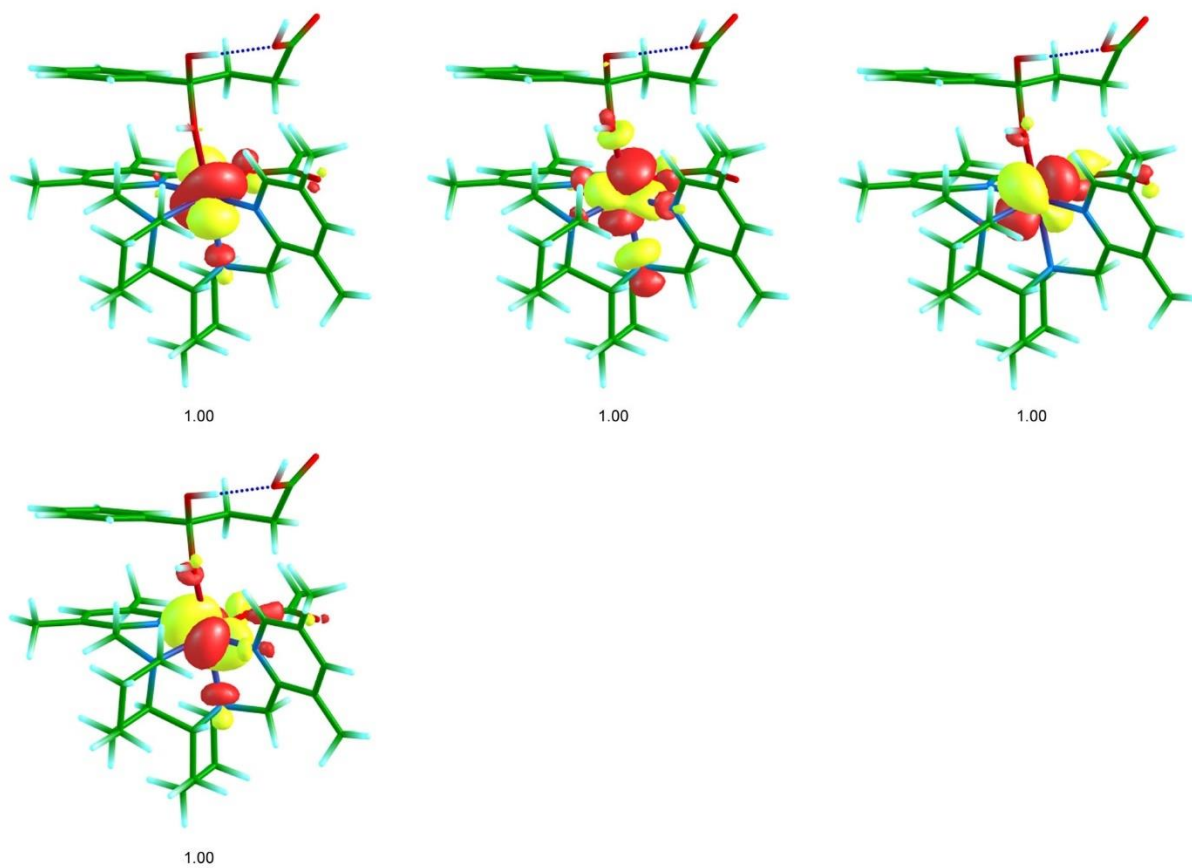
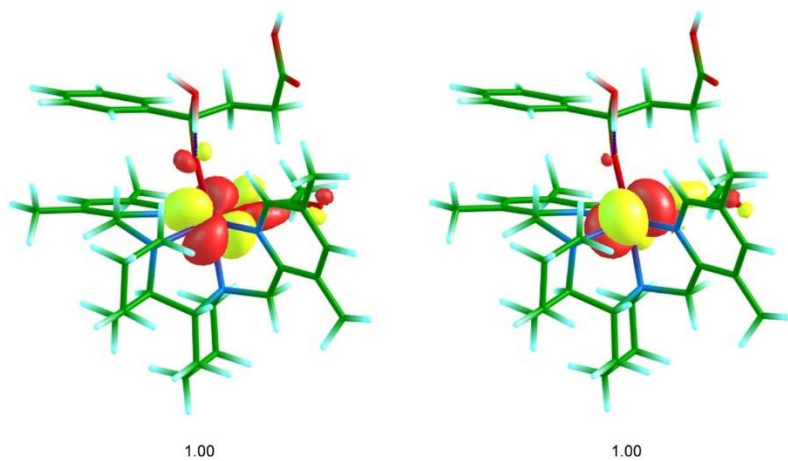


Figure S14. Singly-occupied natural orbitals (SNOs) of key moieties by the approach of the oxo to the benzylic C-H group of 4-OH-PBA. Calculations were done at the UB3LYP-D3(BJ)/B1 level in solvent. Positive values represent alpha-electron occupations. (To be continued)

³TS3



⁵TS3

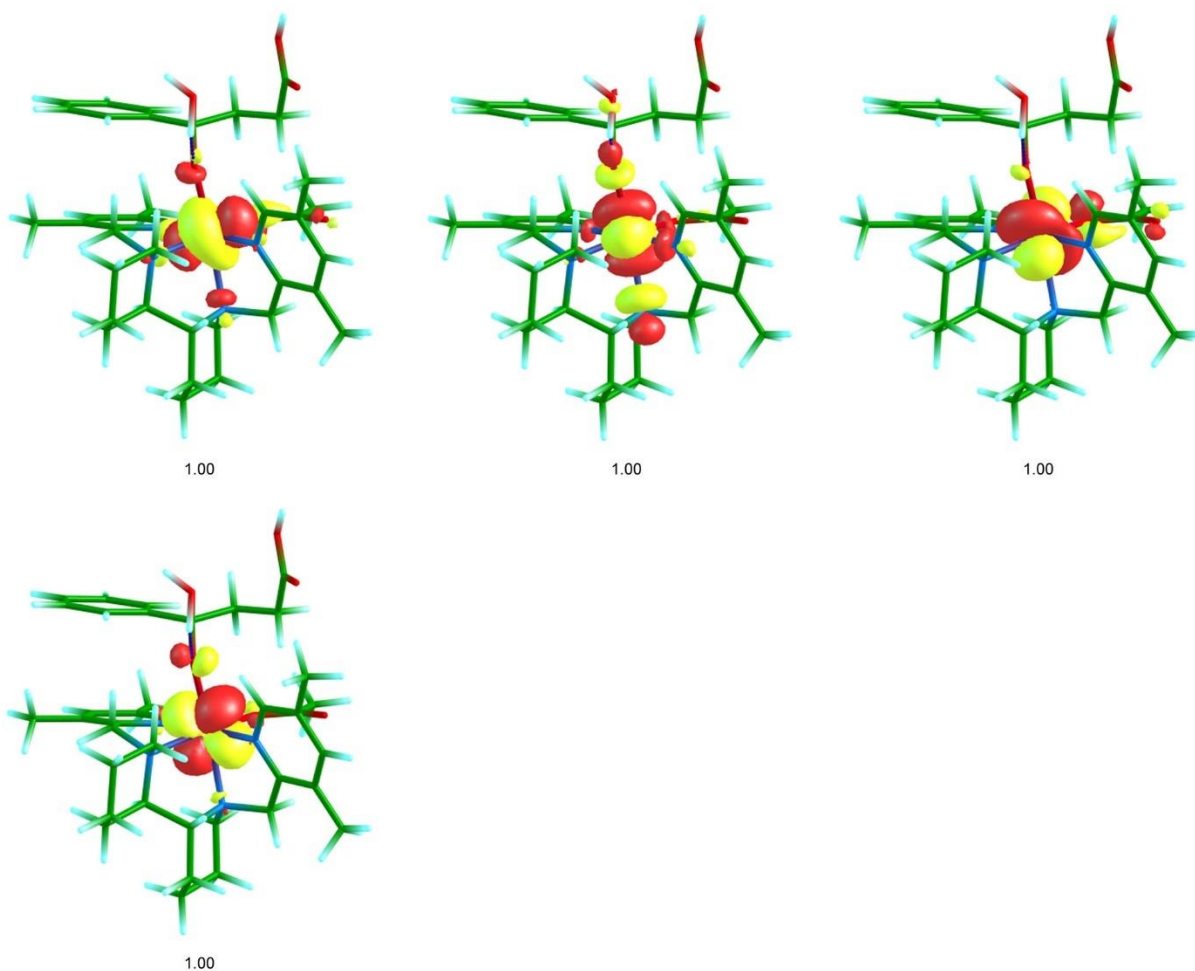
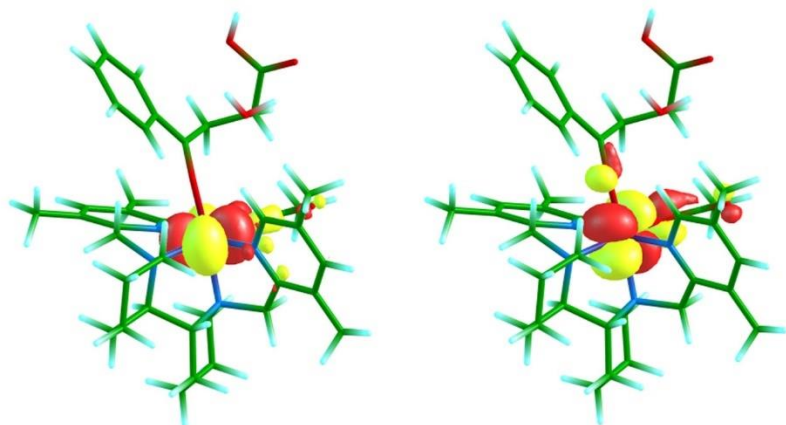


Figure S14. Singly-occupied natural orbitals (SNOs) of key moieties by the approach of the oxo to the benzylic C-H group of 4-OH-PBA. Calculations were done at the UB3LYP-D3(BJ)/B1 level in solvent. Positive values represent alpha-electron occupations. (To be continued)

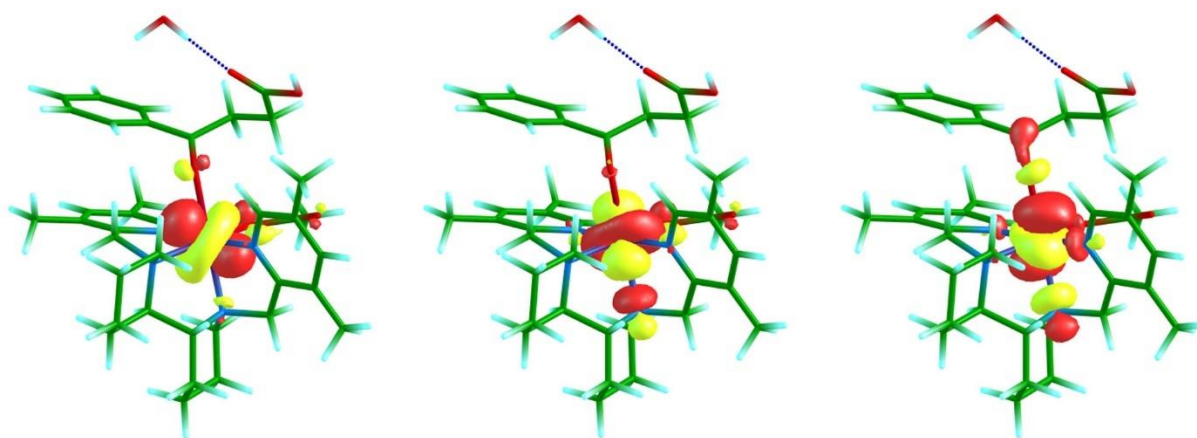
³PC



1.00

1.00

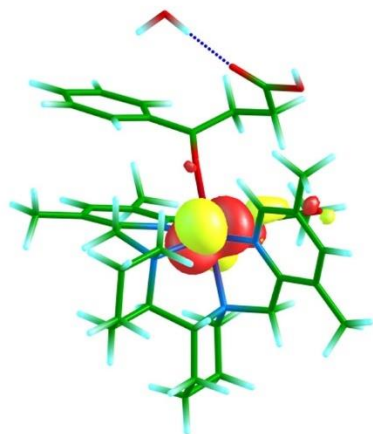
⁵PC



1.00

1.00

1.00



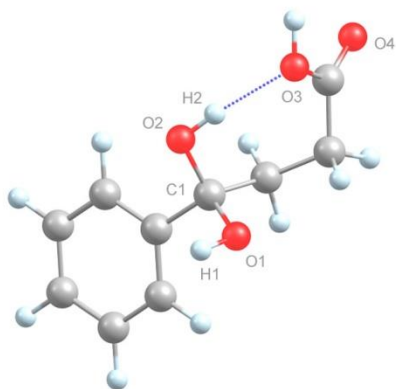
1.00

Figure S14. Singly-occupied natural orbitals (SNOs) of key moieties by the approach of the oxo to the benzylic C-H group of 4-OH-PBA. Calculations were done at the UB3LYP-D3(BJ)/B1 level in solvent. Positive values represent alpha-electron occupations.

Table S13. Various SCF and Gibbs free energies of the water-assisted dehydration of the *gem*-diol complex. Calculations were done at the UB3LYP-D3(BJ)/B2//B1 level in solvent.

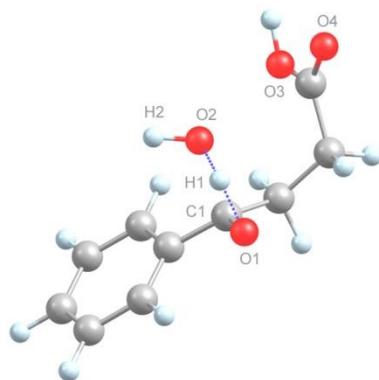
1. without water						
	OPT/B1+ZPE	ΔE	SPE/B2+ZPE	ΔE	G	ΔG
RC₀	-689.194258	0.0	-689.345546	0.0	-689.235452	0.0
TS₀	-689.139326	34.5	-689.290366	34.6	-689.180384	34.6
PC₀	-689.207875	-8.5	-689.358430	-8.1	-689.252232	-10.5
2. one water						
	OPT/B1+ZPE	ΔE	SPE/B2+ZPE	ΔE	G	ΔG
RC₁	-765.649675	0.0	-765.806056	0.0	-765.694391	0.0
TS₁	-765.618317	19.7	-765.773474	20.4	-765.661275	20.8
PC₁	-765.665310	-9.8	-765.821687	-9.8	-765.714121	-12.4
3. two water						
	OPT/B1+ZPE	ΔE	SPE/B2+ZPE	ΔE	G	ΔG
RC₂	-842.110563	0.0	-842.270757	0.0	-842.158104	0.0
TS₂	-842.082319	17.7	-842.241032	18.7	-842.127555	19.2
PC₂	-842.125754	-9.5	-842.287249	-10.3	-842.174841	-10.5

C1-O1 = 1.425
 C1-O2 = 1.415
 H1-O2 = 2.507
 H1-O1 = 0.966
 \angle O2-H2-O3 = 158.4



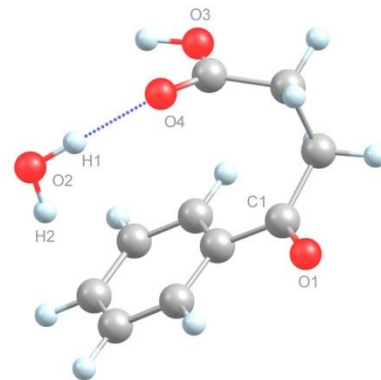
RC₀

H1-O2 = 1.233
 H1-O1 = 1.230
 C1-O1 = 1.330
 C1-O2 = 1.815
 \angle O1-H1-O2 = 127.4
 $\nu_{\text{img}} = i 1818.8$



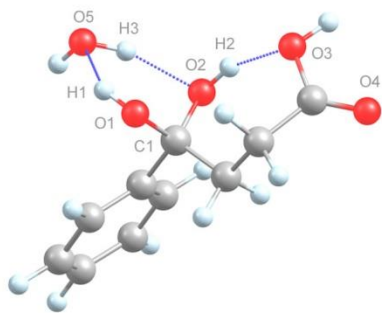
TS₀

H1-O2 = 0.971
 H1-O1 = 4.819
 C1-O1 = 1.225
 C1-O2 = 4.818
 \angle O2-H1-O4 = 179.5



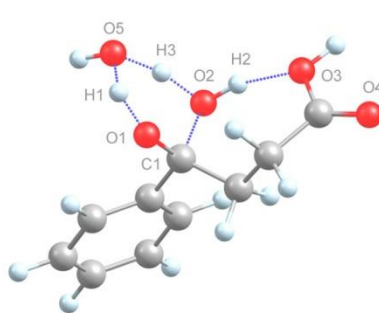
PC₀

C1-O1 = 1.415
 \angle O1-H1-O5 = 148.4
 C1-O2 = 1.432
 \angle O5-H3-O2 = 146.0
 H2-O3 = 1.865
 H3-O2 = 1.933
 H1-O5 = 1.960



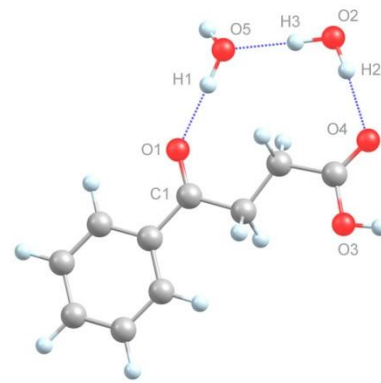
RC₁

H1-O1 = 1.278
 \angle O1-H1-O5 = 148.4
 H1-O5 = 1.162
 \angle C1-O2-H2 = 107.6
 H3-O5 = 1.266
 \angle O2-H3-O5 = 146.0
 $\nu_{\text{img}} = i 1370.5$
 H3-O2 = 1.167
 C1-O2 = 1.659
 C1-O1 = 1.324



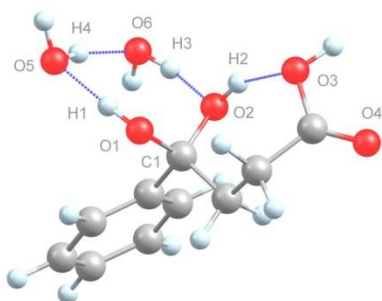
TS₁

H1-O1 = 1.824
 \angle O1-H1-O5 = 178.3
 H3-O5 = 1.855
 \angle O2-H3-O5 = 178.8
 H2-O4 = 1.963
 C1-O1 = 1.231



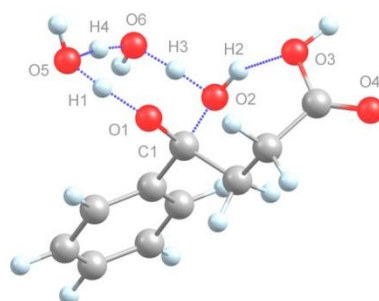
PC₁

C1-O1 = 1.402
 \angle O1-H1-O5 = 176.2
 C1-O2 = 1.440
 \angle O5-H4-O6 = 163.4
 H2-O3 = 1.887
 \angle O6-H3-O2 = 166.8
 H3-O2 = 1.778
 H1-O5 = 1.767
 O6-H4 = 1.764



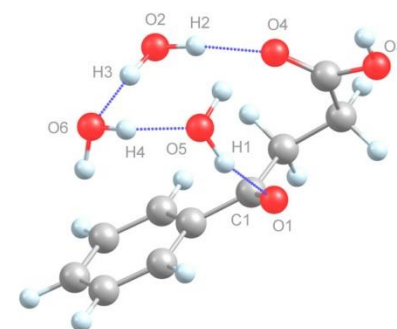
RC₂

H1-O5 = 1.119
 H1-O1 = 1.331
 O5-H4 = 1.337
 O6-H4 = 1.109
 H3-O2 = 1.240
 H3-O6 = 1.178
 H2-O3 = 1.848
 C1-O2 = 1.595
 C1-O1 = 1.322
 \angle O6-H3-O2 = 172.9
 \angle C1-O2-H2 = 106.5
 \angle O1-H1-O5 = 172.7
 \angle O5-H4-O6 = 165.7
 $\nu_{\text{img}} = i 1018.8$



TS₂

C1-O1 = 1.231
 \angle O1-H1-O5 = 149.4
 H1-O1 = 1.966
 \angle O5-H4-O6 = 168.2
 H4-O5 = 1.807
 \angle O6-H3-O2 = 170.8
 H3-O6 = 1.856
 \angle O2-H2-O4 = 172.4
 H2-O4 = 1.967



PC₂

Figure S15. Optimized structures of the intermediates of the water-assisted dehydration of the *gem*-diol complex. Calculations were done at the UB3LYP-D3(BJ)/B1 level in solvent. Hydrogen atoms of *rac*-L are omitted for clarity. Lengths are in Å units, angles are in degree units and imaginary frequencies are in cm⁻¹ units.

Part V Alcohol oxidation of 4-OH-PBA by the Mn^{IV}(O)(AcO[•]) species 2 via the DHA and R-DHA mechanisms.

Table S14. Various SCF and Gibbs free energies of the alcohol oxidation via the dual hydrogen abstraction (DHA) mechanism. Calculations were done at the UB3LYP-D3(BJ)/B2//B1 level in solvent.

	OPT/B1+ZPE	ΔE	SPE/B2+ZPE	ΔE	G	ΔG
³ RC	-3300.863742	0.0	-3301.392463	0.0	-3300.949328	0.0
⁵ RC	-3300.857928	3.6	-3301.379967	7.8	-3300.939823	6.0
³ TS1	-3300.862878	0.5	-3301.389706	1.7	-3300.944997	2.7
⁵ TS1	-3300.845133	11.7	-3301.371437	13.2	-3300.929341	12.5
³ IM1	-3300.932137	-42.9	-3301.458993	-41.7	-3301.015303	-41.4
⁵ IM1	-3300.952417	-55.6	-3301.478231	-53.8	-3301.039626	-56.7
³ TS2 _{DHA}	-3300.931139	-42.3	-3301.458500	-41.4	-3301.014142	-40.7
⁵ TS2 _{DHA}	-3300.950728	-54.6	-3301.476601	-52.8	-3301.036120	-54.5
³ PC	-3300.977673	-71.5	-3301.504299	-70.2	-3301.063147	-71.4
⁵ PC	-3300.990461	-79.5	-3301.515431	-77.2	-3301.075405	-79.1

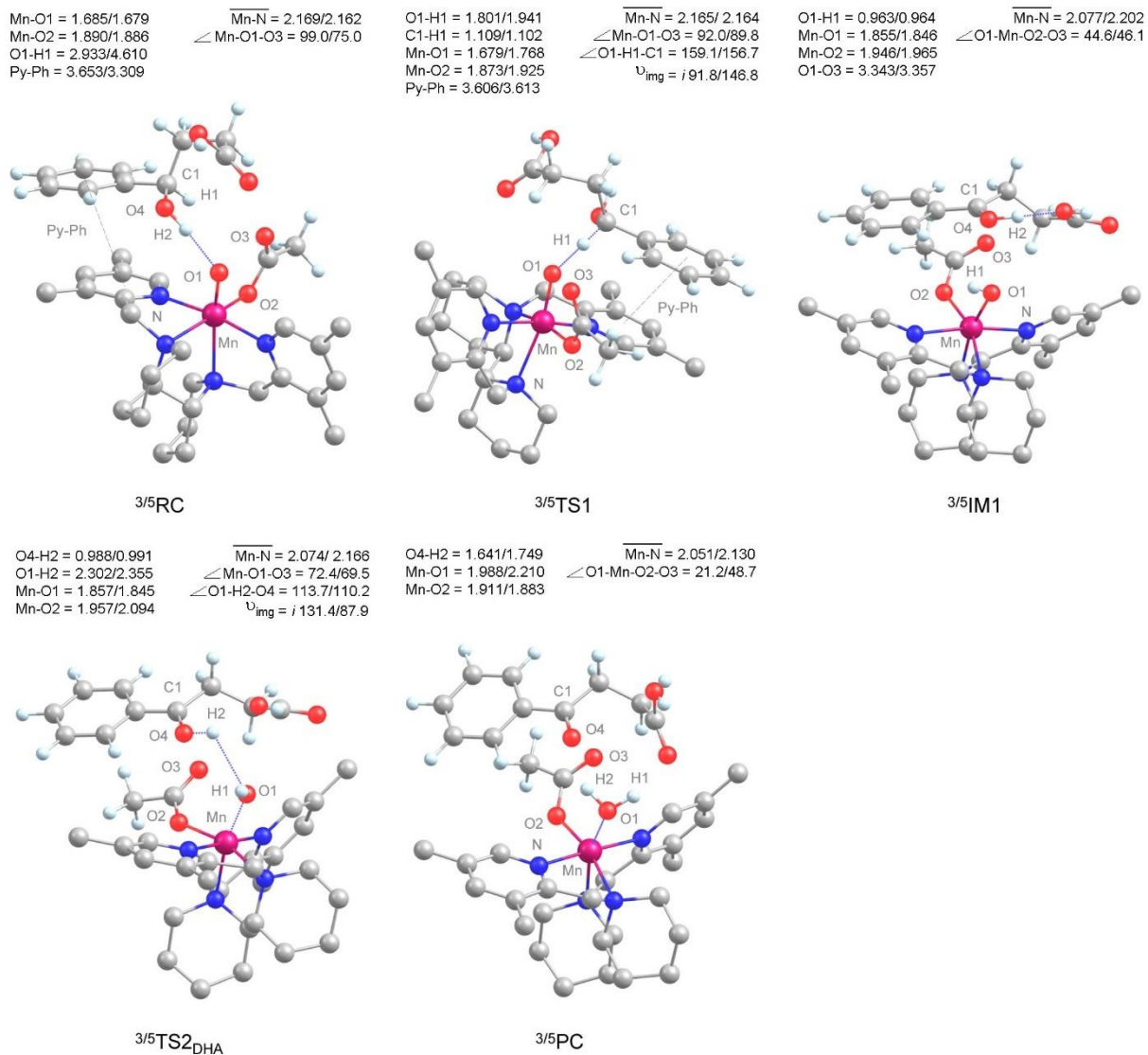


Figure S16. Optimized structures of key intermediates of the alcohol oxidation via the dual hydrogen abstraction (DHA) mechanism. Calculations were done at the UB3LYP-D3(BJ)/B1 level in solvent. Hydrogen atoms of *rac*-L are omitted for clarity. Lengths are in Å units, angles are in degree units and imaginary frequencies are in cm^{-1} units.

Table S15. Mulliken charges and spin densities of key intermediates of the alcohol oxidation via the dual hydrogen abstraction (DHA) mechanism.

	Mulliken charge						spin densities					
	Mn	O1	<i>rac</i> -L	OAc	H1	Sub-H1	Mn	O1	<i>rac</i> -L	OAc	H1	Sub-H1
³RC	0.49	-0.25	1.81	-0.09	0.14	-0.10	2.95	-0.41	-0.28	-0.27	0.00	0.00
⁵RC	0.63	-0.57	1.77	-0.37	0.14	0.40	2.71	0.44	0.23	-0.01	0.00	0.63
³TS1	0.51	-0.27	1.81	-0.19	0.12	0.01	2.97	-0.45	-0.28	-0.12	0.00	-0.12
⁵TS1	0.54	-0.32	1.75	-0.13	0.13	0.03	3.04	0.81	-0.26	0.26	0.00	0.16
³IM1	0.66	-0.70	1.29	-0.55	0.32	0.97	2.09	0.05	-0.15	-0.01	0.01	0.00
⁵IM1	0.91	-0.69	1.04	-0.56	0.32	0.97	3.97	0.00	0.00	0.02	0.01	0.00
³TS2_{DHA}	0.67	-0.69	1.32	-0.55	0.32	0.94	2.09	0.05	-0.14	-0.01	0.01	0.00
⁵TS2_{DHA}	0.88	-0.69	1.19	-0.65	0.33	0.95	3.97	-0.01	-0.04	0.07	0.01	0.00
³PC	0.57	-0.60	1.57	-0.39	0.38	0.48	2.15	-0.01	-0.16	0.02	0.00	0.00
⁵PC	0.83	-0.69	1.43	-0.44	0.38	0.49	4.03	0.03	-0.06	-0.01	0.00	0.00

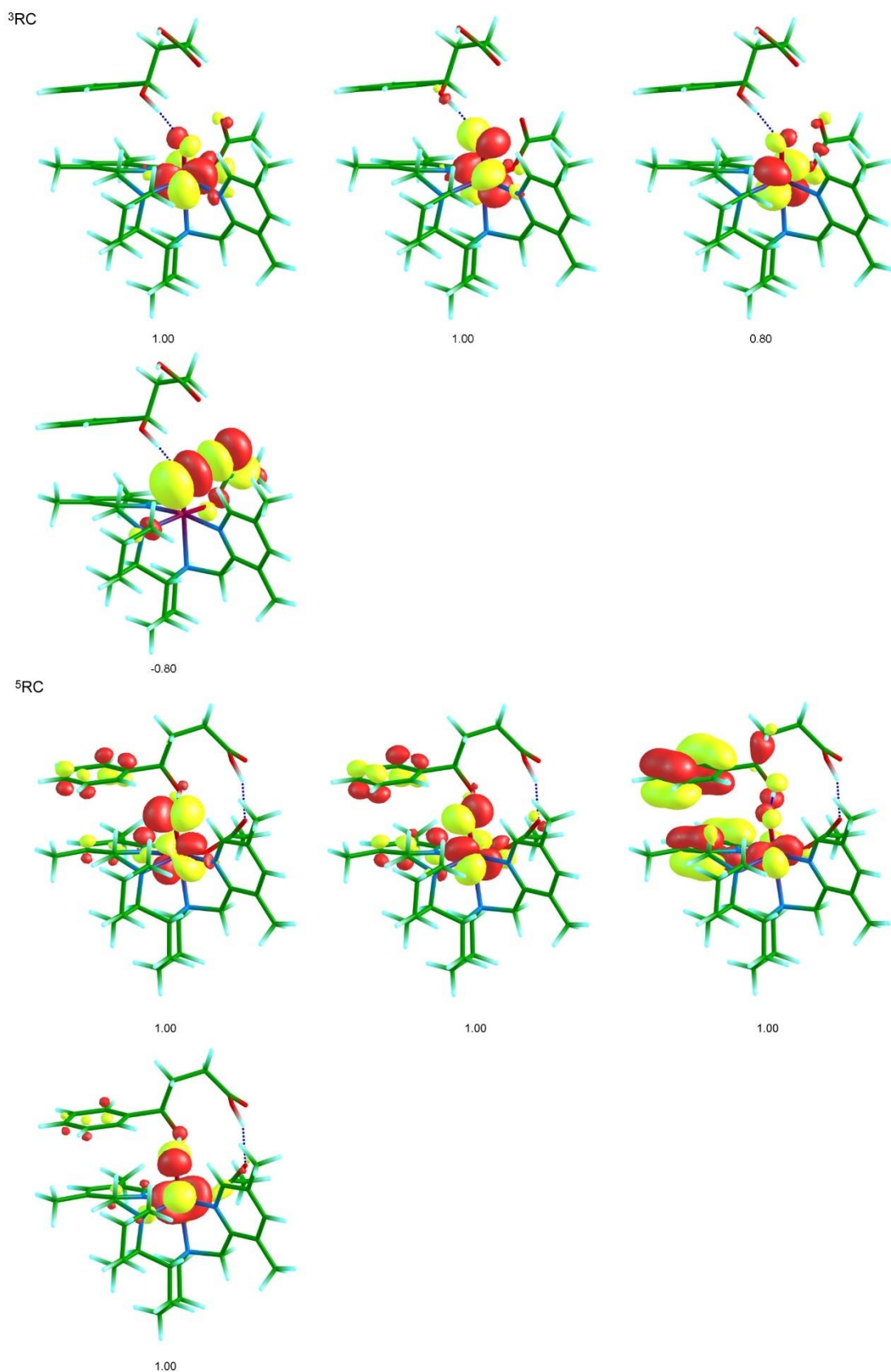
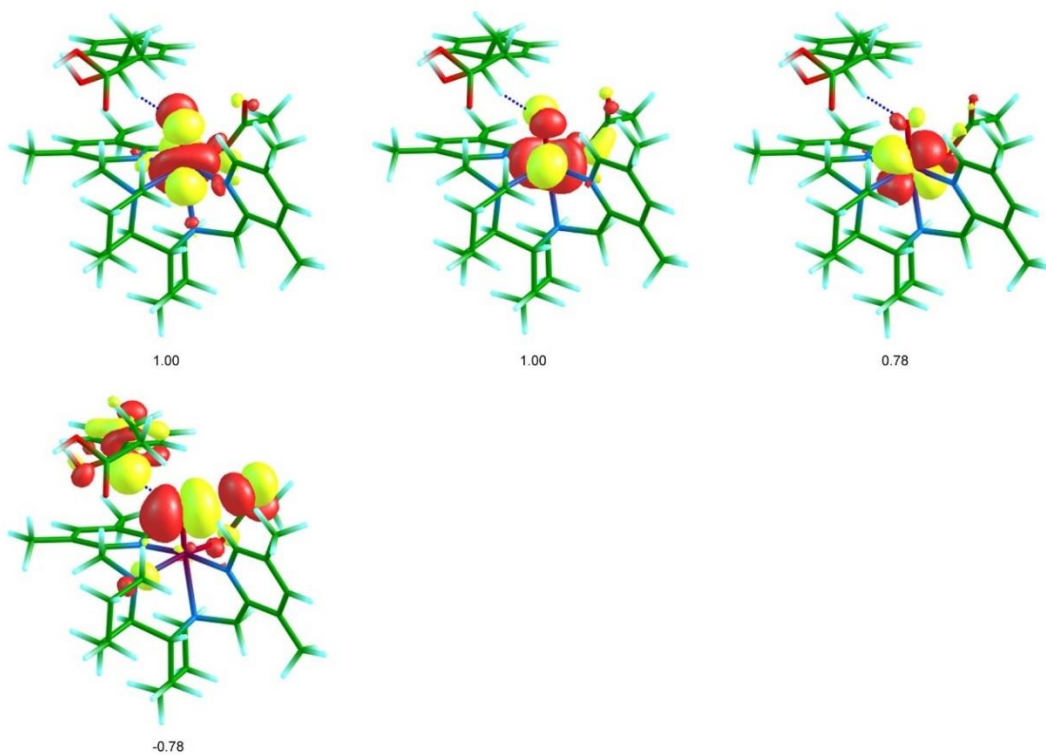


Figure S17. Singly-occupied natural orbitals (SNOs) of key intermediates of the alcohol oxidation via the dual hydrogen abstraction (DHA) mechanism. Calculations were done at the UB3LYP-D3(BJ)/B1 level in solvent. Positive values represent alpha-electron occupations and negative ones represent beta occupations. (To be continued)

³TS1



⁵TS1

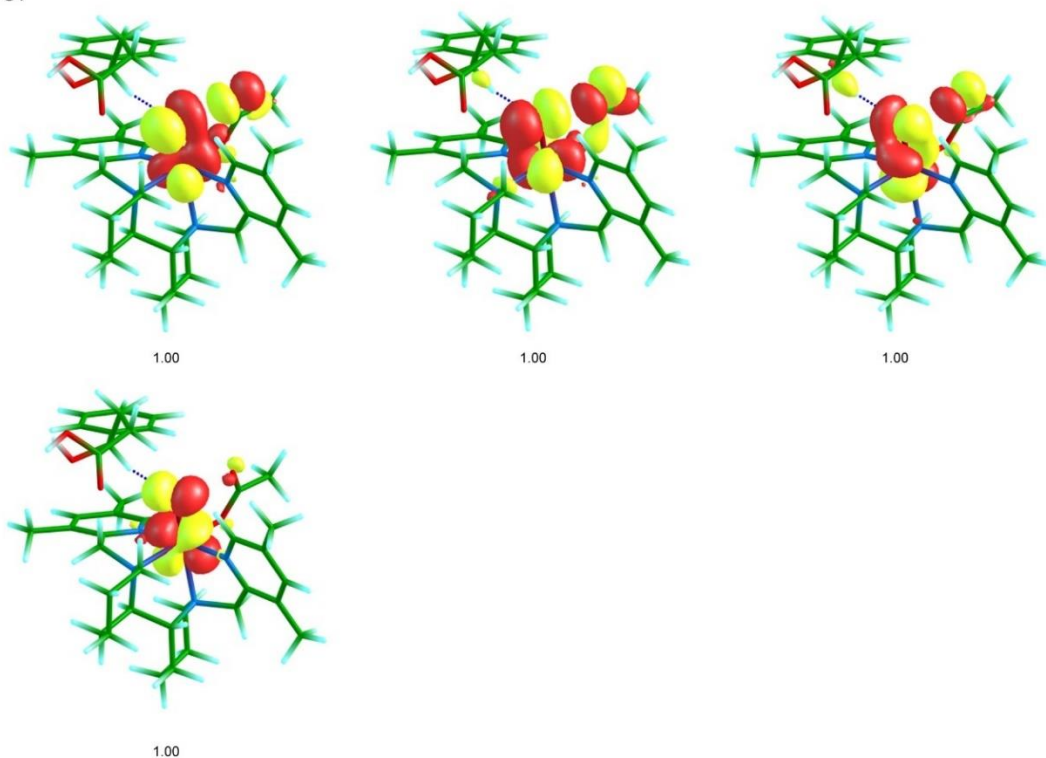
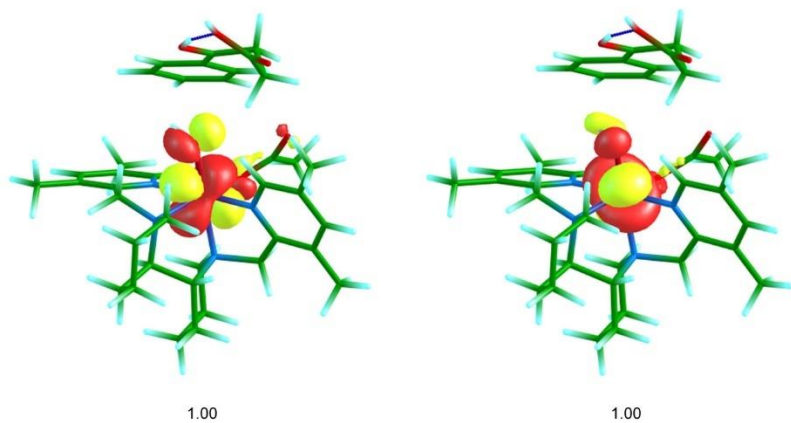


Figure S17. Singly-occupied natural orbitals (SNOs) of key intermediates of the alcohol oxidation via the dual hydrogen abstraction (DHA) mechanism. Calculations were done at the UB3LYP-D3(BJ)/B1 level in solvent. Positive and negative values represent alpha and netative ones represent beta occupations. (To be continued)

³IM1



⁵IM1

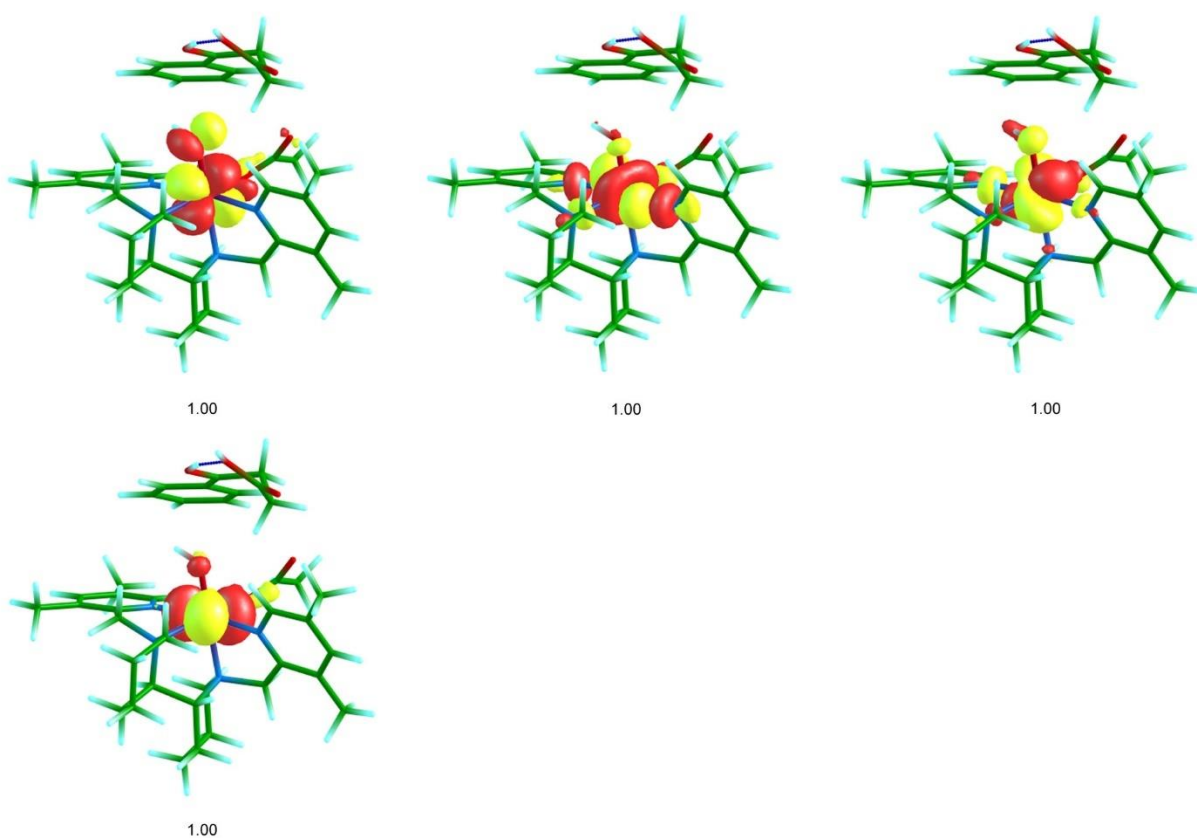
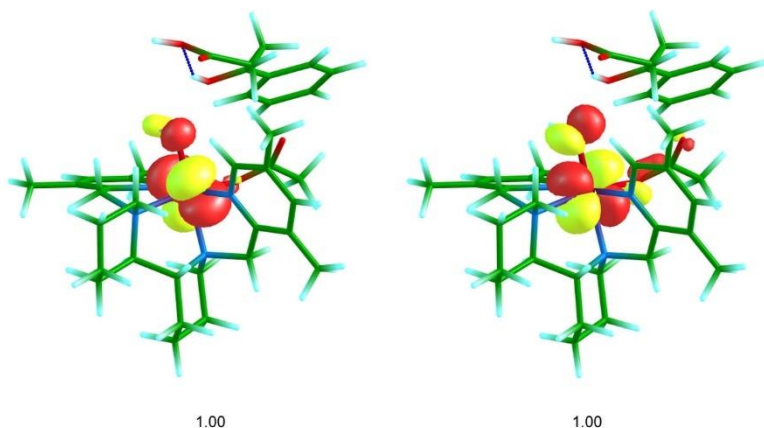


Figure S17. Singly-occupied natural orbitals (SNOs) of key intermediates of the alcohol oxidation via the dual hydrogen abstraction (DHA) mechanism. Calculations were done at the UB3LYP-D3(BJ)/B1 level in solvent. Positive values represent alpha-electron occupations. (To be continued)

$^3\text{TS2}_{\text{DHA}}$



$^5\text{TS2}_{\text{DHA}}$

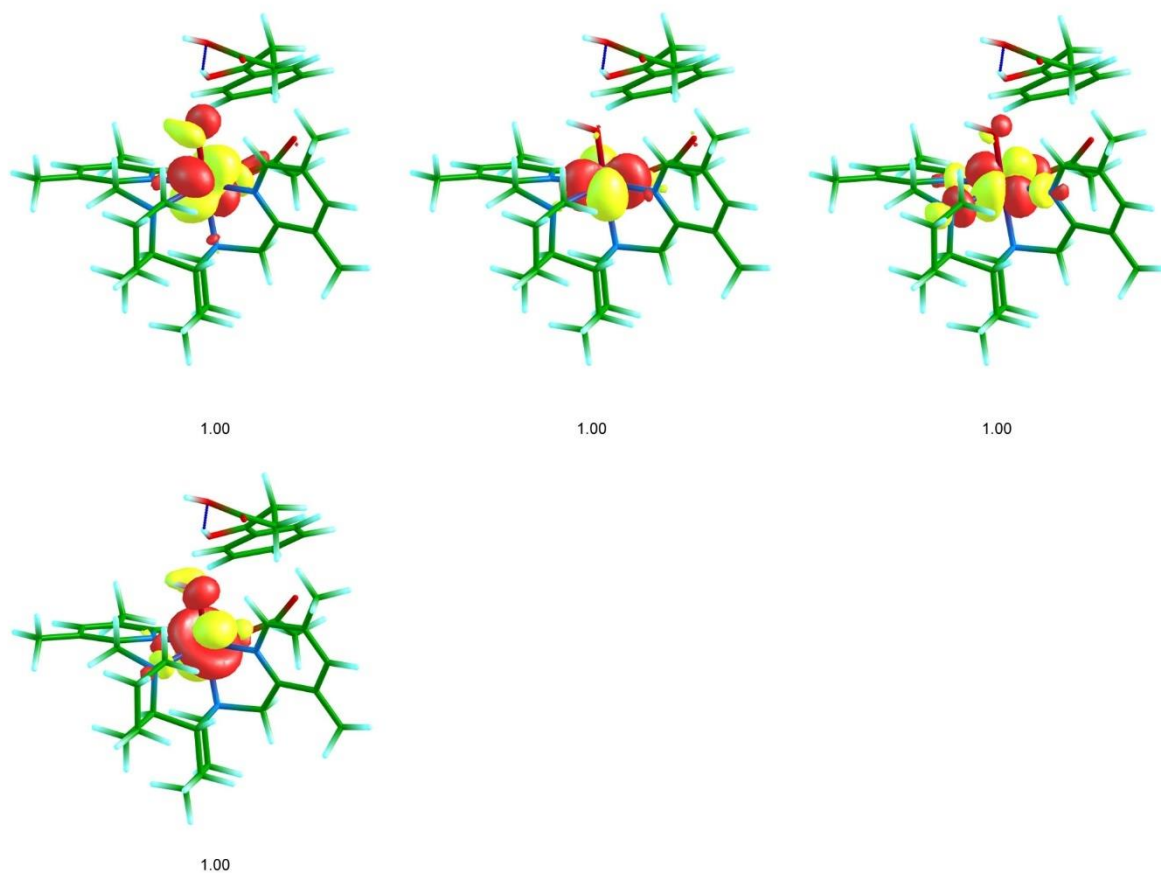
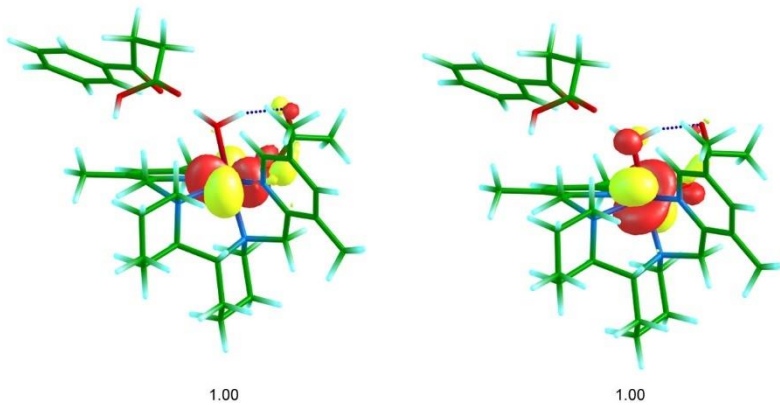


Figure S17. Singly-occupied natural orbitals (SNOs) of key intermediates of the alcohol oxidation via the dual hydrogen abstraction (DHA) mechanism. Calculations were done at the UB3LYP-D3(BJ)/B1 level in solvent. Positive values represent alpha-electron occupations. (To be continued)

^3PC



^5PC

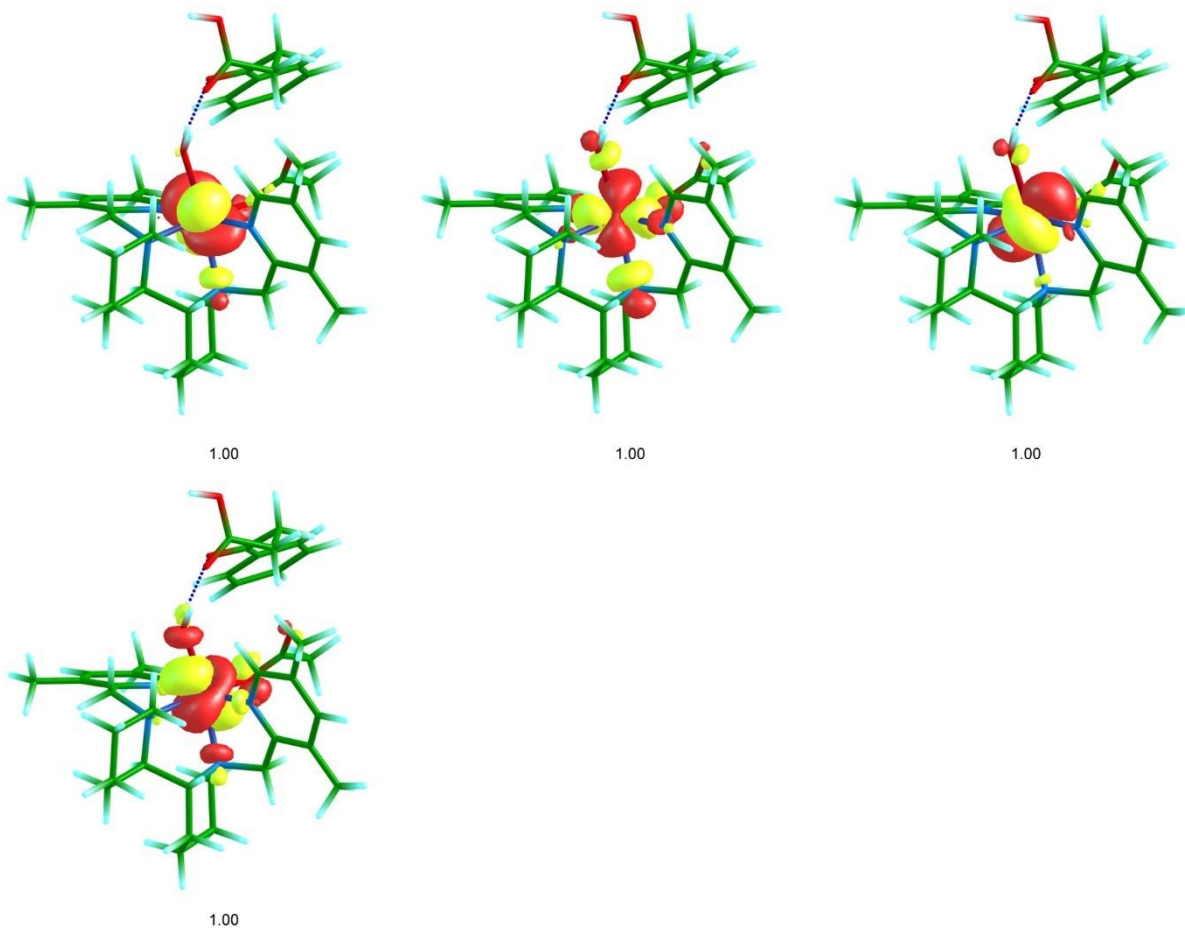


Figure S17. Singly-occupied natural orbitals (SNOs) of key intermediates of the alcohol oxidation via the dual hydrogen abstraction (DHA) mechanism. Calculations were done at the UB3LYP-D3(BJ)/B1 level in solvent. Positive values represent alpha-electron occupations.

Table S16. Various SCF and Gibbs free energies of key intermediates of the alcohol oxidation via the reversed-dual hydrogen abstraction (R-DHA) mechanism. Calculations were done at the UB3LYP-D3(BJ)/B2//B1 level in solvent.

	OPT/B1+ZPE	ΔE	SPE/B2+ZPE	ΔE	G	ΔG
³RC	-3300.863742 ^a	0.0	-3301.392463	0.0	-3300.949328	0.0
⁵RC	-3300.857928	3.6	-3301.379967	7.8	-3300.939823	6.0
³TS1_{OH}	-3300.862077	1.0	-3301.386804	3.6	-3300.948573	0.5
⁵TS1_{OH}	-3300.856629	4.5	-3301.379831	7.9	-3300.940961	5.3
³IM1_{OH}	-3300.875001	-7.1	-3301.399817	-4.6	-3300.958342	-5.7
⁵IM1_{OH}	-3300.875028	-7.1	-3301.399844	-4.6	-3300.958859	-6.0
³TS2_{CH}	-3300.862650	0.7	-3301.386318	3.9	-3300.943775	3.5
⁵TS2_{CH}	-3300.867065	-2.1	-3301.391130	0.8	-3300.951719	-1.5
³PC	-3300.976571	-70.8	-3301.501783	-68.6	-3301.059945	-69.4
⁵PC	-3300.990511	-79.5	-3301.514005	-76.3	-3301.077113	-80.2

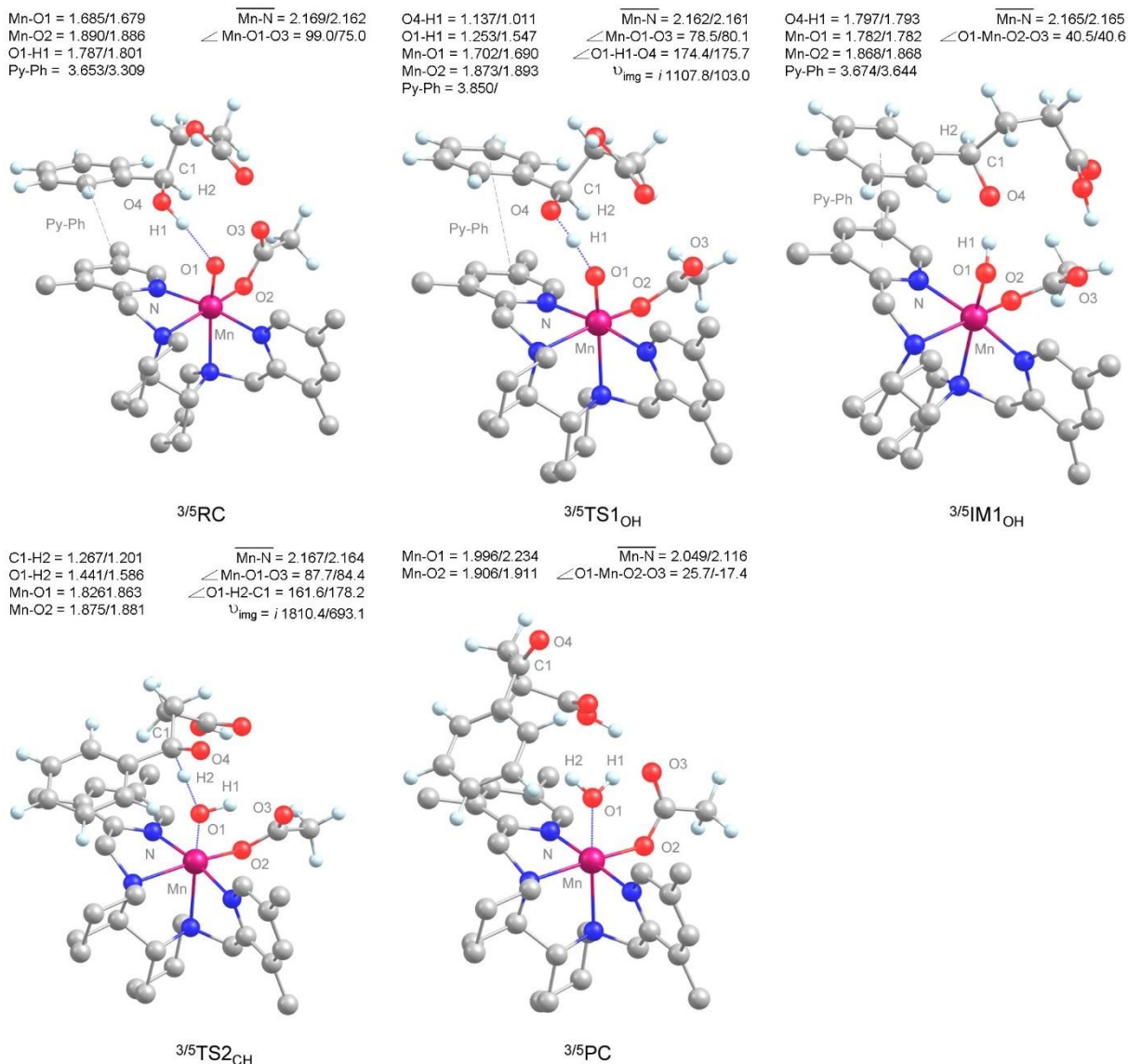


Figure S18. Optimized structures of key intermediates of the alcohol oxidation via the reversed-dual hydrogen abstraction (R-DHA) mechanism. Calculations were done at the UB3LYP-D3(BJ)/B1 level in solvent. Hydrogen atoms of *rac-L* are omitted for clarity. Lengths are in Å units, angles are in degree units and imaginary frequencies are in cm^{-1} units.

Table S17. Mulliken charges and spin densities of key intermediates of the alcohol oxidation via the reversed-dual hydrogen abstraction (R-DHA) mechanism. Calculations were done at the UB3LYP-D3(BJ)/B2//B1 level in solvent.

	Mulliken charge						spin densities					
	Mn	O1	<i>rac</i> -L	OAc	H1	Sub-H1	Mn	O1	<i>rac</i> -L	OAc	H1	Sub-H1
³RC	0.49	-0.25	1.81	-0.09	0.34	-0.30	2.95	-0.41	-0.28	-0.27	0.00	0.00
⁵RC	0.63	-0.57	1.77	-0.37	0.34	0.21	2.71	0.44	0.23	-0.01	0.00	0.63
³TS1_{OH}	0.63	-0.54	1.60	-0.36	0.31	0.35	2.90	0.22	-0.20	-0.01	0.01	-0.93
⁵TS1_{OH}	0.62	-0.56	1.53	-0.37	0.34	0.44	2.82	0.40	-0.15	-0.01	0.00	0.94
³IM1_{OH}	0.57	-0.50	1.82	-0.29	0.36	0.04	3.20	0.09	-0.32	0.00	0.02	-0.99
⁵IM1_{OH}	0.57	-0.50	1.82	-0.29	0.36	0.04	3.20	0.09	-0.29	0.00	0.00	1.00
³TS2_{CH}	0.60	-0.54	1.78	-0.26	0.38	0.04	3.05	0.08	-0.32	0.01	0.01	-0.82
⁵TS2_{CH}	0.61	-0.58	1.79	-0.29	0.37	0.08	3.49	-0.03	-0.32	0.00	0.01	0.86
³PC	0.56	-0.57	1.55	-0.38	0.36	0.48	2.15	-0.01	-0.16	0.02	0.00	0.00
⁵PC	0.78	-0.68	1.51	-0.41	0.40	0.39	4.03	0.02	-0.07	0.00	0.00	0.01

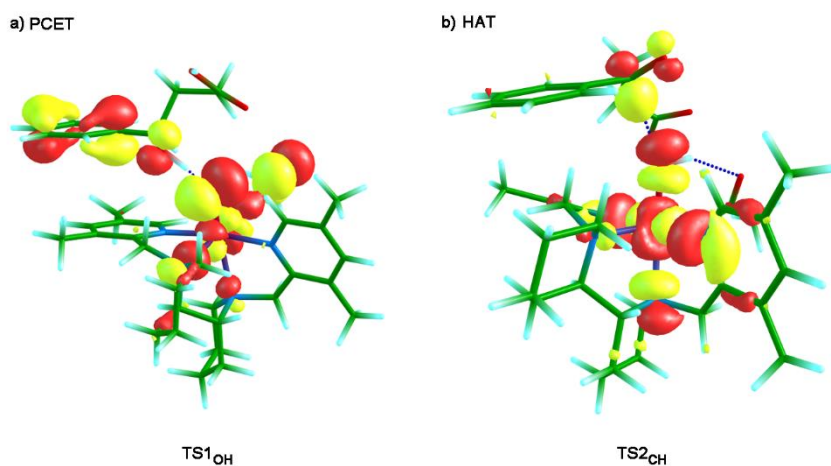


Fig. S19 the singly-occupied natural orbitals of oxidants TS1_{OH} on the triplet ground state and TS2_{CH} on the quintet ground state. Calculations were performed at the UB3LYP/B1 level in a solvent.

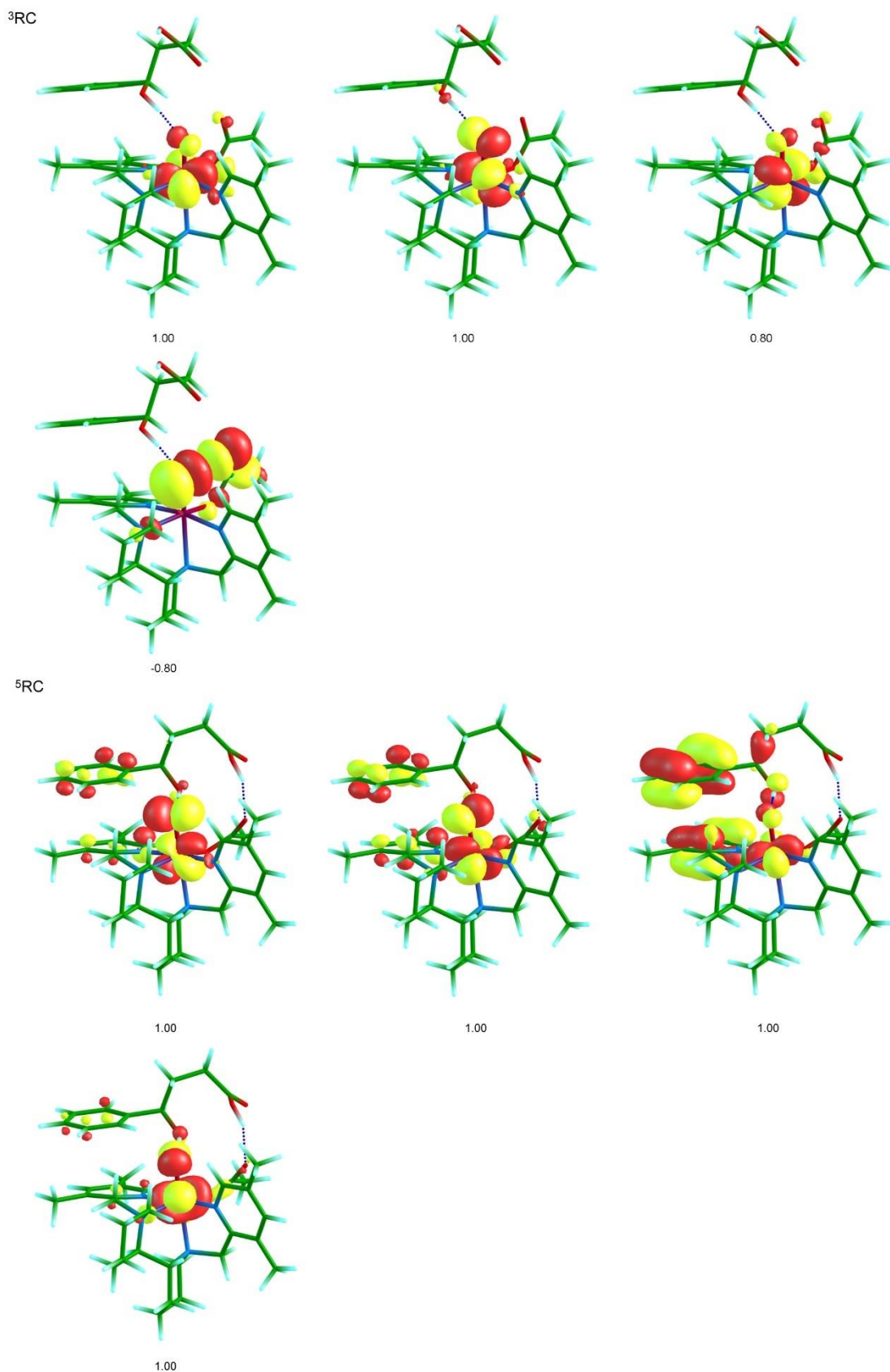


Figure S20. Singly-occupied natural orbitals (SNOs) of key intermediates of the alcohol oxidation via the reversed-dual hydrogen abstraction (R-DHA) mechanism. Calculations were done at the UB3LYP-D3(BJ)/B1 level in solvent. Positive and beta values represent alpha and netative ones represent beta occupations. (To be continued)

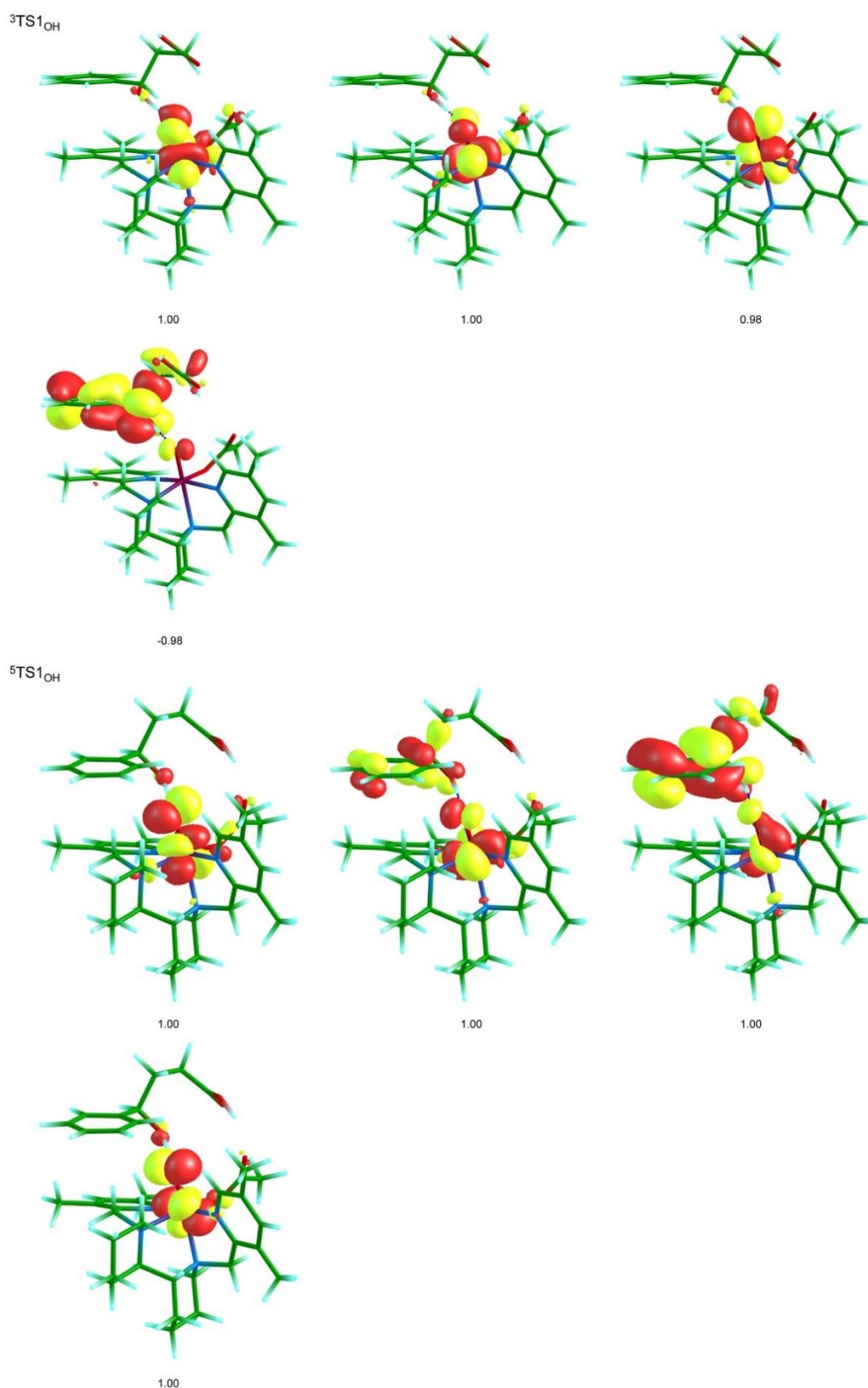


Figure S20. Singly-occupied natural orbitals (SNOs) of key intermediates of the alcohol oxidation via the reversed-dual hydrogen abstraction (R-DHA) mechanism. Calculations were done at the UB3LYP-D3(BJ)/B1 level in solvent. Positive and beta values represent alpha and netative ones represent beta occupations. (To be continued)

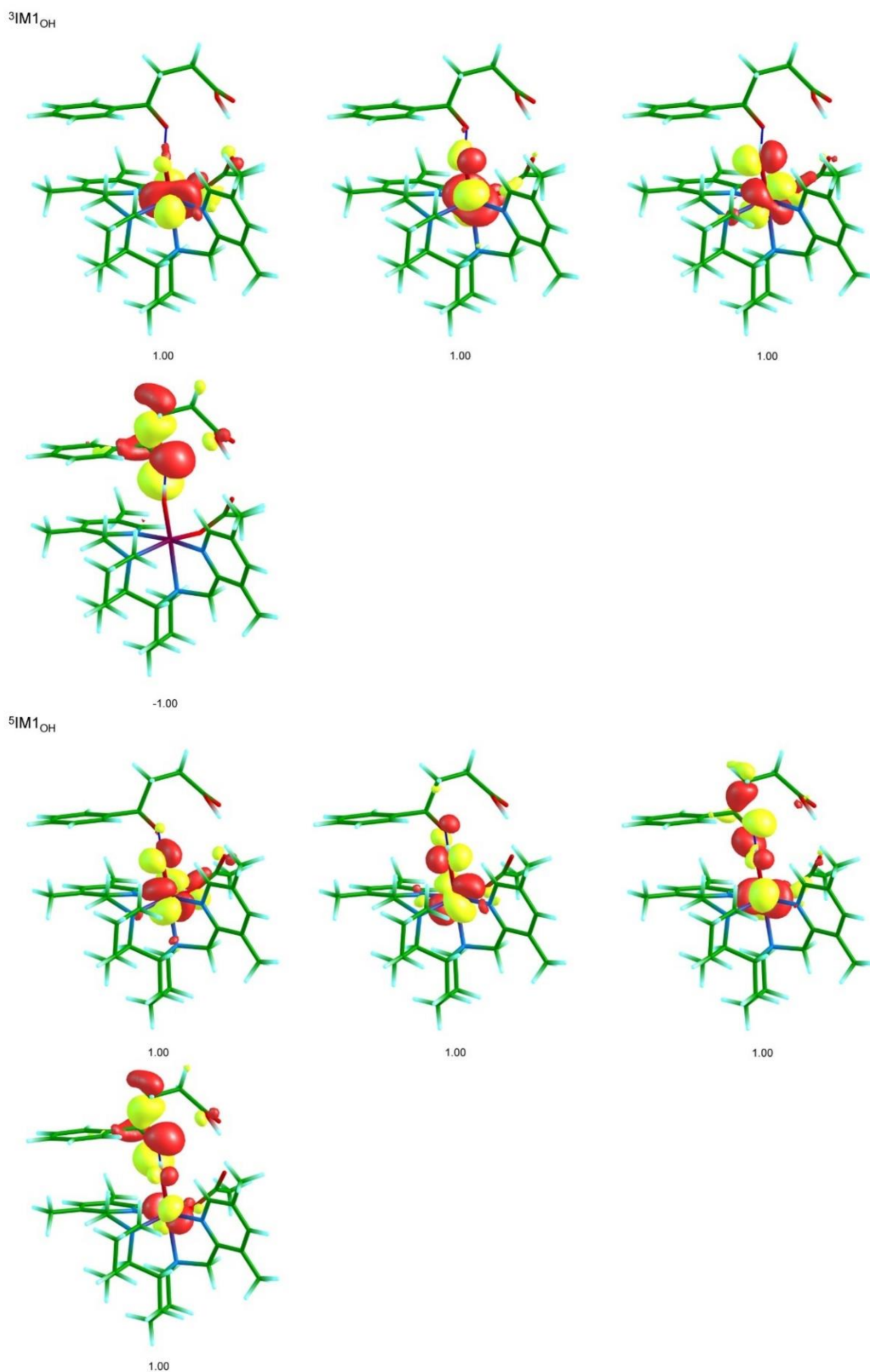


Figure S20. Singly-occupied natural orbitals (SNOs) of key intermediates of the alcohol oxidation via the reversed-dual hydrogen abstraction (R-DHA) mechanism. Calculations were done at the UB3LYP-D3(BJ)/B1 level in solvent. Positive and negative values represent alpha and netative ones represent beta occupations. (To be continued)

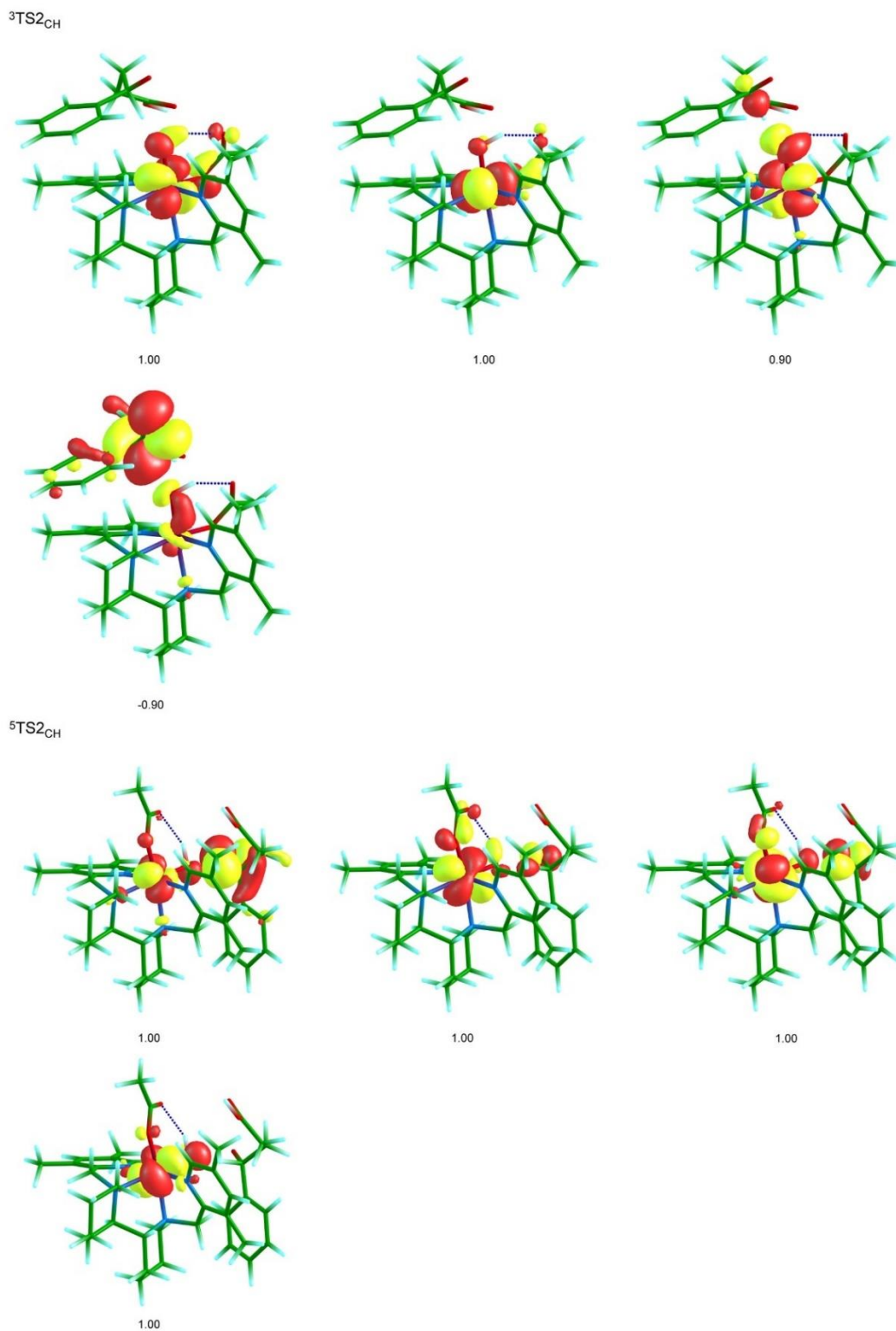
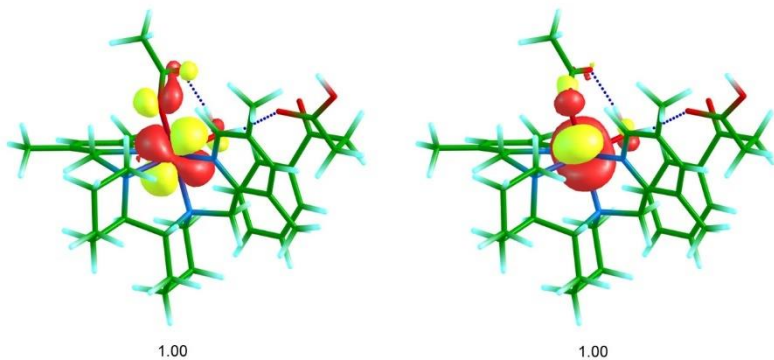


Figure S20. Singly-occupied natural orbitals (SNOs) of key intermediates of the alcohol oxidation via the reversed-dual hydrogen abstraction (R-DHA) mechanism. Calculations were done at the UB3LYP-D3(BJ)/B1 level in solvent. Positive and negative values represent alpha and netative ones represent beta occupations. (To be continued)

^3PC



^5PC

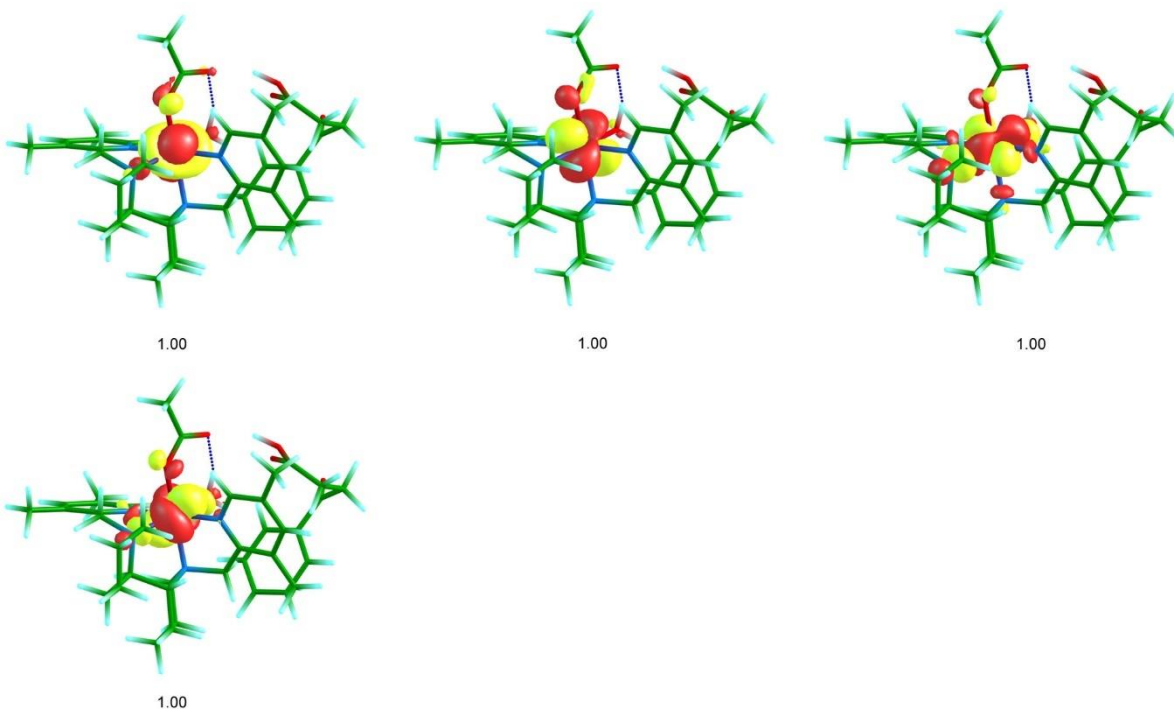


Figure S20. Singly-occupied natural orbitals (SNOs) of key intermediates of the alcohol oxidation via the reversed-dual hydrogen abstraction (R-DHA) mechanism. Calculations were done at the UB3LYP-D3(BJ)/B1 level in solvent. Positive values represent alpha-electron occupations and netative ones represent beta occupations.

Part VI Cartesian coordinates

Part I Conversion of the Mn^{III}-OOH species 1 to a Mn^{III}-peracetate species 3 via a Mn^{IV}(O)(AcO•) species 2.

³1

Mn	0.012757000	0.561184000	-0.406462000	H	1.761082000	-0.723256000	-2.701720000
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N	0.631719000	-1.374519000	-1.054074000	H	1.710048000	-1.840946000	0.682187000
N	-2.066102000	0.286757000	-0.457336000	H	2.089529000	-3.762871000	-0.628352000
N	-0.386298000	-0.525898000	1.488980000	H	1.169305000	-4.278268000	0.753605000
C	2.763514000	-0.153616000	-0.905980000	H	0.340494000	-5.318819000	-1.382781000
C	4.163067000	-0.140062000	-0.888055000	H	-0.923083000	-4.339598000	-0.650510000
C	4.780603000	0.855778000	-0.128499000	H	-0.804228000	-3.784335000	-3.064462000
C	4.039697000	1.804008000	0.586352000	H	0.923597000	-3.482666000	-2.948947000
C	2.654693000	1.711499000	0.507033000	H	-0.364820000	-1.328260000	-2.894155000
C	4.702878000	2.874768000	1.407962000	H	-1.327761000	-1.941513000	-1.556999000
C	4.966189000	-1.154603000	-1.658199000	H	-5.875924000	-0.095715000	-0.312648000
C	1.955230000	-1.138060000	-1.708836000	H	-2.239476000	0.678795000	-2.471440000
C	0.818581000	-2.232695000	0.190158000	H	-5.715258000	1.286811000	-2.730261000
C	1.097490000	-3.700583000	-0.169970000	H	-5.522032000	-0.430087000	-3.085660000
C	0.062774000	-4.291848000	-1.129735000	H	-4.328785000	0.734172000	-3.686235000
C	-0.018379000	-3.428568000	-2.391555000	H	-4.370370000	-1.416184000	2.531291000
C	-0.342367000	-1.982649000	-2.021344000	H	-5.798239000	-0.511985000	2.009785000
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C	-4.052444000	-0.144702000	0.814484000	H	-1.655647000	0.889881000	2.373711000
C	-4.796121000	0.015486000	-0.355025000	H	-2.157733000	-0.771763000	2.659215000
C	-4.182585000	0.313903000	-1.576498000	H	-1.299811000	-2.149820000	0.536339000
C	-2.797658000	0.442999000	-1.573390000	H	-1.450127000	-2.782356000	2.804574000
C	-4.976447000	0.487204000	-2.842443000	H	-0.404166000	-3.940936000	2.036430000
C	-4.715031000	-0.456903000	2.130575000	H	0.476638000	-3.205637000	4.276462000
C	-1.748380000	-0.095049000	1.908325000	H	1.611200000	-2.775160000	3.004368000
C	-0.386767000	-1.993660000	1.113257000	H	1.307827000	-0.806321000	4.480389000
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C	0.609026000	-2.565972000	3.399413000	H	0.510122000	0.853755000	2.782132000
C	0.507522000	-1.088286000	3.789737000	H	1.615224000	-0.335777000	2.110008000
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H	2.006266000	2.400750000	1.033537000	H	1.451416000	2.384025000	-2.508479000
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H	5.325128000	2.430318000	2.190977000	C	-0.819169000	3.509323000	0.461765000
H	3.965180000	3.524500000	1.883188000	O	-0.715793000	4.098107000	-0.702493000
H	4.758423000	-2.171450000	-1.308715000	H	-0.251604000	3.510527000	-1.365280000
H	6.034618000	-0.968659000	-1.537739000	C	-1.467358000	4.319043000	1.537293000
H	4.733120000	-1.119206000	-2.726889000	H	-1.214195000	5.374602000	1.433920000
				H	-2.552639000	4.214741000	1.427860000
				H	-1.176864000	3.939254000	2.515937000
				⁵ 1			

Mn	-0.030976000	0.511103000	-0.421124000	H	-0.174671000	-1.557781000	-2.881536000
N	2.043669000	0.774891000	-0.239071000	H	-1.195349000	-2.083272000	-1.552304000
N	0.750075000	-1.504254000	-1.006473000	H	-5.871517000	-0.197230000	-0.377372000
N	-2.080546000	0.270840000	-0.512528000	H	-2.240875000	0.611053000	-2.537832000
N	-0.376370000	-0.472251000	1.426189000	H	-5.733121000	1.130511000	-2.824673000
C	2.801300000	-0.144051000	-0.865941000	H	-5.504715000	-0.591391000	-3.133414000
C	4.201452000	-0.061155000	-0.852124000	H	-4.334538000	0.580462000	-3.764678000
C	4.773265000	1.011388000	-0.166837000	H	-4.353557000	-1.413998000	2.507610000
C	3.988502000	1.971369000	0.482387000	H	-5.799732000	-0.556347000	1.958337000
C	2.610421000	1.805505000	0.413765000	H	-4.520138000	0.317316000	2.813027000
C	4.598662000	3.127332000	1.225980000	H	-1.664044000	0.950578000	2.281632000
C	5.055546000	-1.084872000	-1.552860000	H	-2.133921000	-0.708886000	2.624696000
C	2.067456000	-1.230742000	-1.616000000	H	-1.242922000	-2.166965000	0.546624000
C	0.891576000	-2.269405000	0.279363000	H	-1.454731000	-2.650765000	2.859548000
C	1.178368000	-3.759431000	0.031046000	H	-0.391124000	-3.848394000	2.184690000
C	0.173812000	-4.408589000	-0.925277000	H	0.439228000	-2.969742000	4.395057000
C	0.135175000	-3.625180000	-2.241398000	H	1.601605000	-2.631533000	3.120699000
C	-0.187757000	-2.156880000	-1.968719000	H	1.287133000	-0.565735000	4.447694000
C	-2.671302000	-0.002129000	0.666746000	H	-0.457681000	-0.664197000	4.266822000
C	-4.056369000	-0.178097000	0.763037000	H	0.509814000	0.984446000	2.646233000
C	-4.794351000	-0.062361000	-0.416788000	H	1.620658000	-0.245698000	2.059408000
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C	-2.802749000	0.383864000	-1.639576000	O	0.389163000	2.421245000	-2.400955000
C	-4.978433000	0.343220000	-2.915443000	H	1.350488000	2.395833000	-2.537510000
C	-4.718851000	-0.473135000	2.082606000	O	-0.387622000	2.415399000	0.681387000
C	-1.746845000	-0.049592000	1.848598000	C	-0.924985000	3.508680000	0.457610000
C	-0.349223000	-1.968727000	1.141283000	O	-0.914291000	4.067335000	-0.732310000
C	-0.454701000	-2.788243000	2.436994000	H	-0.418253000	3.495226000	-1.378189000
C	0.593142000	-2.391347000	3.479859000	C	-1.659609000	4.269675000	1.513720000
C	0.492176000	-0.890985000	3.770100000	H	-1.653302000	5.339711000	1.307222000
C	0.627992000	-0.086618000	2.478089000	H	-2.698957000	3.921663000	1.512930000
H	5.855522000	1.099973000	-0.137081000	H	-1.227614000	4.055009000	2.491066000
H	1.930460000	2.498781000	0.892562000	³ TS ₁₂			
H	5.239930000	3.717775000	0.564457000	Mn	-0.008269000	0.636138000	-0.395274000
H	5.221410000	2.769734000	2.052065000	N	2.038499000	0.714228000	-0.184884000
H	3.829855000	3.785033000	1.636740000	N	0.564947000	-1.313334000	-1.124147000
H	4.902501000	-2.084456000	-1.132304000	N	-2.075277000	0.377100000	-0.412537000
H	6.112702000	-0.834445000	-1.450025000	N	-0.405271000	-0.601698000	1.496755000
H	4.821482000	-1.138260000	-2.620593000	C	2.724831000	-0.166510000	-0.945416000
H	1.898173000	-0.893525000	-2.643390000	C	4.123402000	-0.203016000	-0.929430000
H	2.682566000	-2.131265000	-1.671083000	C	4.775720000	0.705095000	-0.093026000
H	1.764720000	-1.849436000	0.782092000	C	4.068609000	1.613344000	0.702911000
H	2.182448000	-3.841370000	-0.398802000	C	2.681098000	1.579729000	0.620180000
H	1.225831000	-4.285888000	0.986371000	C	4.767439000	2.584446000	1.613619000
H	0.456396000	-5.449824000	-1.104934000	C	4.889217000	-1.181775000	-1.779406000
H	-0.827695000	-4.426948000	-0.476550000	C	1.876015000	-1.064411000	-1.800844000
H	-0.625688000	-4.026045000	-2.917949000	C	0.754353000	-2.235504000	0.074022000
H	1.098736000	-3.711422000	-2.757407000	C	1.006554000	-3.684839000	-0.372221000

C	-0.057951000	-4.209472000	-1.337663000	H	0.430361000	-3.469594000	4.093968000
C	-0.153312000	-3.279915000	-2.550214000	H	1.562214000	-2.973635000	2.843427000
C	-0.444473000	-1.848961000	-2.101067000	H	1.301511000	-1.102307000	4.450147000
C	-2.663838000	0.024220000	0.749850000	H	-0.448565000	-1.154430000	4.283109000
C	-4.054907000	-0.115734000	0.841254000	H	0.521371000	0.677699000	2.866389000
C	-4.801957000	0.125049000	-0.312800000	H	1.601385000	-0.484966000	2.112537000
C	-4.194693000	0.496398000	-1.517383000	O	-0.024528000	1.230986000	-2.004462000
C	-2.810235000	0.615380000	-1.514007000	O	0.673463000	2.789487000	-2.361456000
C	-4.993924000	0.757180000	-2.764349000	H	1.613933000	2.570760000	-2.270830000
C	-4.718480000	-0.504410000	2.136342000	O	-0.306617000	2.267840000	0.727927000
C	-1.750977000	-0.157338000	1.933127000	C	-0.616054000	3.478059000	0.537674000
C	-0.436732000	-2.034389000	1.026304000	O	-0.417781000	4.104412000	-0.564453000
C	-0.514801000	-3.019615000	2.204181000	H	0.076811000	3.535657000	-1.314741000
C	0.566536000	-2.775134000	3.260198000	C	-1.255478000	4.233447000	1.657826000
C	0.492613000	-1.324758000	3.747857000	H	-1.249667000	5.304538000	1.462775000
C	0.615273000	-0.366721000	2.563464000	H	-2.289313000	3.884056000	1.752287000
H	5.861160000	0.699172000	-0.056650000	H	-0.741713000	4.003272000	2.593024000
H	2.058554000	2.244538000	1.204651000	⁵ TS ₁₂			
H	5.434023000	3.237081000	1.041696000	Mn	-0.001201000	0.597645000	-0.381553000
H	5.379871000	2.051060000	2.347087000	N	2.015552000	0.855382000	-0.206815000
H	4.052176000	3.209434000	2.151881000	N	0.684849000	-1.243243000	-1.163171000
H	4.657039000	-2.214577000	-1.499049000	N	-2.028890000	0.205234000	-0.337434000
H	5.963303000	-1.033474000	-1.658348000	N	-0.265068000	-0.686923000	1.514426000
H	4.646392000	-1.063949000	-2.839769000	C	2.751738000	0.065180000	-1.015118000
H	1.665679000	-0.572679000	-2.754320000	C	4.146674000	0.156415000	-1.043372000
H	2.383544000	-2.004091000	-2.016005000	C	4.738599000	1.101363000	-0.202129000
H	1.657605000	-1.882508000	0.572950000	C	3.976813000	1.922734000	0.636763000
H	1.987675000	-3.735270000	-0.854435000	C	2.595597000	1.762141000	0.597145000
H	1.089688000	-4.310836000	0.518194000	C	4.612396000	2.937771000	1.546123000
H	0.198452000	-5.224945000	-1.651801000	C	4.969346000	-0.727258000	-1.943058000
H	-1.033369000	-4.269031000	-0.839110000	C	1.952749000	-0.872251000	-1.872786000
H	-0.962019000	-3.584771000	-3.220870000	C	0.979817000	-2.176871000	0.006891000
H	0.773149000	-3.320442000	-3.133660000	C	1.336785000	-3.586749000	-0.490560000
H	-0.470183000	-1.149717000	-2.937729000	C	0.290510000	-4.170674000	-1.441497000
H	-1.418597000	-1.816479000	-1.613912000	C	0.083479000	-3.221218000	-2.624070000
H	-5.882328000	0.020491000	-0.270966000	C	-0.311047000	-1.830804000	-2.127839000
H	-2.253230000	0.907386000	-2.395712000	C	-2.571470000	-0.198972000	0.830452000
H	-5.728925000	1.549701000	-2.593674000	C	-3.951515000	-0.412055000	0.947349000
H	-5.543356000	-0.140440000	-3.064925000	C	-4.734164000	-0.193088000	-0.187037000
H	-4.349338000	1.058147000	-3.592604000	C	-4.173433000	0.229913000	-1.397258000
H	-4.381400000	-1.489777000	2.474981000	C	-2.798076000	0.424448000	-1.421351000
H	-5.801976000	-0.542786000	2.012863000	C	-5.012664000	0.469829000	-2.621863000
H	-4.492119000	0.212824000	2.931381000	C	-4.566280000	-0.853666000	2.249540000
H	-1.635288000	0.804007000	2.442357000	C	-1.626122000	-0.357852000	1.990724000
H	-2.186374000	-0.853230000	2.651974000	C	-0.199042000	-2.099489000	0.995168000
H	-1.357469000	-2.140196000	0.450148000	C	-0.170038000	-3.128341000	2.137314000
H	-1.500146000	-2.912718000	2.669743000	C	0.917329000	-2.837207000	3.175393000
H	-0.483461000	-4.041383000	1.820744000	C	0.747718000	-1.413195000	3.715097000

C	0.762762000	-0.409909000	2.562373000	H	-2.231560000	3.746874000	2.337403000
H	5.820620000	1.195305000	-0.197631000	H	-0.516086000	3.966577000	2.708796000
H	1.930948000	2.352415000	1.214286000	³ 2			
H	5.160954000	3.685033000	0.964331000	Mn	0.025179000	-0.746953000	-0.171598000
H	5.327479000	2.456596000	2.220166000	N	-2.021425000	-0.541634000	0.084500000
H	3.863574000	3.454475000	2.149673000	N	-0.404563000	1.143083000	-1.247069000
H	4.845841000	-1.783115000	-1.679529000	N	2.096187000	-0.664732000	-0.283286000
H	6.028476000	-0.480362000	-1.856075000	N	0.595589000	0.795900000	1.451927000
H	4.677510000	-0.610642000	-2.991148000	C	-2.648231000	0.254203000	-0.807680000
H	1.672999000	-0.370683000	-2.803104000	C	-4.036358000	0.421580000	-0.774420000
H	2.521012000	-1.765359000	-2.130122000	C	-4.738864000	-0.270314000	0.213964000
H	1.864541000	-1.762710000	0.491161000	C	-4.090516000	-1.095255000	1.140177000
H	2.304879000	-3.541853000	-0.999105000	C	-2.708575000	-1.204098000	1.031834000
H	1.496764000	-4.226611000	0.379213000	C	-4.843707000	-1.832579000	2.212160000
H	0.619555000	-5.152627000	-1.792105000	C	-4.739214000	1.303091000	-1.771936000
H	-0.661267000	-4.323552000	-0.917945000	C	-1.758464000	0.895289000	-1.831838000
H	-0.718979000	-3.572525000	-3.279213000	C	-0.458859000	2.263444000	-0.218388000
H	0.990904000	-3.170060000	-3.235512000	C	-0.593372000	3.632076000	-0.907562000
H	-0.418106000	-1.112594000	-2.941314000	C	0.477764000	3.876158000	-1.971655000
H	-1.268493000	-1.892468000	-1.612306000	C	0.442939000	2.748192000	-3.005806000
H	-5.806451000	-0.354861000	-0.124899000	C	0.616007000	1.391839000	-2.321697000
H	-2.276228000	0.767057000	-2.305593000	C	2.757594000	-0.158054000	0.780543000
H	-5.781923000	1.221901000	-2.421675000	C	4.156903000	-0.114064000	0.798720000
H	-5.523591000	-0.449432000	-2.924901000	C	4.830090000	-0.615876000	-0.316969000
H	-4.402672000	0.815425000	-3.458737000	C	4.144948000	-1.149865000	-1.413669000
H	-4.175065000	-1.827076000	2.563611000	C	2.756889000	-1.157468000	-1.347406000
H	-5.649185000	-0.942046000	2.148819000	C	4.866981000	-1.697820000	-2.613272000
H	-4.356604000	-0.139433000	3.051952000	C	4.905745000	0.448443000	1.978175000
H	-1.570350000	0.589914000	2.534994000	C	1.908383000	0.297912000	1.935145000
H	-2.001442000	-1.106825000	2.690954000	C	0.744903000	2.112644000	0.726939000
H	-1.123068000	-2.259771000	0.436729000	C	0.959466000	3.275435000	1.710073000
H	-1.148338000	-3.111115000	2.629272000	C	-0.103764000	3.331505000	2.810017000
H	-0.072891000	-4.131805000	1.718191000	C	-0.154089000	1.990972000	3.549270000
H	0.855375000	-3.567133000	3.987431000	C	-0.408807000	0.854198000	2.560023000
H	1.913945000	-2.946585000	2.728654000	H	-5.818151000	-0.161562000	0.264851000
H	1.556484000	-1.153652000	4.404778000	H	-2.127872000	-1.818276000	1.707386000
H	-0.188740000	-1.333834000	4.279225000	H	-5.605586000	-2.481214000	1.769769000
H	0.597864000	0.613439000	2.904773000	H	-5.355865000	-1.127292000	2.873977000
H	1.743178000	-0.434194000	2.083495000	H	-4.174796000	-2.447811000	2.816847000
O	-0.108160000	1.457098000	-1.908104000	H	-4.400861000	2.341299000	-1.690970000
O	-0.880655000	2.875657000	-2.694095000	H	-5.816832000	1.286227000	-1.602948000
H	-0.048647000	3.176625000	-3.093934000	H	-4.549375000	0.969815000	-2.796740000
O	-0.377244000	2.238547000	0.832182000	H	-1.641126000	0.217740000	-2.682797000
C	-0.945908000	3.349808000	0.714854000	H	-2.185625000	1.825017000	-2.206359000
O	-1.300036000	3.888717000	-0.404998000	H	-1.371034000	2.090956000	0.353146000
H	-1.075294000	3.403139000	-1.293731000	H	-1.583831000	3.691282000	-1.368902000
C	-1.280935000	4.129121000	1.948851000	H	-0.585596000	4.406039000	-0.137896000
H	-1.393937000	5.188956000	1.723980000	H	0.301686000	4.841364000	-2.454030000

H	1.472176000	3.929240000	-1.511826000	C	-1.878476000	1.034221000	-1.813636000
H	1.252458000	2.851294000	-3.734049000	C	-0.754358000	2.252410000	0.032810000
H	-0.496038000	2.775934000	-3.569184000	C	-1.001850000	3.692660000	-0.447273000
H	0.541364000	0.562807000	-3.026875000	C	0.062691000	4.189367000	-1.427284000
H	1.600689000	1.344699000	-1.857571000	C	0.156195000	3.230331000	-2.616839000
H	5.915769000	-0.590395000	-0.330258000	C	0.443737000	1.809244000	-2.131450000
H	2.142460000	-1.560020000	-2.142557000	C	2.660289000	-0.007572000	0.730982000
H	5.506433000	-2.538109000	-2.325793000	C	4.051007000	0.140276000	0.792668000
H	5.510043000	-0.932255000	-3.057782000	C	4.779236000	-0.138434000	-0.365675000
H	4.165995000	-2.044229000	-3.375039000	C	4.154959000	-0.555955000	-1.545764000
H	4.662567000	1.504560000	2.134522000	C	2.771110000	-0.682294000	-1.517243000
H	5.981990000	0.371232000	1.817003000	C	4.934415000	-0.859817000	-2.795117000
H	4.660495000	-0.088663000	2.899364000	C	4.733947000	0.573620000	2.063061000
H	1.719092000	-0.553727000	2.596092000	C	1.762167000	0.207164000	1.917547000
H	2.427031000	1.056057000	2.523068000	C	0.440964000	2.069010000	0.979752000
H	1.648855000	2.021522000	0.122820000	C	0.522951000	3.070641000	2.144183000
H	1.945867000	3.153297000	2.169172000	C	-0.553844000	2.841636000	3.207560000
H	1.013583000	4.210531000	1.149381000	C	-0.478342000	1.399271000	3.716826000
H	0.129005000	4.144051000	3.503655000	C	-0.608029000	0.421859000	2.548780000
H	-1.089098000	3.554748000	2.381743000	H	-5.864099000	-0.694924000	-0.043879000
H	-0.958268000	1.978141000	4.290710000	H	-2.063072000	-2.238669000	1.232558000
H	0.782311000	1.823300000	4.093084000	H	-5.456801000	-3.210953000	1.084099000
H	-0.403318000	-0.123270000	3.045858000	H	-5.375439000	-2.021086000	2.384867000
H	-1.392588000	0.987501000	2.108904000	H	-4.064228000	-3.196756000	2.181737000
O	-0.106959000	-1.727156000	-1.535927000	H	-4.650349000	2.197992000	-1.524745000
O	-2.638830000	-2.420873000	-2.661113000	H	-5.961955000	1.020070000	-1.660680000
H	-1.758890000	-2.362449000	-2.253912000	H	-4.649348000	1.025691000	-2.847146000
O	0.133108000	-2.168248000	1.064849000	H	-1.665403000	0.516529000	-2.752679000
C	0.206669000	-3.418757000	0.643535000	H	-2.388689000	1.966835000	-2.052683000
O	0.148990000	-3.728832000	-0.546775000	H	-1.657221000	1.914139000	0.542364000
H	-3.201116000	-2.837502000	-1.999081000	H	-1.984222000	3.734093000	-0.927177000
C	0.364884000	-4.440891000	1.736590000	H	-1.080119000	4.338986000	0.429002000
H	0.403690000	-5.444155000	1.316056000	H	-0.193598000	5.196388000	-1.767400000
H	1.283501000	-4.222521000	2.287661000	H	1.038686000	4.261785000	-0.931853000
H	-0.475732000	-4.350483000	2.429468000	H	0.966869000	3.515148000	-3.293601000
s^2				H	-0.769371000	3.257500000	-3.202075000
Mn	0.007592000	-0.672752000	-0.353284000	H	0.467412000	1.089397000	-2.950883000
N	-2.044641000	-0.718757000	-0.167090000	H	1.417186000	1.787564000	-1.642342000
N	-0.571158000	1.307962000	-1.144435000	H	5.859506000	-0.028446000	-0.345439000
N	2.056038000	-0.404265000	-0.411229000	H	2.201245000	-1.010481000	-2.377730000
N	0.413874000	0.643758000	1.477563000	H	5.677078000	-1.640587000	-2.605388000
C	-2.725365000	0.154502000	-0.941086000	H	5.472374000	0.029502000	-3.137823000
C	-4.123722000	0.193143000	-0.925318000	H	4.278261000	-1.196159000	-3.600129000
C	-4.778721000	-0.703804000	-0.078737000	H	4.389617000	1.563187000	2.381049000
C	-4.075180000	-1.605523000	0.727592000	H	5.813941000	0.622977000	1.916573000
C	-2.687485000	-1.577308000	0.646131000	H	4.533090000	-0.125605000	2.880701000
C	-4.776852000	-2.565235000	1.647845000	H	1.647028000	-0.737460000	2.456621000
C	-4.887836000	1.162051000	-1.788064000	H	2.200773000	0.924455000	2.612324000

H	1.359785000	2.165737000	0.399417000	C	-1.085337000	3.477822000	-1.277711000
H	1.510851000	2.973597000	2.605759000	C	-0.036509000	3.733992000	-2.363308000
H	0.487928000	4.085137000	1.742473000	C	0.055612000	2.517610000	-3.290176000
H	-0.412153000	3.547567000	4.030492000	C	0.354063000	1.255875000	-2.480446000
H	-1.551195000	3.035704000	2.793280000	H	5.824958000	-0.076661000	-0.413309000
H	-1.285436000	1.186042000	4.423704000	H	2.130292000	-1.577872000	-2.004131000
H	0.464089000	1.234575000	4.251140000	H	5.607655000	-2.216382000	-2.163103000
H	-0.512597000	-0.617713000	2.865804000	H	5.344989000	-0.753344000	-3.114116000
H	-1.593827000	0.536567000	2.097140000	H	4.168327000	-2.076361000	-3.189108000
O	-0.017241000	-1.247298000	-2.056144000	H	4.413264000	2.176333000	1.835941000
O	-0.850883000	-3.261017000	-2.340002000	H	5.834370000	1.147563000	1.608782000
H	-1.720687000	-3.141665000	-1.933279000	H	4.578331000	0.683086000	2.765917000
O	0.233002000	-2.172643000	0.743695000	H	1.721131000	-0.043061000	2.609660000
C	0.737379000	-3.393030000	0.643692000	H	2.205561000	1.617192000	2.281403000
O	0.771173000	-4.028110000	-0.405517000	H	1.306659000	2.190436000	-0.139671000
H	-0.232807000	-3.583433000	-1.626565000	H	1.501391000	3.541807000	1.785452000
C	1.264683000	-3.929035000	1.947645000	H	0.449016000	4.384725000	0.688462000
H	1.435788000	-5.002222000	1.871940000	H	-0.398644000	4.452795000	3.057027000
H	2.211329000	-3.426227000	2.172417000	H	-1.555875000	3.629671000	2.020195000
H	0.568774000	-3.704718000	2.758701000	H	-1.230178000	2.266548000	4.067653000
³ TS ₂₃				H	0.513933000	2.283105000	3.846624000
Mn	-0.011491000	-0.714825000	0.002612000	H	-0.468253000	0.129682000	3.019774000
N	2.027231000	-0.485564000	-0.249456000	H	-1.583173000	1.031998000	2.000236000
N	0.405708000	0.984178000	1.315603000	H	-5.918250000	-0.741831000	0.187954000
N	-2.093899000	-0.719221000	0.129875000	H	-2.118401000	-1.838213000	1.864667000
N	-0.636249000	1.000320000	-1.387296000	H	-5.491834000	-2.878680000	1.930919000
C	2.660801000	0.207390000	0.720732000	H	-5.460536000	-1.391526000	2.879997000
C	4.049291000	0.379267000	0.697247000	H	-4.124398000	-2.548627000	3.010008000
C	4.746134000	-0.193596000	-0.368043000	H	-4.737551000	1.681342000	-1.980601000
C	4.092471000	-0.912032000	-1.376087000	H	-6.014442000	0.467974000	-1.827811000
C	2.712049000	-1.035391000	-1.269263000	H	-4.674383000	0.207449000	-2.952865000
C	4.840076000	-1.526660000	-2.526879000	H	-1.733130000	-0.198749000	-2.713311000
C	4.758050000	1.138185000	1.787029000	H	-2.480920000	1.363100000	-2.408270000
C	1.784277000	0.720004000	1.828494000	H	-1.703400000	1.984704000	0.120550000
C	0.400665000	2.247118000	0.464916000	H	-2.071275000	3.385847000	-1.745018000
C	0.503312000	3.508728000	1.337418000	H	-1.168766000	4.319229000	-0.587015000
C	-0.548054000	3.557290000	2.447701000	H	-0.305019000	4.629253000	-2.930959000
C	-0.441472000	2.296855000	3.310252000	H	0.944198000	3.929444000	-1.911341000
C	-0.586836000	1.048154000	2.442170000	H	0.854477000	2.642226000	-4.027165000
C	-2.774139000	-0.094042000	-0.855520000	H	-0.878025000	2.400039000	-3.851868000
C	-4.174476000	-0.083392000	-0.870768000	H	0.373718000	0.363377000	-3.108833000
C	-4.832225000	-0.738828000	0.171696000	H	1.338611000	1.349202000	-2.020495000
C	-4.130436000	-1.388382000	1.193044000	O	0.167828000	-1.987854000	1.224320000
C	-2.742878000	-1.354777000	1.123706000	O	2.623798000	-2.431659000	2.642540000
C	-4.835922000	-2.093177000	2.318497000	H	1.785817000	-2.419286000	2.151671000
C	-4.941272000	0.605378000	-1.969135000	O	-0.113273000	-2.257093000	-1.319832000
C	-1.939602000	0.542811000	-1.934677000	C	-0.075900000	-3.381357000	-0.741977000
C	-0.814785000	2.193566000	-0.477420000	O	0.042261000	-3.491443000	0.535372000

H	3.290979000	-2.711185000	2.006131000	H	-1.710125000	3.749334000	-1.214096000
C	-0.156027000	-4.657499000	-1.518323000	H	-0.768552000	4.417113000	0.086975000
H	-0.180838000	-5.523209000	-0.859052000	H	0.162863000	5.023090000	-2.172806000
H	-1.052013000	-4.623778000	-2.142634000	H	1.338851000	4.091769000	-1.256886000
H	0.718866000	-4.707806000	-2.172745000	H	1.215008000	3.149944000	-3.545399000
⁵ TS ₂₃				H	-0.533337000	3.005160000	-3.435393000
Mn	0.002420000	-0.717840000	-0.216895000	H	0.568913000	0.795742000	-2.992433000
N	-2.041652000	-0.616295000	-0.068024000	H	1.563609000	1.545963000	-1.749255000
N	-0.449981000	1.237657000	-1.217713000	H	5.880317000	-0.357026000	-0.327521000
N	2.066054000	-0.562556000	-0.328163000	H	2.162997000	-1.328935000	-2.246965000
N	0.499582000	0.736625000	1.467754000	H	5.595929000	-2.137202000	-2.449747000
C	-2.666052000	0.236754000	-0.912227000	H	5.467514000	-0.503652000	-3.105322000
C	-4.057732000	0.376487000	-0.893295000	H	4.210889000	-1.700422000	-3.466911000
C	-4.766324000	-0.395132000	0.030978000	H	4.526449000	1.526146000	2.259555000
C	-4.121519000	-1.273163000	0.910832000	H	5.893796000	0.472120000	1.876808000
C	-2.736927000	-1.353328000	0.821634000	H	4.584873000	-0.115399000	2.912018000
C	-4.882575000	-2.097752000	1.910724000	H	1.650092000	-0.645591000	2.545060000
C	-4.761518000	1.319840000	-1.832346000	H	2.304386000	0.990463000	2.583135000
C	-1.766985000	0.970675000	-1.864654000	H	1.533080000	2.090037000	0.252034000
C	-0.572591000	2.285321000	-0.127170000	H	1.747523000	3.084393000	2.376642000
C	-0.731169000	3.692151000	-0.728309000	H	0.794203000	4.175826000	1.413810000
C	0.358694000	4.035595000	-1.746212000	H	-0.129715000	3.910578000	3.738910000
C	0.390936000	2.973211000	-2.848274000	H	-1.303864000	3.359738000	2.552132000
C	0.591165000	1.585169000	-2.239650000	H	-1.149893000	1.655939000	4.347668000
C	2.700060000	-0.103551000	0.774236000	H	0.598548000	1.578026000	4.176269000
C	4.096607000	-0.014898000	0.810634000	H	-0.497282000	-0.330022000	2.968377000
C	4.796115000	-0.419885000	-0.327947000	H	-1.507687000	0.813812000	2.091843000
C	4.139864000	-0.902194000	-1.465761000	O	0.033104000	-1.625673000	-1.782379000
C	2.752218000	-0.960508000	-1.414614000	O	-1.810720000	-3.024395000	-2.197383000
C	4.890388000	-1.337319000	-2.693549000	H	-2.566964000	-2.883884000	-1.612889000
C	4.814283000	0.494275000	2.032786000	O	0.160903000	-2.160158000	0.958498000
C	1.822596000	0.251192000	1.942538000	C	0.373631000	-3.435083000	0.610316000
C	0.612781000	2.107829000	0.837311000	O	0.121243000	-3.872993000	-0.500874000
C	0.765752000	3.202282000	1.906828000	H	-1.104506000	-3.416469000	-1.637063000
C	-0.319273000	3.142008000	2.984673000	C	0.961247000	-4.249093000	1.731850000
C	-0.333101000	1.751681000	3.626391000	H	1.031074000	-5.296004000	1.439522000
C	-0.529513000	0.679239000	2.554795000	H	1.955431000	-3.858328000	1.969300000
H	-5.847874000	-0.306058000	0.068777000	H	0.344205000	-4.144401000	2.627818000
H	-2.155878000	-2.004466000	1.461711000	³ B			
H	-5.589745000	-2.759957000	1.402183000	Mn	-0.024103000	-0.566307000	-0.042262000
H	-5.459002000	-1.451762000	2.579667000	N	1.977764000	-0.458773000	-0.308800000
H	-4.210485000	-2.709437000	2.515254000	N	0.399864000	0.942470000	1.296586000
H	-4.464237000	2.357100000	-1.645682000	N	-2.038743000	-0.653653000	0.161413000
H	-5.842240000	1.250902000	-1.700976000	N	-0.579693000	0.979624000	-1.326877000
H	-4.529284000	1.089210000	-2.876230000	C	2.635528000	0.136818000	0.703593000
H	-1.581802000	0.343177000	-2.741516000	C	4.032596000	0.219182000	0.717894000
H	-2.225879000	1.897314000	-2.208689000	C	4.713370000	-0.348940000	-0.359783000
H	-1.493302000	2.049029000	0.407688000	C	4.034220000	-0.976748000	-1.411541000

C	2.646766000	-1.008700000	-1.337823000	H	-4.601994000	0.123401000	-2.971407000
C	4.765546000	-1.590781000	-2.573098000	H	-1.674987000	-0.189244000	-2.688700000
C	4.761789000	0.878791000	1.857423000	H	-2.399187000	1.385182000	-2.383807000
C	1.764700000	0.636615000	1.817680000	H	-1.669940000	2.014351000	0.135326000
C	0.429400000	2.241545000	0.506020000	H	-2.004326000	3.403364000	-1.733274000
C	0.529456000	3.475831000	1.414789000	H	-1.075868000	4.329218000	-0.590037000
C	-0.514780000	3.492683000	2.532745000	H	-0.226845000	4.588320000	-2.948991000
C	-0.414781000	2.199427000	3.345746000	H	1.018348000	3.896833000	-1.918159000
C	-0.590630000	0.991777000	2.428239000	H	0.910501000	2.567702000	-4.005530000
C	-2.729739000	-0.078479000	-0.841475000	H	-0.821818000	2.339517000	-3.819775000
C	-4.128103000	-0.112565000	-0.877691000	H	0.447364000	0.319514000	-3.032634000
C	-4.774087000	-0.771672000	0.169515000	H	1.396232000	1.344029000	-1.963448000
C	-4.060179000	-1.378775000	1.210165000	O	0.199843000	-1.976759000	1.174527000
C	-2.673896000	-1.295907000	1.158671000	O	2.593218000	-2.545728000	2.598688000
C	-4.754946000	-2.090266000	2.338094000	H	3.262292000	-2.792248000	1.950824000
C	-4.895906000	0.533202000	-2.000178000	O	-0.177535000	-2.044493000	-1.352785000
C	-1.883637000	0.550041000	-1.909093000	C	-0.212480000	-3.160488000	-0.787296000
C	-0.769061000	2.204716000	-0.450336000	O	-0.061499000	-3.280252000	0.504899000
C	-1.014181000	3.478511000	-1.271960000	H	1.765469000	-2.451358000	2.095893000
C	0.034703000	3.702550000	-2.363744000	C	-0.429336000	-4.438286000	-1.522094000
C	0.113344000	2.465926000	-3.263293000	H	-0.419801000	-5.291978000	-0.846772000
C	0.417327000	1.225776000	-2.425326000	H	-1.388486000	-4.376482000	-2.042987000
H	5.798341000	-0.303580000	-0.379916000	H	0.360129000	-4.539706000	-2.271751000
H	2.047581000	-1.476402000	-2.108678000	53			
H	5.472084000	-2.350562000	-2.225484000	Mn	-0.038553000	-0.593149000	-0.122966000
H	5.339912000	-0.830434000	-3.111478000	N	1.989863000	-0.451758000	-0.369042000
H	4.073810000	-2.059367000	-3.275928000	N	0.494966000	1.009421000	1.363709000
H	4.491091000	1.936742000	1.941670000	N	-2.064539000	-0.674218000	0.050453000
H	5.840835000	0.817040000	1.708308000	N	-0.578152000	1.058583000	-1.317766000
H	4.521270000	0.398780000	2.811075000	C	2.679934000	0.167877000	0.607343000
H	1.678782000	-0.145373000	2.577680000	C	4.080093000	0.238579000	0.564872000
H	2.200499000	1.510795000	2.301546000	C	4.721357000	-0.361850000	-0.518101000
H	1.343660000	2.199059000	-0.087644000	C	4.005409000	-1.018032000	-1.527583000
H	1.529866000	3.496833000	1.858822000	C	2.622969000	-1.039378000	-1.402704000
H	0.470279000	4.371192000	0.792588000	C	4.693365000	-1.669340000	-2.695069000
H	-0.353018000	4.364042000	3.173059000	C	4.858386000	0.921730000	1.657362000
H	-1.525031000	3.589204000	2.115726000	C	1.884921000	0.713973000	1.767386000
H	-1.196654000	2.150196000	4.109231000	C	0.440417000	2.290235000	0.573695000
H	0.545009000	2.152371000	3.872201000	C	0.517061000	3.529566000	1.480198000
H	-0.498875000	0.047244000	2.966966000	C	-0.504021000	3.501387000	2.620162000
H	-1.587117000	1.025853000	1.990237000	C	-0.324991000	2.216313000	3.434333000
H	-5.859460000	-0.813220000	0.174892000	C	-0.450902000	0.998804000	2.520817000
H	-2.041002000	-1.741534000	1.915391000	C	-2.741035000	-0.027899000	-0.920583000
H	-5.367920000	-2.912486000	1.956333000	C	-4.138841000	-0.022875000	-0.952640000
H	-5.420679000	-1.405668000	2.872686000	C	-4.798346000	-0.708099000	0.070524000
H	-4.037082000	-2.498833000	3.051978000	C	-4.099992000	-1.370965000	1.086816000
H	-4.717814000	1.613433000	-2.030003000	C	-2.711423000	-1.328555000	1.031641000
H	-5.967464000	0.371402000	-1.873410000	C	-4.811064000	-2.098668000	2.193728000

C	-4.895336000	0.691133000	-2.040902000	O	-0.151393000	-2.494388000	-1.338975000
C	-1.874176000	0.643914000	-1.944079000	C	-0.253087000	-3.459160000	-0.587149000
C	-0.785044000	2.225350000	-0.357606000	O	-0.133826000	-3.340030000	0.738534000
C	-1.096699000	3.522210000	-1.120029000	H	1.808234000	-2.386572000	2.050376000
C	-0.048963000	3.854011000	-2.185264000	C	-0.527063000	-4.864631000	-1.012228000
C	0.101248000	2.674475000	-3.150050000	H	-0.602663000	-5.535679000	-0.157829000
C	0.432520000	1.393637000	-2.385232000	H	-1.456926000	-4.876743000	-1.586111000
H	5.805247000	-0.321757000	-0.575886000	H	0.284884000	-5.187087000	-1.669609000
H	1.994626000	-1.532729000	-2.134793000	Part II Hydroxylation of PBA to 4-OH-PBA by the proximal and distal oxygen of the Mn^{III}(OOH) species 1.			
H	5.417600000	-2.413432000	-2.350076000	³ RC			
H	5.241335000	-0.925691000	-3.282191000	Mn	0.885752000	0.312146000	-0.221143000
H	3.976594000	-2.164855000	-3.352918000	N	2.264155000	1.828269000	0.113894000
H	4.596092000	1.982714000	1.728342000	N	2.537537000	-0.369116000	-1.365831000
H	5.929912000	0.850851000	1.464125000	N	-0.363168000	-1.304345000	-0.497386000
H	4.656771000	0.466046000	2.631791000	N	1.688876000	-1.146488000	1.267154000
H	1.870496000	-0.044823000	2.556170000	C	3.233495000	1.918673000	-0.820421000
H	2.380393000	1.594166000	2.183390000	C	4.206798000	2.923881000	-0.770687000
H	1.337225000	2.290462000	-0.047622000	C	4.135874000	3.827177000	0.290892000
H	1.524586000	3.570503000	1.907584000	C	3.143833000	3.729273000	1.273293000
H	0.421885000	4.430413000	0.871015000	C	2.221127000	2.698076000	1.138297000
H	-0.371639000	4.382328000	3.254498000	C	3.072088000	4.689283000	2.428420000
H	-1.526372000	3.548627000	2.223187000	C	5.283541000	3.020898000	-1.818539000
H	-1.082687000	2.136251000	4.219594000	C	3.170471000	0.877107000	-1.902463000
H	0.652039000	2.219179000	3.931879000	C	3.493224000	-1.074150000	-0.406182000
H	-0.286428000	0.062936000	3.058754000	C	4.651131000	-1.744106000	-1.161501000
H	-1.465408000	0.962100000	2.116973000	C	4.178846000	-2.669847000	-2.284972000
H	-5.884347000	-0.720271000	0.078518000	C	3.280316000	-1.892497000	-3.250790000
H	-2.088902000	-1.813427000	1.772841000	C	2.109667000	-1.264719000	-2.496415000
H	-5.448492000	-2.889737000	1.787079000	C	-0.345565000	-2.255634000	0.461260000
H	-5.454958000	-1.412862000	2.752797000	C	-1.090753000	-3.433370000	0.328576000
H	-4.102893000	-2.550907000	2.890635000	C	-1.858542000	-3.578530000	-0.827083000
H	-4.704667000	1.769189000	-2.011869000	C	-1.895678000	-2.586796000	-1.812578000
H	-5.969018000	0.536251000	-1.924424000	C	-1.124276000	-1.451991000	-1.596668000
H	-4.604216000	0.329423000	-3.031626000	C	-2.730343000	-2.734960000	-3.053305000
H	-1.644403000	-0.056349000	-2.753728000	C	-1.062096000	-4.505418000	1.385464000
H	-2.378807000	1.498423000	-2.393632000	C	0.500056000	-1.945261000	1.668362000
H	-1.662287000	1.966284000	0.236802000	C	2.656861000	-2.006208000	0.486137000
H	-2.078150000	3.424010000	-1.594016000	C	3.456892000	-2.948349000	1.400244000
H	-1.206718000	4.330719000	-0.394882000	C	4.128681000	-2.224504000	2.569623000
H	-0.348650000	4.754523000	-2.728112000	C	3.073623000	-1.451847000	3.366660000
H	0.917776000	4.075243000	-1.716646000	C	2.327100000	-0.486573000	2.447353000
H	0.911969000	2.848412000	-3.863496000	H	4.876400000	4.618757000	0.359084000
H	-0.813280000	2.545716000	-3.738948000	H	1.435606000	2.547021000	1.866351000
H	0.494814000	0.530052000	-3.049439000	H	2.932890000	5.713684000	2.069330000
H	1.400533000	1.501618000	-1.899295000	H	4.001207000	4.667581000	3.006041000
O	0.190229000	-2.004266000	1.177084000	H	2.244757000	4.445075000	3.097770000
O	2.654159000	-2.469970000	2.523856000	H	5.927304000	2.134901000	-1.805313000
H	3.294260000	-2.752210000	1.861514000				

H	5.911619000	3.895323000	-1.641503000	C	-4.443763000	-3.312589000	1.722495000
H	4.857351000	3.104922000	-2.822789000	H	-3.098010000	-2.303819000	3.074213000
H	2.548012000	1.230765000	-2.728757000	H	-2.825377000	-0.328568000	1.622129000
H	4.160903000	0.664548000	-2.303492000	H	-5.514654000	-2.040775000	-1.247482000
H	3.914835000	-0.284999000	0.217934000	H	-5.757218000	-4.049777000	0.179426000
H	5.291741000	-0.962639000	-1.582354000	H	-4.550426000	-4.191531000	2.350396000
H	5.276178000	-2.271967000	-0.438605000	C	-4.002634000	0.187732000	-0.779731000
H	5.044487000	-3.079997000	-2.812264000	H	-2.968001000	0.546278000	-0.740337000
H	3.626017000	-3.523199000	-1.872688000	H	-4.207484000	-0.061247000	-1.826773000
H	2.861883000	-2.550991000	-4.017659000	C	-4.940407000	1.322067000	-0.335914000
H	3.859675000	-1.125251000	-3.775832000	H	-4.772539000	1.540456000	0.724410000
H	1.472363000	-0.663435000	-3.146298000	H	-5.981361000	0.995323000	-0.431690000
H	1.494268000	-2.056394000	-2.071786000	C	-4.711590000	2.600622000	-1.165598000
H	-2.450281000	-4.479296000	-0.955845000	H	-3.671460000	2.920749000	-1.071685000
H	-1.092685000	-0.630886000	-2.302413000	H	-4.928817000	2.405250000	-2.219270000
H	-3.771869000	-2.937316000	-2.788416000	C	-5.582430000	3.723905000	-0.666338000
H	-2.375510000	-3.573598000	-3.660833000	O	-6.815054000	3.708159000	-1.223543000
H	-2.697568000	-1.831105000	-3.665130000	H	-7.339697000	4.423677000	-0.827927000
H	-0.065473000	-4.952670000	1.466973000	O	-5.261609000	4.542632000	0.170719000
H	-1.770136000	-5.298288000	1.139806000	⁵ RC			
H	-1.332108000	-4.107678000	2.366952000	Mn	0.877804000	0.285588000	-0.169573000
H	-0.083371000	-1.343190000	2.370978000	N	2.269135000	1.843307000	0.121411000
H	0.792974000	-2.859426000	2.186027000	N	2.633784000	-0.372812000	-1.422176000
H	2.040518000	-2.631080000	-0.161808000	N	-0.383796000	-1.317662000	-0.471718000
H	2.767078000	-3.700836000	1.796502000	N	1.700895000	-1.115643000	1.197881000
H	4.179253000	-3.503738000	0.798721000	C	3.237960000	1.933763000	-0.809179000
H	4.639436000	-2.951208000	3.207679000	C	4.184802000	2.968449000	-0.776003000
H	4.896387000	-1.531062000	2.203008000	C	4.084745000	3.897079000	0.260071000
H	3.533457000	-0.868271000	4.169881000	C	3.084632000	3.803650000	1.234506000
H	2.374402000	-2.149649000	3.841700000	C	2.191748000	2.745931000	1.116089000
H	1.536393000	0.053531000	2.971151000	C	2.974935000	4.794323000	2.360515000
H	3.030995000	0.255476000	2.067416000	C	5.266762000	3.075062000	-1.818329000
O	0.175348000	1.180534000	-1.699385000	C	3.229996000	0.890534000	-1.899500000
O	-0.235262000	2.576562000	-1.542803000	C	3.546722000	-1.082192000	-0.460490000
H	0.558493000	3.084857000	-1.772958000	C	4.708091000	-1.782644000	-1.184192000
O	-0.409014000	1.010805000	1.326369000	C	4.234831000	-2.699750000	-2.315945000
C	-1.235191000	1.920356000	1.535514000	C	3.369737000	-1.903638000	-3.298872000
O	-1.529030000	2.845868000	0.667304000	C	2.207254000	-1.242956000	-2.558421000
H	-0.995140000	2.762857000	-0.188412000	C	-0.344946000	-2.263490000	0.487159000
C	-1.940658000	2.031120000	2.848985000	C	-1.088845000	-3.442736000	0.376241000
H	-1.506559000	2.872764000	3.399185000	C	-1.864742000	-3.598252000	-0.773724000
H	-2.998650000	2.249665000	2.691528000	C	-1.906272000	-2.618867000	-1.771709000
H	-1.812048000	1.118404000	3.427976000	C	-1.139951000	-1.476778000	-1.569103000
C	-3.627500000	-2.254526000	2.127440000	C	-2.741858000	-2.784614000	-3.009460000
C	-3.477870000	-1.135652000	1.308830000	C	-1.057093000	-4.497680000	1.449393000
C	-4.148083000	-1.043101000	0.082288000	C	0.529323000	-1.924480000	1.659779000
C	-4.979868000	-2.101341000	-0.303440000	C	2.671182000	-1.994086000	0.419412000
C	-5.119555000	-3.232594000	0.502861000	C	3.438729000	-2.946790000	1.349069000

C	4.130227000	-2.225733000	2.507953000	C	-1.938001000	1.743802000	3.182356000
C	3.098303000	-1.413007000	3.294233000	H	-1.520390000	2.576761000	3.758753000
C	2.366712000	-0.443680000	2.367024000	H	-3.015355000	1.895978000	3.105480000
H	4.805511000	4.708121000	0.312131000	H	-1.710496000	0.810884000	3.696299000
H	1.397241000	2.598847000	1.835147000	C	-3.616656000	-2.137905000	2.061554000
H	2.825365000	5.806168000	1.971156000	C	-3.514124000	-1.062190000	1.181556000
H	3.892715000	4.805077000	2.956523000	C	-4.229494000	-1.038368000	-0.022733000
H	2.139226000	4.553993000	3.021014000	C	-5.058176000	-2.125867000	-0.323165000
H	5.927889000	2.202095000	-1.793820000	C	-5.152709000	-3.215824000	0.545306000
H	5.876289000	3.963493000	-1.645465000	C	-4.433243000	-3.225072000	1.741908000
H	4.846837000	3.141816000	-2.826662000	H	-3.050624000	-2.131789000	2.988294000
H	2.621228000	1.253521000	-2.733818000	H	-2.859919000	-0.234398000	1.425938000
H	4.241838000	0.742687000	-2.282698000	H	-5.626992000	-2.121901000	-1.249050000
H	3.977092000	-0.305899000	0.174874000	H	-5.790324000	-4.056066000	0.287538000
H	5.361306000	-1.008592000	-1.601403000	H	-4.505224000	-4.071709000	2.417287000
H	5.319641000	-2.319991000	-0.456473000	C	-4.118072000	0.144520000	-0.955041000
H	5.099920000	-3.132034000	-2.826860000	H	-3.065087000	0.426827000	-1.066889000
H	3.655242000	-3.539833000	-1.911919000	H	-4.476041000	-0.133378000	-1.952356000
H	2.957088000	-2.553478000	-4.076585000	C	-4.902597000	1.368231000	-0.455675000
H	3.978512000	-1.146557000	-3.806704000	H	-4.558355000	1.638301000	0.548160000
H	1.597783000	-0.625328000	-3.221596000	H	-5.965492000	1.117537000	-0.374900000
H	1.554884000	-2.020921000	-2.156986000	C	-4.718050000	2.573412000	-1.398799000
H	-2.458477000	-4.499609000	-0.888710000	H	-3.656454000	2.813042000	-1.495517000
H	-1.116139000	-0.660795000	-2.281661000	H	-5.115307000	2.334210000	-2.389361000
H	-3.778429000	-3.006019000	-2.741020000	C	-5.415477000	3.793666000	-0.856590000
H	-2.372278000	-3.617012000	-3.616842000	O	-6.733627000	3.810275000	-1.160586000
H	-2.727750000	-1.881143000	-3.622448000	H	-7.133951000	4.593071000	-0.747544000
H	-0.060591000	-4.943755000	1.536737000	O	-4.895691000	4.662621000	-0.186828000
H	-1.765500000	-5.294826000	1.219184000	³ TS _{dis}			
H	-1.324901000	-4.082011000	2.424422000	Mn	0.918295000	0.297671000	-0.267942000
H	-0.032390000	-1.312960000	2.370741000	N	2.298284000	1.970790000	-0.037278000
H	0.858666000	-2.820122000	2.185055000	N	2.736539000	-0.356546000	-1.375447000
H	2.047025000	-2.604538000	-0.234531000	N	-0.271957000	-1.398406000	-0.381125000
H	2.736382000	-3.683133000	1.752069000	N	1.808415000	-0.922910000	1.260617000
H	4.147834000	-3.521225000	0.750028000	C	3.262495000	2.019392000	-0.968853000
H	4.619776000	-2.956575000	3.157601000	C	4.167180000	3.090346000	-1.035468000
H	4.916862000	-1.559961000	2.131446000	C	4.021182000	4.107984000	-0.092767000
H	3.576144000	-0.820804000	4.080314000	C	3.018965000	4.062500000	0.883215000
H	2.387612000	-2.082227000	3.791728000	C	2.173909000	2.958581000	0.862882000
H	1.591194000	0.117510000	2.889198000	C	2.858922000	5.148273000	1.911638000
H	3.082019000	0.274408000	1.967539000	C	5.246890000	3.143502000	-2.084263000
O	0.106728000	1.187745000	-1.625395000	C	3.301495000	0.879232000	-1.958061000
O	-0.429582000	2.482283000	-1.304223000	C	3.671861000	-0.956045000	-0.360161000
H	0.281927000	3.095820000	-1.550176000	C	4.858532000	-1.669477000	-1.030060000
O	-0.338970000	1.029507000	1.542094000	C	4.421785000	-2.686077000	-2.088419000
C	-1.301262000	1.752942000	1.829303000	C	3.528983000	-1.999581000	-3.127006000
O	-1.820816000	2.608700000	0.977434000	C	2.339838000	-1.330648000	-2.437410000
H	-1.314853000	2.596771000	0.119928000	C	-0.157736000	-2.248236000	0.659610000

C	-0.803140000	-3.487882000	0.660813000	H	1.620932000	0.466847000	2.816647000
C	-1.573142000	-3.807174000	-0.460926000	H	3.113540000	0.599349000	1.899673000
C	-1.710557000	-2.921943000	-1.532264000	O	0.268928000	1.047674000	-1.663199000
C	-1.032825000	-1.709732000	-1.444057000	O	-1.935797000	1.203217000	-1.542154000
C	-2.528642000	-3.257565000	-2.748547000	H	-1.948993000	1.782677000	-2.321319000
C	-0.692564000	-4.433710000	1.826827000	O	-0.260596000	1.128267000	1.326421000
C	0.676402000	-1.735437000	1.796409000	C	-1.216135000	1.881513000	1.591576000
C	2.828512000	-1.825374000	0.586492000	O	-2.083910000	2.283991000	0.712908000
C	3.628366000	-2.647205000	1.609279000	H	-1.955601000	1.877492000	-0.241655000
C	4.267422000	-1.784685000	2.700057000	C	-1.417797000	2.405692000	2.981511000
C	3.188738000	-0.944780000	3.389595000	H	-0.984120000	3.410665000	3.035221000
C	2.427460000	-0.108326000	2.362339000	H	-2.481092000	2.487110000	3.211054000
H	4.705759000	4.951281000	-0.116214000	H	-0.910027000	1.765876000	3.702284000
H	1.384272000	2.843470000	1.592971000	C	-3.533766000	-2.102755000	1.936806000
H	2.677141000	6.114247000	1.430205000	C	-3.650698000	-1.023149000	1.071959000
H	3.767389000	5.248927000	2.513797000	C	-4.375265000	-1.136443000	-0.133495000
H	2.024063000	4.938110000	2.583781000	C	-4.956051000	-2.378598000	-0.452403000
H	5.934744000	2.296191000	-1.991233000	C	-4.844458000	-3.460646000	0.415185000
H	5.829164000	4.061293000	-1.986582000	C	-4.134940000	-3.326926000	1.614258000
H	4.826131000	3.114500000	-3.094319000	H	-2.973316000	-1.998432000	2.860260000
H	2.699437000	1.142432000	-2.833474000	H	-3.184141000	-0.078426000	1.324582000
H	4.323520000	0.721537000	-2.308155000	H	-5.508824000	-2.480502000	-1.381137000
H	4.072410000	-0.116219000	0.209830000	H	-5.308377000	-4.408294000	0.161719000
H	5.488669000	-0.908905000	-1.503083000	H	-4.041394000	-4.172185000	2.288133000
H	5.482986000	-2.128912000	-0.261137000	C	-4.539803000	0.041051000	-1.035191000
H	5.303535000	-3.121698000	-2.567042000	H	-3.516032000	0.370512000	-1.371387000
H	3.874422000	-3.515234000	-1.622073000	H	-5.084025000	-0.240627000	-1.942211000
H	3.140246000	-2.720742000	-3.852336000	C	-5.204416000	1.255385000	-0.367444000
H	4.107818000	-1.260156000	-3.692277000	H	-4.654274000	1.533425000	0.536463000
H	1.704641000	-0.790957000	-3.142018000	H	-6.217824000	0.978983000	-0.056244000
H	1.721360000	-2.099962000	-1.971564000	C	-5.262898000	2.464881000	-1.318346000
H	-2.085828000	-4.763262000	-0.490584000	H	-4.254652000	2.745175000	-1.631166000
H	-1.098463000	-0.960575000	-2.220279000	H	-5.850919000	2.215876000	-2.205946000
H	-3.389657000	-3.872447000	-2.479057000	C	-5.871109000	3.657203000	-0.624295000
H	-1.927510000	-3.819869000	-3.471477000	O	-7.222409000	3.642115000	-0.667139000
H	-2.888902000	-2.352923000	-3.243770000	H	-7.554829000	4.406343000	-0.167808000
H	0.346643000	-4.729978000	2.003009000	O	-5.249850000	4.527068000	-0.049853000
H	-1.274057000	-5.337978000	1.639678000	⁵ TS _{dis}			
H	-1.067288000	-3.976139000	2.747373000	Mn	0.823814000	0.256342000	-0.230577000
H	0.069067000	-1.079017000	2.425651000	N	2.099896000	1.978421000	-0.087329000
H	1.038263000	-2.549624000	2.422837000	N	2.678435000	-0.355287000	-1.359275000
H	2.246765000	-2.525131000	-0.015369000	N	-0.213642000	-1.535242000	-0.307611000
H	2.957009000	-3.376487000	2.073437000	N	1.792385000	-0.845857000	1.333262000
H	4.373673000	-3.240237000	1.075602000	C	3.039084000	2.061909000	-1.044145000
H	4.778772000	-2.424848000	3.424424000	C	3.864872000	3.190658000	-1.164937000
H	5.030129000	-1.124196000	2.268621000	C	3.672383000	4.226456000	-0.251241000
H	3.629617000	-0.255515000	4.116050000	C	2.702420000	4.142103000	0.753890000
H	2.502786000	-1.592593000	3.946828000	C	1.935851000	2.983404000	0.788013000

C	2.495009000	5.243474000	1.756906000	H	0.055770000	-1.044483000	2.497771000
C	4.914808000	3.283854000	-2.241064000	H	1.105356000	-2.456979000	2.570321000
C	3.143980000	0.893515000	-1.994360000	H	2.306275000	-2.462177000	0.103641000
C	3.644325000	-0.833343000	-0.309949000	H	3.069943000	-3.207347000	2.210755000
C	4.888981000	-1.488316000	-0.930913000	H	4.472239000	-3.033342000	1.197225000
C	4.542427000	-2.585351000	-1.941798000	H	4.855494000	-2.123126000	3.514121000
C	3.615062000	-2.017698000	-3.021611000	H	5.025952000	-0.846997000	2.316330000
C	2.372649000	-1.404303000	-2.376353000	H	3.597287000	0.001764000	4.151905000
C	-0.089947000	-2.313112000	0.786436000	H	2.542217000	-1.397837000	4.033496000
C	-0.665563000	-3.585033000	0.844665000	H	1.542785000	0.575763000	2.850755000
C	-1.351631000	-4.024694000	-0.290448000	H	3.020439000	0.759260000	1.916238000
C	-1.469808000	-3.228155000	-1.432164000	O	0.041478000	0.982422000	-1.638041000
C	-0.883967000	-1.967233000	-1.385661000	O	-1.891833000	0.811658000	-1.502635000
C	-2.178782000	-3.705004000	-2.669160000	H	-1.956722000	1.179670000	-2.400387000
C	-0.566963000	-4.441111000	2.079248000	O	-0.463933000	1.078057000	1.408103000
C	0.701532000	-1.696091000	1.903061000	C	-1.299067000	1.983971000	1.530417000
C	2.854538000	-1.713724000	0.677101000	O	-1.997564000	2.448874000	0.522107000
C	3.701756000	-2.461234000	1.717988000	H	-1.854347000	1.900187000	-0.312327000
C	4.304068000	-1.533942000	2.775910000	C	-1.585426000	2.645340000	2.842871000
C	3.187893000	-0.731563000	3.450516000	H	-1.376283000	3.716018000	2.759446000
C	2.375185000	0.030565000	2.404926000	H	-2.647134000	2.537459000	3.081296000
H	4.295955000	5.113492000	-0.318956000	H	-0.975420000	2.204275000	3.628995000
H	1.182465000	2.838979000	1.549619000	C	-3.690220000	-2.330812000	1.809221000
H	2.241847000	6.182239000	1.254491000	C	-3.726801000	-1.164939000	1.054720000
H	3.407647000	5.417846000	2.335469000	C	-4.275962000	-1.167166000	-0.244822000
H	1.689572000	4.999737000	2.453207000	C	-4.755417000	-2.381842000	-0.772015000
H	5.668107000	2.496203000	-2.131304000	C	-4.735354000	-3.544723000	-0.007777000
H	5.425910000	4.246887000	-2.192967000	C	-4.202293000	-3.523384000	1.284159000
H	4.476749000	3.181545000	-3.238828000	H	-3.262988000	-2.315106000	2.806481000
H	2.507030000	1.082665000	-2.865089000	H	-3.329264000	-0.246771000	1.472922000
H	4.168139000	0.802888000	-2.363229000	H	-5.164544000	-2.398137000	-1.777337000
H	3.977176000	0.059400000	0.221798000	H	-5.128618000	-4.468698000	-0.419092000
H	5.465550000	-0.706083000	-1.436508000	H	-4.173228000	-4.432566000	1.875809000
H	5.537787000	-1.861543000	-0.135700000	C	-4.369396000	0.073821000	-1.044022000
H	5.459707000	-2.979137000	-2.389092000	H	-3.226402000	0.367396000	-1.292780000
H	4.050169000	-3.427892000	-1.438954000	H	-4.804711000	-0.104392000	-2.031549000
H	3.291766000	-2.800167000	-3.715101000	C	-4.986863000	1.290644000	-0.361959000
H	4.147809000	-1.266225000	-3.616048000	H	-4.476839000	1.504096000	0.581519000
H	1.708416000	-0.948719000	-3.113382000	H	-6.024173000	1.039313000	-0.110536000
H	1.804530000	-2.194107000	-1.881448000	C	-4.965932000	2.540036000	-1.258825000
H	-1.806212000	-5.010437000	-0.280009000	H	-3.942844000	2.818222000	-1.516830000
H	-0.940625000	-1.276463000	-2.215075000	H	-5.514325000	2.337640000	-2.184599000
H	-3.047951000	-4.312781000	-2.408575000	C	-5.596138000	3.727038000	-0.571936000
H	-1.511082000	-4.321587000	-3.280988000	O	-6.931108000	3.576398000	-0.422041000
H	-2.514251000	-2.864407000	-3.280739000	H	-7.278628000	4.354135000	0.044741000
H	0.474990000	-4.668895000	2.327616000	O	-5.004303000	4.707391000	-0.172870000
H	-1.092246000	-5.386179000	1.931265000	³ IM1 _{dis}			
H	-1.010740000	-3.939782000	2.945016000	Mn	0.806887000	0.143655000	-0.131987000

N	0.579380000	2.102970000	0.470287000	H	2.582786000	-0.703910000	-2.461201000
N	2.138589000	1.087362000	-1.455514000	H	1.790161000	-5.577517000	-1.219382000
N	1.204746000	-1.835710000	-0.631659000	H	0.010794000	-1.814016000	-2.302735000
N	2.666362000	-0.288279000	0.993683000	H	-0.594016000	-5.205660000	-2.767002000
C	0.961908000	3.000843000	-0.459341000	H	0.861092000	-4.982293000	-3.739774000
C	0.822484000	4.379296000	-0.251250000	H	-0.395383000	-3.730900000	-3.726464000
C	0.269284000	4.788668000	0.962608000	H	4.155910000	-4.277599000	0.955339000
C	-0.125885000	3.863944000	1.935827000	H	3.155684000	-5.715063000	0.707369000
C	0.052696000	2.518634000	1.634381000	H	2.771709000	-4.578967000	2.008436000
C	-0.715903000	4.294255000	3.250592000	H	1.944406000	-1.829702000	2.218940000
C	1.250675000	5.375846000	-1.295955000	H	3.571424000	-2.122468000	1.619165000
C	1.509399000	2.414178000	-1.730524000	H	3.716895000	-0.856510000	-0.723047000
C	3.459535000	1.275421000	-0.725633000	H	5.354693000	-1.153769000	0.947194000
C	4.557342000	1.807679000	-1.659700000	H	5.928616000	0.121953000	-0.088041000
C	4.717590000	0.977318000	-2.935074000	H	6.275461000	0.647308000	2.349940000
C	3.372882000	0.890404000	-3.662409000	H	5.209195000	1.836652000	1.614702000
C	2.307258000	0.314972000	-2.731740000	H	4.200212000	1.099242000	3.756896000
C	2.003017000	-2.522288000	0.204136000	H	4.332946000	-0.588368000	3.280595000
C	2.243793000	-3.892658000	0.028159000	H	2.004696000	0.264286000	2.901053000
C	1.626263000	-4.516042000	-1.056400000	H	2.647888000	1.588740000	1.943801000
C	0.808571000	-3.801457000	-1.940122000	O	-0.536834000	0.258567000	-1.332636000
C	0.629589000	-2.447381000	-1.679281000	O	-3.065964000	0.634301000	-0.131318000
C	0.132571000	-4.462092000	-3.110694000	H	-1.410423000	0.460048000	-0.948750000
C	3.128720000	-4.657741000	0.976682000	O	-0.229548000	-0.699492000	1.579843000
C	2.590224000	-1.732989000	1.343000000	C	-1.145775000	-0.716812000	2.408638000
C	3.780960000	-0.041549000	-0.000664000	O	-2.269163000	-0.049997000	2.284517000
C	5.167144000	-0.114339000	0.658162000	H	-2.447287000	0.305800000	1.366294000
C	5.289373000	0.778738000	1.895483000	C	-1.061574000	-1.531490000	3.662360000
C	4.182950000	0.426294000	2.894301000	H	-1.451529000	-0.965258000	4.510193000
C	2.813946000	0.549005000	2.227166000	H	-1.695878000	-2.413494000	3.526569000
H	0.148617000	5.850776000	1.155870000	H	-0.036916000	-1.848806000	3.847304000
H	-0.221066000	1.749468000	2.342948000	C	-4.030473000	-3.307843000	1.779165000
H	-1.623846000	4.884588000	3.092854000	C	-4.424991000	-2.142902000	1.119192000
H	-0.010205000	4.920781000	3.805009000	C	-3.689371000	-1.664350000	0.028905000
H	-0.970613000	3.432892000	3.871664000	C	-2.558545000	-2.375328000	-0.392567000
H	2.326527000	5.308227000	-1.489999000	C	-2.153270000	-3.530623000	0.274262000
H	1.031143000	6.393133000	-0.967497000	C	-2.890813000	-4.000004000	1.363661000
H	0.734092000	5.206067000	-2.245715000	H	-4.610127000	-3.669811000	2.622326000
H	0.686762000	2.242717000	-2.429535000	H	-5.301861000	-1.609699000	1.468344000
H	2.218544000	3.092600000	-2.204580000	H	-1.984789000	-2.005936000	-1.234611000
H	3.270190000	2.041865000	0.027109000	H	-1.266277000	-4.061274000	-0.054943000
H	4.309589000	2.838803000	-1.931682000	H	-2.581406000	-4.901427000	1.883312000
H	5.492071000	1.872276000	-1.099098000	C	-4.019195000	-0.360376000	-0.666302000
H	5.475970000	1.432488000	-3.578358000	H	-3.354946000	1.533881000	-0.336947000
H	5.072364000	-0.032665000	-2.693638000	H	-3.789462000	-0.456808000	-1.733354000
H	3.439027000	0.237480000	-4.537941000	C	-5.457440000	0.119929000	-0.498455000
H	3.075895000	1.879819000	-4.028450000	H	-5.637065000	0.383775000	0.548707000
H	1.322922000	0.274084000	-3.199086000	H	-6.119038000	-0.714183000	-0.745857000

C	-5.796604000	1.315675000	-1.407636000	H	2.234784000	2.708272000	-2.676047000
H	-5.174805000	2.188907000	-1.196175000	H	3.031634000	2.378500000	-0.166593000
H	-5.642881000	1.034312000	-2.455184000	H	4.346800000	2.749601000	-2.089488000
C	-7.231154000	1.762272000	-1.243534000	H	5.438846000	2.216270000	-0.841740000
O	-8.104960000	0.794685000	-1.595981000	H	5.920745000	1.116005000	-3.051304000
H	-9.006979000	1.129497000	-1.462760000	H	5.473530000	-0.093961000	-1.857131000
O	-7.587315000	2.849088000	-0.842478000	H	4.205381000	-0.542808000	-3.941398000
⁵ IM1 _{dis}				H	3.620185000	1.116638000	-3.983527000
Mn	0.798651000	0.084881000	-0.041738000	H	1.867548000	-0.401747000	-3.024092000
N	0.249556000	2.122662000	-0.114923000	H	3.027242000	-0.996678000	-1.850685000
N	2.294853000	0.937936000	-1.480408000	H	2.792577000	-5.418498000	0.517998000
N	1.399236000	-1.884416000	0.117236000	H	0.388058000	-2.511570000	-1.558350000
N	2.442893000	0.286119000	1.309580000	H	0.717905000	-6.029035000	-1.249581000
C	0.671101000	2.778867000	-1.208755000	H	2.128779000	-5.543468000	-2.189092000
C	0.259841000	4.095569000	-1.472125000	H	0.564419000	-4.765797000	-2.483583000
C	-0.610398000	4.691413000	-0.560211000	H	4.546790000	-3.155314000	2.490923000
C	-1.049837000	4.012736000	0.582747000	H	3.924033000	-4.810132000	2.501911000
C	-0.580314000	2.717270000	0.759405000	H	3.132152000	-3.557251000	3.468174000
C	-1.982894000	4.646063000	1.577779000	H	1.700834000	-0.956275000	2.830885000
C	0.728888000	4.832063000	-2.699320000	H	3.435490000	-1.119031000	2.587041000
C	1.559805000	2.018290000	-2.163758000	H	3.849279000	-0.536755000	-0.005905000
C	3.415944000	1.472547000	-0.639281000	H	5.164138000	-0.159640000	1.928781000
C	4.630342000	1.876051000	-1.492204000	H	5.796293000	0.868710000	0.677850000
C	5.091850000	0.758970000	-2.433137000	H	5.622407000	2.055919000	2.893770000
C	3.920107000	0.304671000	-3.310378000	H	4.619889000	2.849057000	1.686703000
C	2.741283000	-0.118553000	-2.434542000	H	3.278632000	2.580823000	3.749950000
C	2.215806000	-2.157772000	1.151667000	H	3.656705000	0.866479000	3.822793000
C	2.736737000	-3.442112000	1.347506000	H	1.378900000	1.232829000	2.847395000
C	2.391928000	-4.414800000	0.406410000	H	2.063445000	2.327389000	1.655287000
C	1.555310000	-4.129061000	-0.678696000	O	-0.363259000	-0.318171000	-1.371313000
C	1.061711000	-2.831363000	-0.772385000	O	-2.977388000	0.458603000	-0.512238000
C	1.218041000	-5.171106000	-1.709596000	H	-1.284267000	-0.066498000	-1.179582000
C	3.633028000	-3.758369000	2.515915000	O	-0.462574000	-0.217359000	1.811475000
C	2.483830000	-0.999930000	2.070236000	C	-1.479715000	-0.388154000	2.486462000
C	3.699831000	0.436238000	0.465480000	O	-2.681514000	-0.047767000	2.068082000
C	4.933988000	0.729192000	1.332756000	H	-2.694851000	0.232731000	1.105849000
C	4.735587000	1.925207000	2.267200000	C	-1.456019000	-1.016495000	3.845493000
C	3.492510000	1.702426000	3.133585000	H	-0.469136000	-0.909281000	4.294127000
C	2.270299000	1.441511000	2.254825000	H	-2.224492000	-0.583970000	4.487251000
H	-0.951082000	5.706895000	-0.741620000	H	-1.675047000	-2.083514000	3.726003000
H	-0.862785000	2.133408000	1.624794000	C	-2.563285000	-3.825492000	-0.013456000
H	-2.908082000	4.968022000	1.089974000	C	-3.164258000	-2.568661000	0.040161000
H	-1.525354000	5.532173000	2.029103000	C	-3.366331000	-1.828184000	-1.133257000
H	-2.241523000	3.949089000	2.377834000	C	-2.964019000	-2.371219000	-2.358347000
H	1.816774000	4.958819000	-2.694554000	C	-2.375515000	-3.635473000	-2.415129000
H	0.274351000	5.823091000	-2.747161000	C	-2.174330000	-4.364324000	-1.241853000
H	0.466259000	4.293188000	-3.615077000	H	-2.408910000	-4.387974000	0.901836000
H	0.926335000	1.557130000	-2.927644000	H	-3.476125000	-2.171991000	0.999481000

H	-3.113553000	-1.801815000	-3.271049000	H	-2.347969000	-5.391372000	-0.217400000
H	-2.076361000	-4.049878000	-3.372730000	H	0.214405000	-2.718934000	-2.396197000
H	-1.722040000	-5.349241000	-1.283762000	H	-2.197712000	-5.244372000	-2.984675000
C	-3.982834000	-0.449084000	-1.098058000	H	-0.750314000	-6.092685000	-2.439215000
H	-3.179992000	1.373360000	-0.751564000	H	-0.599041000	-4.696761000	-3.520128000
H	-4.148439000	-0.106177000	-2.123503000	H	-1.696487000	-4.056540000	2.946694000
C	-5.296137000	-0.381371000	-0.318615000	H	-2.939127000	-4.902943000	2.014199000
H	-5.135906000	-0.715756000	0.710907000	H	-3.111513000	-3.178648000	2.363930000
H	-5.987956000	-1.088680000	-0.785486000	H	-1.613102000	-0.802555000	1.779890000
C	-5.915665000	1.028508000	-0.315066000	H	-0.763366000	-1.963636000	2.773639000
H	-5.267449000	1.740139000	0.200164000	H	1.553702000	-2.441613000	1.660678000
H	-6.071685000	1.369199000	-1.343901000	H	0.923429000	-2.211193000	3.932186000
C	-7.241621000	1.037676000	0.407185000	H	2.657241000	-2.106329000	3.878519000
O	-8.213140000	0.433552000	-0.311474000	H	1.644384000	-0.379580000	5.405218000
H	-9.032888000	0.440237000	0.209637000	H	2.524553000	0.399034000	4.097032000
O	-7.438730000	1.502165000	1.509581000	H	0.322295000	1.509637000	4.313654000
³ TS _{pro}				H	-0.511945000	-0.035343000	4.223337000
Mn	0.678033000	-0.385023000	-0.468926000	H	-0.547942000	1.142771000	2.009144000
N	-0.244747000	-2.198392000	-0.453731000	H	1.196286000	1.278925000	2.047867000
N	0.475834000	-0.646838000	1.619637000	H	3.509228000	4.780607000	-0.794392000
N	1.594097000	1.469068000	-0.484313000	H	-0.137773000	2.580511000	-0.278946000
N	2.780844000	-0.936463000	-0.069956000	H	-0.228682000	5.016174000	-0.766083000
C	-0.884387000	-2.490960000	0.695626000	H	1.267994000	5.931207000	-1.052188000
C	-1.665447000	-3.647106000	0.826414000	H	0.772335000	5.515285000	0.592642000
C	-1.748344000	-4.488061000	-0.284818000	H	5.668362000	2.144419000	-0.110407000
C	-1.076721000	-4.197215000	-1.477982000	H	5.551346000	3.635289000	-1.055009000
C	-0.330447000	-3.024093000	-1.511014000	H	5.442401000	2.063037000	-1.859068000
C	-1.157511000	-5.104339000	-2.674887000	H	3.647563000	-0.186151000	-1.821634000
C	-2.392623000	-3.963055000	2.106567000	H	4.603870000	0.131182000	-0.387518000
C	-0.752026000	-1.474810000	1.798569000	H	2.934759000	0.254659000	1.634918000
C	1.691784000	-1.440624000	2.073362000	H	5.079631000	-0.718089000	1.531854000
C	1.747217000	-1.569298000	3.604149000	H	4.339436000	-1.314829000	2.989965000
C	1.648182000	-0.221274000	4.323158000	H	5.541606000	-3.129145000	1.729425000
C	0.376209000	0.506841000	3.878910000	H	3.826567000	-3.500724000	1.836676000
C	0.360684000	0.652862000	2.359379000	H	4.564017000	-3.857006000	-0.506521000
C	2.932791000	1.455119000	-0.653174000	H	5.254147000	-2.239648000	-0.571111000
C	3.670334000	2.641309000	-0.764054000	H	2.997197000	-2.273146000	-1.662731000
C	2.965738000	3.844652000	-0.702274000	H	2.304553000	-2.977603000	-0.211761000
C	1.579340000	3.868185000	-0.527451000	O	-1.267233000	0.470353000	-0.521490000
C	0.935002000	2.638965000	-0.419872000	O	-1.737126000	0.792702000	-1.852872000
C	0.804004000	5.153393000	-0.440806000	H	-2.187440000	-0.023929000	-2.130210000
C	5.163828000	2.619628000	-0.958647000	O	1.089365000	-0.475680000	-2.472228000
C	3.580495000	0.096883000	-0.767313000	C	1.075078000	0.236899000	-3.487286000
C	2.938086000	-0.815962000	1.422428000	O	0.201478000	1.201601000	-3.662871000
C	4.287156000	-1.377644000	1.901165000	H	-0.476816000	1.190473000	-2.938202000
C	4.551172000	-2.800678000	1.401412000	C	2.070763000	0.070662000	-4.587240000
C	4.449313000	-2.837138000	-0.126878000	H	1.587635000	0.169533000	-5.560541000
C	3.087388000	-2.308802000	-0.575498000	H	2.813794000	0.871301000	-4.498322000

H	2.570593000	-0.892266000	-4.495705000	C	-0.579182000	-2.529775000	-1.195928000
C	-3.161972000	4.966361000	-0.362345000	C	-1.168317000	-4.601061000	-2.513132000
C	-3.388293000	3.593295000	-0.325691000	C	0.853568000	-4.782664000	2.125079000
C	-2.987184000	2.822909000	0.788373000	C	1.066239000	-1.768117000	1.996899000
C	-2.326422000	3.488297000	1.846999000	C	3.061006000	-1.214504000	0.652552000
C	-2.100015000	4.859682000	1.806175000	C	4.169386000	-1.698719000	1.602633000
C	-2.521966000	5.608686000	0.702824000	C	4.593412000	-0.625894000	2.608982000
H	-3.487944000	5.540718000	-1.224123000	C	3.366793000	-0.152185000	3.394621000
H	-3.885285000	3.112335000	-1.161029000	C	2.274906000	0.329596000	2.438110000
H	-2.017578000	2.916809000	2.717944000	H	2.991669000	5.721049000	-0.658635000
H	-1.601412000	5.348570000	2.637406000	H	0.367232000	3.053621000	1.420846000
H	-2.348164000	6.679373000	0.670302000	H	0.882250000	6.516218000	0.968513000
C	-3.180176000	1.371803000	0.850067000	H	2.163974000	5.963297000	2.046595000
H	-2.094155000	0.889389000	0.160770000	H	0.527367000	5.305351000	2.212768000
H	-3.045461000	0.978996000	1.863240000	H	4.723009000	3.307947000	-2.423070000
C	-4.355556000	0.724796000	0.134880000	H	4.171423000	4.982719000	-2.544701000
H	-4.335064000	0.961492000	-0.934714000	H	3.394441000	3.720190000	-3.509138000
H	-5.303217000	1.123797000	0.519032000	H	1.771496000	1.284562000	-2.924841000
C	-4.335986000	-0.805713000	0.321049000	H	3.488220000	1.407090000	-2.586813000
H	-3.372195000	-1.224001000	0.024587000	H	3.609340000	0.794354000	0.110352000
H	-4.498817000	-1.044487000	1.378072000	H	5.146889000	0.409242000	-1.658526000
C	-5.385763000	-1.517799000	-0.493681000	H	5.620340000	-0.622241000	-0.338759000
O	-6.639681000	-1.158889000	-0.141790000	H	5.706172000	-1.822581000	-2.548677000
H	-7.267486000	-1.639775000	-0.705894000	H	4.539555000	-2.591492000	-1.481934000
O	-5.162139000	-2.321112000	-1.375121000	H	3.485584000	-2.312570000	-3.703065000
⁵ TS _{pro}				H	3.904476000	-0.604923000	-3.731766000
Mn	0.461898000	0.239766000	-0.121239000	H	1.512236000	-0.901009000	-3.058785000
N	1.348964000	2.277436000	-0.221686000	H	1.999145000	-2.015227000	-1.796420000
N	2.390711000	0.008673000	-1.391533000	H	-0.234094000	-5.720152000	-0.184500000
N	-0.049066000	-1.894023000	-0.142807000	H	-0.941152000	-1.903413000	-2.004268000
N	1.876485000	-0.672276000	1.406969000	H	-1.787851000	-5.462371000	-2.251893000
C	2.234606000	2.473414000	-1.212604000	H	-0.337681000	-4.964955000	-3.128076000
C	2.855966000	3.717805000	-1.412871000	H	-1.764955000	-3.918937000	-3.122441000
C	2.527502000	4.746982000	-0.530702000	H	1.927594000	-4.637851000	2.283485000
C	1.624408000	4.547117000	0.518743000	H	0.679234000	-5.849264000	1.971494000
C	1.061857000	3.279845000	0.622900000	H	0.342767000	-4.485273000	3.046048000
C	1.277025000	5.640005000	1.492202000	H	0.285305000	-1.303094000	2.605814000
C	3.837801000	3.943407000	-2.533772000	H	1.659795000	-2.402755000	2.657555000
C	2.509995000	1.293261000	-2.114874000	H	2.694265000	-2.089195000	0.113949000
C	3.504595000	-0.167673000	-0.394871000	H	3.794180000	-2.570487000	2.150179000
C	4.841759000	-0.476213000	-1.090380000	H	5.017159000	-2.063461000	1.019001000
C	4.747022000	-1.671773000	-2.044143000	H	5.354758000	-1.026998000	3.284821000
C	3.630848000	-1.433164000	-3.067529000	H	5.050020000	0.226124000	2.088626000
C	2.313203000	-1.130189000	-2.351546000	H	3.622405000	0.672023000	4.068237000
C	0.431275000	-2.592915000	0.901437000	H	2.989624000	-0.968412000	4.022361000
C	0.359539000	-3.992449000	0.940863000	H	1.368102000	0.613893000	2.973324000
C	-0.181691000	-4.634961000	-0.175074000	H	2.626760000	1.219964000	1.911424000
C	-0.646456000	-3.917609000	-1.280373000	O	-1.427020000	0.638861000	-1.177890000

O	-1.635065000	2.059369000	-1.111276000	C	3.442856000	0.512534000	-0.872639000
H	-1.308353000	2.385865000	-1.964838000	C	4.583775000	0.748861000	-1.873893000
O	-0.760505000	0.809414000	1.727434000	C	4.472605000	-0.137370000	-3.117422000
C	-1.630014000	1.533341000	2.207710000	C	3.106967000	0.071494000	-3.779371000
O	-2.230881000	2.488779000	1.509525000	C	1.984083000	-0.176810000	-2.771782000
H	-1.926577000	2.488954000	0.571108000	C	1.092496000	-2.682310000	0.132386000
C	-2.106615000	1.428175000	3.621993000	C	1.019367000	-4.042842000	-0.203252000
H	-1.938572000	2.380616000	4.132610000	C	0.221776000	-4.398477000	-1.292013000
H	-3.183303000	1.236185000	3.631672000	C	-0.485913000	-3.435219000	-2.017291000
H	-1.576550000	0.627976000	4.134973000	C	-0.370951000	-2.117314000	-1.589871000
C	-3.228456000	-2.952277000	1.393103000	C	-1.337029000	-3.796943000	-3.203925000
C	-3.344129000	-1.704158000	0.798376000	C	1.777860000	-5.086685000	0.574774000
C	-3.724616000	-1.583285000	-0.558646000	C	1.954586000	-2.170601000	1.264008000
C	-3.977416000	-2.763480000	-1.294022000	C	3.484655000	-0.849923000	-0.143983000
C	-3.902720000	-4.008656000	-0.682658000	C	4.867069000	-1.292275000	0.364539000
C	-3.514799000	-4.109719000	0.657421000	C	5.342577000	-0.484111000	1.575053000
H	-2.914995000	-3.030646000	2.428818000	C	4.294496000	-0.571012000	2.689073000
H	-3.120265000	-0.813615000	1.373414000	C	2.937747000	-0.097927000	2.167148000
H	-4.262174000	-2.683533000	-2.338535000	H	1.766145000	5.930615000	0.814810000
H	-4.130182000	-4.904039000	-1.251129000	H	0.371477000	2.199162000	2.381568000
H	-3.428040000	-5.084638000	1.125506000	H	0.036241000	5.636768000	2.993021000
C	-3.862675000	-0.279421000	-1.199991000	H	1.663153000	5.229302000	3.539591000
H	-2.573901000	0.166822000	-1.243529000	H	0.327773000	4.099993000	3.825498000
H	-4.123589000	-0.343604000	-2.259408000	H	3.405610000	4.630885000	-1.938814000
C	-4.610410000	0.821278000	-0.459992000	H	2.521756000	6.069196000	-1.413655000
H	-4.072503000	1.134871000	0.439477000	H	1.782443000	4.941402000	-2.559354000
H	-5.563249000	0.405820000	-0.108662000	H	0.907574000	2.101913000	-2.495668000
C	-4.892509000	2.042110000	-1.354965000	H	2.609730000	2.528391000	-2.442315000
H	-3.968161000	2.439651000	-1.771652000	H	3.491553000	1.302763000	-0.121356000
H	-5.549471000	1.743911000	-2.178476000	H	4.570581000	1.800474000	-2.178772000
C	-5.558590000	3.153541000	-0.582255000	H	5.538469000	0.607539000	-1.362970000
O	-6.806746000	2.820643000	-0.183254000	H	5.279905000	0.099005000	-3.816728000
H	-7.175270000	3.560776000	0.326610000	H	4.591057000	-1.193441000	-2.843500000
O	-5.056996000	4.225526000	-0.316096000	H	2.966397000	-0.617780000	-4.617780000
³ IM _{pro}				H	3.040544000	1.084917000	-4.191400000
Mn	0.690671000	0.198426000	0.014371000	H	1.002120000	0.014339000	-3.209402000
N	1.006252000	2.185263000	0.413530000	H	2.000886000	-1.223121000	-2.469930000
N	2.079258000	0.656008000	-1.530495000	H	0.155356000	-5.443366000	-1.581473000
N	0.398429000	-1.750515000	-0.551377000	H	-0.890870000	-1.320461000	-2.110266000
N	2.466330000	-0.819304000	0.955123000	H	-2.045149000	-4.591667000	-2.949663000
C	1.544067000	2.877845000	-0.611986000	H	-0.716594000	-4.165918000	-4.027217000
C	1.830183000	4.246626000	-0.512521000	H	-1.901954000	-2.934653000	-3.565552000
C	1.554840000	4.870697000	0.704446000	H	2.859737000	-4.930991000	0.501862000
C	1.026859000	4.157546000	1.786417000	H	1.555644000	-6.084415000	0.191836000
C	0.769274000	2.807338000	1.582296000	H	1.514564000	-5.064227000	1.636722000
C	0.746312000	4.812338000	3.111178000	H	1.347934000	-2.095971000	2.171372000
C	2.415234000	5.013583000	-1.669460000	H	2.762207000	-2.876796000	1.473617000
C	1.800911000	2.083079000	-1.861817000	H	3.143782000	-1.613391000	-0.845009000

H	4.794153000	-2.347508000	0.651833000	N	1.969888000	-0.799028000	1.172509000
H	5.589619000	-1.258933000	-0.453689000	C	2.078512000	2.796183000	-0.879572000
H	6.308041000	-0.865425000	1.920936000	C	2.657211000	4.074148000	-0.811441000
H	5.498898000	0.566552000	1.297238000	C	2.225080000	4.919822000	0.211112000
H	4.574985000	0.049258000	3.546306000	C	1.256433000	4.512303000	1.133238000
H	4.221544000	-1.603506000	3.051843000	C	0.743901000	3.229312000	0.971640000
H	2.156647000	-0.198301000	2.923352000	C	0.790185000	5.405550000	2.250100000
H	3.002871000	0.964873000	1.916483000	C	3.703053000	4.529194000	-1.797125000
O	-1.791666000	0.659378000	-0.851435000	C	2.456781000	1.803633000	-1.953602000
O	-2.351776000	1.789130000	-0.134325000	C	3.566110000	0.174652000	-0.458431000
H	-2.045877000	2.540575000	-0.666989000	C	4.938405000	0.121194000	-1.150901000
O	-0.371430000	-0.153454000	1.736392000	C	4.979525000	-0.905046000	-2.288080000
C	-1.141434000	0.206522000	2.630675000	C	3.859942000	-0.612678000	-3.293864000
O	-2.077453000	1.117934000	2.451347000	C	2.506594000	-0.554210000	-2.582158000
H	-2.103211000	1.441156000	1.514180000	C	0.678577000	-2.700538000	0.277877000
C	-1.031306000	-0.317510000	4.027718000	C	0.700251000	-4.087811000	0.064060000
H	-0.222223000	0.224824000	4.529980000	C	0.152504000	-4.560025000	-1.130738000
H	-1.954053000	-0.161457000	4.584115000	C	-0.409508000	-3.692828000	-2.072689000
H	-0.768155000	-1.374915000	4.001937000	C	-0.390796000	-2.336952000	-1.758035000
C	-3.456111000	-2.208303000	2.718453000	C	-1.014267000	-4.192206000	-3.356058000
C	-4.019673000	-1.414497000	1.729912000	C	1.281199000	-5.041184000	1.075735000
C	-3.847515000	-1.737248000	0.353040000	C	1.253886000	-2.050869000	1.517848000
C	-3.097810000	-2.908826000	0.041989000	C	3.211843000	-1.081453000	0.373168000
C	-2.518590000	-3.679676000	1.036529000	C	4.349857000	-1.623440000	1.254307000
C	-2.688980000	-3.333666000	2.384514000	C	4.653311000	-0.717093000	2.449902000
H	-3.612075000	-1.953634000	3.761674000	C	3.375025000	-0.512757000	3.268467000
H	-4.598712000	-0.542295000	2.010285000	C	2.253317000	0.028141000	2.381027000
H	-2.990458000	-3.191147000	-0.998527000	H	2.657433000	5.913278000	0.293430000
H	-1.937784000	-4.555742000	0.768069000	H	-0.002967000	2.851254000	1.656263000
H	-2.241054000	-3.939385000	3.165416000	H	0.384396000	6.342481000	1.855909000
C	-4.376136000	-0.945212000	-0.699813000	H	1.621611000	5.663611000	2.913856000
H	-2.556347000	0.033773000	-0.829034000	H	0.014633000	4.920926000	2.847470000
H	-4.264702000	-1.328807000	-1.713052000	H	4.597424000	3.898884000	-1.751822000
C	-5.270302000	0.242631000	-0.512605000	H	4.006270000	5.555771000	-1.583297000
H	-4.936310000	0.851290000	0.334929000	H	3.329151000	4.494620000	-2.825079000
H	-6.287968000	-0.093082000	-0.263527000	H	1.716271000	1.856063000	-2.759796000
C	-5.330142000	1.118781000	-1.780605000	H	3.417299000	2.078268000	-2.393482000
H	-4.332386000	1.457158000	-2.063519000	H	3.564184000	1.038530000	0.209727000
H	-5.746436000	0.535595000	-2.608447000	H	5.158602000	1.114322000	-1.557430000
C	-6.181915000	2.346163000	-1.574228000	H	5.716769000	-0.069333000	-0.408949000
O	-7.490097000	2.039600000	-1.425160000	H	5.956015000	-0.877149000	-2.780966000
H	-7.984200000	2.861927000	-1.273110000	H	4.858064000	-1.920067000	-1.888134000
O	-5.772863000	3.487187000	-1.524136000	H	3.812193000	-1.388078000	-4.065115000
⁵ IM _{pro}				H	4.061096000	0.333422000	-3.810046000
Mn	0.504710000	0.273177000	-0.212848000	H	1.701517000	-0.284271000	-3.270050000
N	1.137370000	2.397689000	-0.005021000	H	2.264765000	-1.543509000	-2.190297000
N	2.458050000	0.413469000	-1.446837000	H	0.162547000	-5.628378000	-1.328747000
N	0.139761000	-1.861569000	-0.622765000	H	-0.798769000	-1.601103000	-2.444233000

H	-1.862182000	-4.854528000	-3.152841000	C	-6.149878000	2.401179000	-1.544863000
H	-0.283837000	-4.766427000	-3.934311000	O	-7.403563000	2.167218000	-1.096335000
H	-1.368788000	-3.365303000	-3.975376000	H	-7.836102000	3.021185000	-0.931437000
H	2.344650000	-4.845292000	1.248427000	O	-5.715112000	3.523167000	-1.699145000
H	1.182658000	-6.071569000	0.729149000	Part III. Hydroxylation of PBA to 4-OH-PBA by the			
H	0.769707000	-4.957862000	2.039784000	Mn^{IV}(O)(AcO•) species 2 generated from the Mn^{III}-OOH			
H	0.431984000	-1.784512000	2.189762000	species 1.			
H	1.894916000	-2.753975000	2.053319000	³ RC			
H	2.941099000	-1.875604000	-0.323993000	Mn	0.885752000	0.312146000	-0.221143000
H	4.053735000	-2.611194000	1.625163000	N	2.264155000	1.828269000	0.113894000
H	5.237158000	-1.795147000	0.641493000	N	2.537537000	-0.369116000	-1.365831000
H	5.441027000	-1.161366000	3.065912000	N	-0.363168000	-1.304345000	-0.497386000
H	5.031213000	0.254659000	2.106271000	N	1.688876000	-1.146488000	1.267154000
H	3.538368000	0.194284000	4.088178000	C	3.233495000	1.918673000	-0.820421000
H	3.071023000	-1.462308000	3.725421000	C	4.206798000	2.923881000	-0.770687000
H	1.316813000	0.119819000	2.931302000	C	4.135874000	3.827177000	0.290892000
H	2.518055000	1.031954000	2.036573000	C	3.143833000	3.729273000	1.273293000
O	-1.644985000	0.577283000	-1.237610000	C	2.221127000	2.698076000	1.138297000
O	-2.208550000	1.861581000	-0.876845000	C	3.072088000	4.689283000	2.428420000
H	-1.911397000	2.429425000	-1.606189000	C	5.283541000	3.020898000	-1.818539000
O	-0.775018000	0.412335000	1.645592000	C	3.170471000	0.877107000	-1.902463000
C	-1.617528000	0.976059000	2.340338000	C	3.493224000	-1.074150000	-0.406182000
O	-2.457115000	1.877780000	1.849477000	C	4.651131000	-1.744106000	-1.161501000
H	-2.314623000	1.992714000	0.880162000	C	4.178846000	-2.669847000	-2.284972000
C	-1.743812000	0.763182000	3.815367000	C	3.280316000	-1.892497000	-3.250790000
H	-1.173080000	1.553000000	4.316969000	C	2.109667000	-1.264719000	-2.496415000
H	-2.782652000	0.842974000	4.136707000	C	-0.345565000	-2.255634000	0.461260000
H	-1.322686000	-0.202693000	4.088600000	C	-1.090753000	-3.433370000	0.328576000
C	-3.247783000	-2.121920000	2.660179000	C	-1.858542000	-3.578530000	-0.827083000
C	-3.806804000	-1.312122000	1.681718000	C	-1.895678000	-2.586796000	-1.812578000
C	-3.743223000	-1.681704000	0.306839000	C	-1.124276000	-1.451991000	-1.596668000
C	-3.114997000	-2.920072000	-0.013726000	C	-2.730343000	-2.734960000	-3.053305000
C	-2.560437000	-3.719228000	0.972709000	C	-1.062096000	-4.505418000	1.385464000
C	-2.609515000	-3.321671000	2.316244000	C	0.500056000	-1.945261000	1.668362000
H	-3.315419000	-1.828891000	3.702768000	C	2.656861000	-2.006208000	0.486137000
H	-4.309074000	-0.394366000	1.966625000	C	3.456892000	-2.948349000	1.400244000
H	-3.085852000	-3.235238000	-1.051242000	C	4.128681000	-2.224504000	2.569623000
H	-2.092237000	-4.658787000	0.702738000	C	3.073623000	-1.451847000	3.366660000
H	-2.172272000	-3.947742000	3.086998000	C	2.327100000	-0.486573000	2.447353000
C	-4.286747000	-0.876326000	-0.729007000	H	4.876400000	4.618757000	0.359084000
H	-2.420227000	-0.019761000	-1.086076000	H	1.435606000	2.547021000	1.866351000
H	-4.267804000	-1.284923000	-1.738388000	H	2.932890000	5.713684000	2.069330000
C	-5.123954000	0.345658000	-0.494887000	H	4.001207000	4.667581000	3.006041000
H	-4.651038000	1.008763000	0.239153000	H	2.244757000	4.445075000	3.097770000
H	-6.086881000	0.053672000	-0.050735000	H	5.927304000	2.134901000	-1.805313000
C	-5.388119000	1.124181000	-1.797788000	H	5.911619000	3.895323000	-1.641503000
H	-4.449942000	1.394308000	-2.283711000	H	4.857351000	3.104922000	-2.822789000
H	-5.968106000	0.499373000	-2.484943000	H	2.548012000	1.230765000	-2.728757000

H	4.160903000	0.664548000	-2.303492000	H	-5.514654000	-2.040775000	-1.247482000
H	3.914835000	-0.284999000	0.217934000	H	-5.757218000	-4.049777000	0.179426000
H	5.291741000	-0.962639000	-1.582354000	H	-4.550426000	-4.191531000	2.350396000
H	5.276178000	-2.271967000	-0.438605000	C	-4.002634000	0.187732000	-0.779731000
H	5.044487000	-3.079997000	-2.812264000	H	-2.968001000	0.546278000	-0.740337000
H	3.626017000	-3.523199000	-1.872688000	H	-4.207484000	-0.061247000	-1.826773000
H	2.861883000	-2.550991000	-4.017659000	C	-4.940407000	1.322067000	-0.335914000
H	3.859675000	-1.125251000	-3.775832000	H	-4.772539000	1.540456000	0.724410000
H	1.472363000	-0.663435000	-3.146298000	H	-5.981361000	0.995323000	-0.431690000
H	1.494268000	-2.056394000	-2.071786000	C	-4.711590000	2.600622000	-1.165598000
H	-2.450281000	-4.479296000	-0.955845000	H	-3.671460000	2.920749000	-1.071685000
H	-1.092685000	-0.630886000	-2.302413000	H	-4.928817000	2.405250000	-2.219270000
H	-3.771869000	-2.937316000	-2.788416000	C	-5.582430000	3.723905000	-0.666338000
H	-2.375510000	-3.573598000	-3.660833000	O	-6.815054000	3.708159000	-1.223543000
H	-2.697568000	-1.831105000	-3.665130000	H	-7.339697000	4.423677000	-0.827927000
H	-0.065473000	-4.952670000	1.466973000	O	-5.261609000	4.542632000	0.170719000
H	-1.770136000	-5.298288000	1.139806000	⁵ RC			
H	-1.332108000	-4.107678000	2.366952000	Mn	0.877804000	0.285588000	-0.169573000
H	-0.083371000	-1.343190000	2.370978000	N	2.269135000	1.843307000	0.121411000
H	0.792974000	-2.859426000	2.186027000	N	2.633784000	-0.372812000	-1.422176000
H	2.040518000	-2.631080000	-0.161808000	N	-0.383796000	-1.317662000	-0.471718000
H	2.767078000	-3.700836000	1.796502000	N	1.700895000	-1.115643000	1.197881000
H	4.179253000	-3.503738000	0.798721000	C	3.237960000	1.933763000	-0.809179000
H	4.639436000	-2.951208000	3.207679000	C	4.184802000	2.968449000	-0.776003000
H	4.896387000	-1.531062000	2.203008000	C	4.084745000	3.897079000	0.260071000
H	3.533457000	-0.868271000	4.169881000	C	3.084632000	3.803650000	1.234506000
H	2.374402000	-2.149649000	3.841700000	C	2.191748000	2.745931000	1.116089000
H	1.536393000	0.053531000	2.971151000	C	2.974935000	4.794323000	2.360515000
H	3.030995000	0.255476000	2.067416000	C	5.266762000	3.075062000	-1.818329000
O	0.175348000	1.180534000	-1.699385000	C	3.229996000	0.890534000	-1.899500000
O	-0.235262000	2.576562000	-1.542803000	C	3.546722000	-1.082192000	-0.460490000
H	0.558493000	3.084857000	-1.772958000	C	4.708091000	-1.782644000	-1.184192000
O	-0.409014000	1.010805000	1.326369000	C	4.234831000	-2.699750000	-2.315945000
C	-1.235191000	1.920356000	1.535514000	C	3.369737000	-1.903638000	-3.298872000
O	-1.529030000	2.845868000	0.667304000	C	2.207254000	-1.242956000	-2.558421000
H	-0.995140000	2.762857000	-0.188412000	C	-0.344946000	-2.263490000	0.487159000
C	-1.940658000	2.031120000	2.848985000	C	-1.088845000	-3.442736000	0.376241000
H	-1.506559000	2.872764000	3.399185000	C	-1.864742000	-3.598252000	-0.773724000
H	-2.998650000	2.249665000	2.691528000	C	-1.906272000	-2.618867000	-1.771709000
H	-1.812048000	1.118404000	3.427976000	C	-1.139951000	-1.476778000	-1.569103000
C	-3.627500000	-2.254526000	2.127440000	C	-2.741858000	-2.784614000	-3.009460000
C	-3.477870000	-1.135652000	1.308830000	C	-1.057093000	-4.497680000	1.449393000
C	-4.148083000	-1.043101000	0.082288000	C	0.529323000	-1.924480000	1.659779000
C	-4.979868000	-2.101341000	-0.303440000	C	2.671182000	-1.994086000	0.419412000
C	-5.119555000	-3.232594000	0.502861000	C	3.438729000	-2.946790000	1.349069000
C	-4.443763000	-3.312589000	1.722495000	C	4.130227000	-2.225733000	2.507953000
H	-3.098010000	-2.303819000	3.074213000	C	3.098303000	-1.413007000	3.294233000
H	-2.825377000	-0.328568000	1.622129000	C	2.366712000	-0.443680000	2.367024000

H	4.805511000	4.708121000	0.312131000	H	-1.710496000	0.810884000	3.696299000
H	1.397241000	2.598847000	1.835147000	C	-3.616656000	-2.137905000	2.061554000
H	2.825365000	5.806168000	1.971156000	C	-3.514124000	-1.062190000	1.181556000
H	3.892715000	4.805077000	2.956523000	C	-4.229494000	-1.038368000	-0.022733000
H	2.139226000	4.553993000	3.021014000	C	-5.058176000	-2.125867000	-0.323165000
H	5.927889000	2.202095000	-1.793820000	C	-5.152709000	-3.215824000	0.545306000
H	5.876289000	3.963493000	-1.645465000	C	-4.433243000	-3.225072000	1.741908000
H	4.846837000	3.141816000	-2.826662000	H	-3.050624000	-2.131789000	2.988294000
H	2.621228000	1.253521000	-2.733818000	H	-2.859919000	-0.234398000	1.425938000
H	4.241838000	0.742687000	-2.282698000	H	-5.626992000	-2.121901000	-1.249050000
H	3.977092000	-0.305899000	0.174874000	H	-5.790324000	-4.056066000	0.287538000
H	5.361306000	-1.008592000	-1.601403000	H	-4.505224000	-4.071709000	2.417287000
H	5.319641000	-2.319991000	-0.456473000	C	-4.118072000	0.144520000	-0.955041000
H	5.099920000	-3.132034000	-2.826860000	H	-3.065087000	0.426827000	-1.066889000
H	3.655242000	-3.539833000	-1.911919000	H	-4.476041000	-0.133378000	-1.952356000
H	2.957088000	-2.553478000	-4.076585000	C	-4.902597000	1.368231000	-0.455675000
H	3.978512000	-1.146557000	-3.806704000	H	-4.558355000	1.638301000	0.548160000
H	1.597783000	-0.625328000	-3.221596000	H	-5.965492000	1.117537000	-0.374900000
H	1.554884000	-2.020921000	-2.156986000	C	-4.718050000	2.573412000	-1.398799000
H	-2.458477000	-4.499609000	-0.888710000	H	-3.656454000	2.813042000	-1.495517000
H	-1.116139000	-0.660795000	-2.281661000	H	-5.115307000	2.334210000	-2.389361000
H	-3.778429000	-3.006019000	-2.741020000	C	-5.415477000	3.793666000	-0.856590000
H	-2.372278000	-3.617012000	-3.616842000	O	-6.733627000	3.810275000	-1.160586000
H	-2.727750000	-1.881143000	-3.622448000	H	-7.133951000	4.593071000	-0.747544000
H	-0.060591000	-4.943755000	1.536737000	O	-4.895691000	4.662621000	-0.186828000
H	-1.765500000	-5.294826000	1.219184000				
H	-1.324901000	-4.082011000	2.424422000	³ TS1			
H	-0.032390000	-1.312960000	2.370741000	Mn	0.852977000	0.360008000	-0.232449000
H	0.858666000	-2.820122000	2.185055000	N	2.260301000	1.839083000	0.111173000
H	2.047025000	-2.604538000	-0.234531000	N	2.538140000	-0.361947000	-1.373909000
H	2.736382000	-3.683133000	1.752069000	N	-0.364949000	-1.302367000	-0.484422000
H	4.147834000	-3.521225000	0.750028000	N	1.702128000	-1.142390000	1.269325000
H	4.619776000	-2.956575000	3.157601000	C	3.233801000	1.921291000	-0.821818000
H	4.916862000	-1.559961000	2.131446000	C	4.221028000	2.911151000	-0.758056000
H	3.576144000	-0.820804000	4.080314000	C	4.161328000	3.804338000	0.313216000
H	2.387612000	-2.082227000	3.791728000	C	3.166757000	3.712170000	1.293126000
H	1.591194000	0.117510000	2.889198000	C	2.226924000	2.698474000	1.145485000
H	3.082019000	0.274408000	1.967539000	C	3.108757000	4.659969000	2.458832000
O	0.106728000	1.187745000	-1.625395000	C	5.302275000	3.003889000	-1.801629000
O	-0.429582000	2.482283000	-1.304223000	C	3.161835000	0.887794000	-1.909398000
H	0.281927000	3.095820000	-1.550176000	C	3.492732000	-1.062339000	-0.413065000
O	-0.338970000	1.029507000	1.542094000	C	4.652281000	-1.729505000	-1.169888000
C	-1.301262000	1.752942000	1.829303000	C	4.180665000	-2.660716000	-2.288657000
O	-1.820816000	2.608700000	0.977434000	C	3.278314000	-1.888714000	-3.254853000
H	-1.314853000	2.596771000	0.119928000	C	2.107833000	-1.259312000	-2.500738000
C	-1.938001000	1.743802000	3.182356000	C	-0.334736000	-2.249028000	0.478565000
H	-1.520390000	2.576761000	3.758753000	C	-1.070298000	-3.433757000	0.351634000
H	-3.015355000	1.895978000	3.105480000	C	-1.839353000	-3.591890000	-0.801322000

C	-1.887919000	-2.605043000	-1.790835000	O	0.196534000	1.089197000	-1.642560000
C	-1.127644000	-1.461992000	-1.581173000	O	-0.340518000	2.746084000	-1.608983000
C	-2.719504000	-2.767110000	-3.031781000	H	0.515058000	3.199416000	-1.663328000
C	-1.029787000	-4.501742000	1.412345000	O	-0.342687000	1.027335000	1.240974000
C	0.514244000	-1.932235000	1.680176000	C	-1.210892000	1.925330000	1.422133000
C	2.662643000	-1.997880000	0.480712000	O	-1.534844000	2.806493000	0.547074000
C	3.469829000	-2.939615000	1.389679000	H	-0.983490000	2.777793000	-0.370261000
C	4.150500000	-2.214043000	2.552906000	C	-1.891289000	2.021379000	2.751388000
C	3.102546000	-1.438337000	3.356531000	H	-1.443918000	2.859283000	3.297266000
C	2.348312000	-0.475395000	2.440407000	H	-2.951505000	2.242204000	2.616099000
H	4.913890000	4.583473000	0.390869000	H	-1.750212000	1.107348000	3.325598000
H	1.435994000	2.553963000	1.868334000	C	-3.631814000	-2.291033000	2.127015000
H	2.995503000	5.691073000	2.110280000	C	-3.485139000	-1.156853000	1.329005000
H	4.033517000	4.609776000	3.041581000	C	-4.144804000	-1.049172000	0.098040000
H	2.271818000	4.426910000	3.119978000	C	-4.963774000	-2.107970000	-0.313112000
H	5.935621000	2.110544000	-1.793090000	C	-5.100292000	-3.254108000	0.472234000
H	5.939667000	3.869401000	-1.614896000	C	-4.434409000	-3.349267000	1.696368000
H	4.880225000	3.101357000	-2.806225000	H	-3.111025000	-2.351492000	3.077903000
H	2.530887000	1.246602000	-2.726822000	H	-2.845847000	-0.347855000	1.664083000
H	4.148771000	0.678409000	-2.320497000	H	-5.490653000	-2.035685000	-1.260717000
H	3.913661000	-0.272290000	0.209889000	H	-5.727649000	-4.071222000	0.129109000
H	5.288331000	-0.946556000	-1.594610000	H	-4.538704000	-4.239906000	2.307950000
H	5.280788000	-2.251701000	-0.445962000	C	-4.004835000	0.197930000	-0.741174000
H	5.046490000	-3.069638000	-2.816535000	H	-2.977644000	0.573476000	-0.679154000
H	3.631557000	-3.514511000	-1.872473000	H	-4.189111000	-0.037099000	-1.795247000
H	2.858235000	-2.550282000	-4.018095000	C	-4.967943000	1.309699000	-0.294312000
H	3.854739000	-1.122290000	-3.784221000	H	-4.815764000	1.517315000	0.770547000
H	1.470498000	-0.659596000	-3.151562000	H	-6.001604000	0.965456000	-0.406379000
H	1.492489000	-2.049467000	-2.073195000	C	-4.752342000	2.602549000	-1.105248000
H	-2.421887000	-4.499236000	-0.924914000	H	-3.720469000	2.941502000	-0.990562000
H	-1.106498000	-0.644886000	-2.291411000	H	-4.950015000	2.415666000	-2.164297000
H	-3.754584000	-3.000271000	-2.767828000	C	-5.653032000	3.701935000	-0.605998000
H	-2.340930000	-3.591076000	-3.645092000	O	-6.875188000	3.671515000	-1.185389000
H	-2.711919000	-1.858491000	-3.637264000	H	-7.419786000	4.371755000	-0.789410000
H	-0.030468000	-4.943524000	1.489698000	O	-5.362591000	4.514443000	0.248095000
H	-1.734695000	-5.299099000	1.172560000	⁵ TS1			
H	-1.297052000	-4.102522000	2.393906000	Mn	0.881867000	0.279850000	-0.218857000
H	-0.064678000	-1.323852000	2.381138000	N	2.247518000	1.840828000	0.134617000
H	0.804751000	-2.844199000	2.203185000	N	2.670966000	-0.354362000	-1.418420000
H	2.043851000	-2.623190000	-0.164421000	N	-0.363049000	-1.337663000	-0.496771000
H	2.782197000	-3.690789000	1.792022000	N	1.704031000	-1.105711000	1.186371000
H	4.187152000	-3.496366000	0.783488000	C	3.224587000	1.961640000	-0.782760000
H	4.664454000	-2.940250000	3.188887000	C	4.138154000	3.025141000	-0.738798000
H	4.916916000	-1.522679000	2.179846000	C	3.993383000	3.953654000	0.291868000
H	3.569306000	-0.852174000	4.153766000	C	2.983126000	3.829488000	1.251835000
H	2.406781000	-2.134001000	3.839543000	C	2.126560000	2.742976000	1.123985000
H	1.561565000	0.065495000	2.969425000	C	2.824696000	4.817507000	2.374493000
H	3.049215000	0.265548000	2.053446000	C	5.231026000	3.161617000	-1.766126000

C	3.272917000	0.918241000	-1.870804000	H	2.074320000	-2.592437000	-0.242929000
C	3.569588000	-1.061045000	-0.438775000	H	2.742346000	-3.671062000	1.753409000
C	4.750207000	-1.750623000	-1.142240000	H	4.163656000	-3.504408000	0.767106000
C	4.307017000	-2.671239000	-2.282309000	H	4.605623000	-2.938155000	3.181659000
C	3.460231000	-1.877152000	-3.281530000	H	4.914218000	-1.543128000	2.157086000
C	2.276421000	-1.223749000	-2.570386000	H	3.550731000	-0.799600000	4.086381000
C	-0.332309000	-2.270229000	0.475376000	H	2.367541000	-2.063869000	3.790509000
C	-1.078264000	-3.449372000	0.376854000	H	1.575429000	0.130571000	2.873483000
C	-1.851319000	-3.618530000	-0.772820000	H	3.074437000	0.290236000	1.967715000
C	-1.885785000	-2.652561000	-1.784052000	O	0.281785000	1.060885000	-1.698107000
C	-1.115077000	-1.511398000	-1.595926000	O	-1.021956000	2.609020000	-1.463092000
C	-2.717999000	-2.831468000	-3.022315000	H	-0.303048000	3.218806000	-1.713896000
C	-1.049518000	-4.490818000	1.463070000	O	-0.347397000	0.984542000	1.510076000
C	0.537473000	-1.921677000	1.646854000	C	-1.294634000	1.700536000	1.860269000
C	2.685850000	-1.980989000	0.422205000	O	-1.869365000	2.565684000	1.058925000
C	3.446686000	-2.932219000	1.358866000	H	-1.458918000	2.565496000	0.147612000
C	4.123352000	-2.208735000	2.525038000	C	-1.851394000	1.666618000	3.248791000
C	3.081622000	-1.395044000	3.297485000	H	-1.392750000	2.482232000	3.818732000
C	2.357451000	-0.429454000	2.360465000	H	-2.929933000	1.828890000	3.237094000
H	4.686362000	4.788036000	0.351184000	H	-1.603291000	0.720769000	3.728431000
H	1.329315000	2.572541000	1.833523000	C	-3.620741000	-2.162322000	2.058071000
H	2.660313000	5.825642000	1.981610000	C	-3.511190000	-1.083823000	1.182199000
H	3.728137000	4.849638000	2.991394000	C	-4.212234000	-1.058796000	-0.030558000
H	1.980192000	4.557467000	3.016136000	C	-5.034796000	-2.147741000	-0.342674000
H	5.919898000	2.310780000	-1.727493000	C	-5.136448000	-3.240272000	0.521759000
H	5.808993000	4.070166000	-1.589460000	C	-4.430476000	-3.250977000	1.726277000
H	4.823938000	3.209687000	-2.780864000	H	-3.065885000	-2.156870000	2.991575000
H	2.699956000	1.273920000	-2.732498000	H	-2.863713000	-0.254196000	1.437599000
H	4.302607000	0.774597000	-2.204925000	H	-5.593509000	-2.142680000	-1.274646000
H	3.981658000	-0.281863000	0.204325000	H	-5.769174000	-4.081286000	0.254632000
H	5.405769000	-0.971769000	-1.546106000	H	-4.507974000	-4.099500000	2.398669000
H	5.350146000	-2.281620000	-0.400505000	C	-4.092365000	0.125319000	-0.960522000
H	5.185293000	-3.097792000	-2.774979000	H	-3.035975000	0.389556000	-1.086973000
H	3.723698000	-3.514708000	-1.891344000	H	-4.468459000	-0.144274000	-1.953453000
H	3.067343000	-2.525945000	-4.070231000	C	-4.848472000	1.361509000	-0.447774000
H	4.076166000	-1.115304000	-3.773320000	H	-4.470220000	1.635222000	0.542851000
H	1.683782000	-0.604850000	-3.246646000	H	-5.911074000	1.123709000	-0.332958000
H	1.614268000	-2.002385000	-2.187288000	C	-4.680220000	2.556190000	-1.407562000
H	-2.447279000	-4.519638000	-0.877488000	H	-3.619708000	2.773993000	-1.554711000
H	-1.080302000	-0.709017000	-2.322384000	H	-5.124853000	2.316022000	-2.377869000
H	-3.755232000	-3.049560000	-2.754333000	C	-5.330848000	3.795591000	-0.851178000
H	-2.347079000	-3.670483000	-3.619692000	O	-6.668742000	3.807979000	-1.052626000
H	-2.701974000	-1.934554000	-3.644811000	H	-7.034074000	4.606213000	-0.636779000
H	-0.054958000	-4.940635000	1.553578000	O	-4.759797000	4.684613000	-0.253250000
H	-1.762419000	-5.287147000	1.244331000	³ IM1			
H	-1.313141000	-4.061951000	2.433470000	Mn	0.821312000	0.387645000	-0.096499000
H	-0.029708000	-1.313737000	2.355908000	N	2.244304000	1.868603000	0.235336000
H	0.871818000	-2.814194000	2.174137000	N	2.467135000	-0.199861000	-1.463197000

N	-0.330845000	-1.303616000	-0.395473000	H	-1.209250000	-0.540800000	-2.100463000
N	1.872313000	-1.217456000	1.185111000	H	-3.854376000	-2.873456000	-2.540262000
C	3.136134000	2.054237000	-0.760962000	H	-2.510144000	-3.452971000	-3.527273000
C	4.098160000	3.067028000	-0.689714000	H	-2.851215000	-1.716385000	-3.435780000
C	4.093800000	3.871868000	0.451741000	H	0.173352000	-5.051131000	1.330004000
C	3.174361000	3.677171000	1.487727000	H	-1.547556000	-5.401715000	1.113314000
C	2.251759000	2.648174000	1.329836000	H	-1.029919000	-4.269366000	2.365726000
C	3.173559000	4.534664000	2.722699000	H	0.213890000	-1.515243000	2.431534000
C	5.094046000	3.278372000	-1.799065000	H	1.086961000	-3.001246000	2.067520000
C	2.998859000	1.119233000	-1.927305000	H	2.111085000	-2.560275000	-0.400095000
C	3.505818000	-0.945200000	-0.634271000	H	3.037965000	-3.766630000	1.389437000
C	4.617465000	-1.512206000	-1.533451000	H	4.341810000	-3.456155000	0.280198000
C	4.081444000	-2.363052000	-2.686021000	H	5.024386000	-3.087748000	2.673640000
C	3.086255000	-1.544455000	-3.511955000	H	5.165663000	-1.588130000	1.767581000
C	1.962538000	-1.014898000	-2.619968000	H	3.992478000	-1.105496000	3.898830000
C	-0.211082000	-2.309327000	0.499127000	H	2.827946000	-2.386802000	3.592282000
C	-0.950208000	-3.488918000	0.354554000	H	1.866129000	-0.148828000	2.983503000
C	-1.799510000	-3.584895000	-0.748607000	H	3.258253000	0.162963000	1.955631000
C	-1.923345000	-2.544119000	-1.673982000	O	-0.026126000	1.289471000	-1.229856000
C	-1.167410000	-1.401400000	-1.445456000	O	-1.623410000	3.919460000	-2.063727000
C	-2.835043000	-2.645729000	-2.863640000	H	-2.473623000	4.174981000	-1.664148000
C	-0.830634000	-4.613763000	1.347701000	O	-0.172730000	0.909484000	1.412151000
C	0.736380000	-2.061255000	1.640097000	C	-1.249430000	1.673149000	1.306716000
C	2.772837000	-1.976220000	0.240676000	O	-1.685804000	2.066065000	0.228922000
C	3.674330000	-2.968739000	0.993449000	H	-1.303937000	3.196970000	-1.507573000
C	4.445393000	-2.323631000	2.147814000	C	-1.879148000	2.040498000	2.624417000
C	3.463639000	-1.639518000	3.103958000	H	-1.259304000	2.814472000	3.088645000
C	2.611053000	-0.624411000	2.343284000	H	-2.883338000	2.431660000	2.466894000
H	4.829398000	4.666210000	0.536481000	H	-1.894607000	1.174260000	3.287821000
H	1.509477000	2.426032000	2.084700000	C	-3.357612000	-2.170103000	2.201976000
H	3.037689000	5.587743000	2.458634000	C	-3.503579000	-1.141373000	1.273664000
H	4.128486000	4.448155000	3.250130000	C	-4.359407000	-1.272478000	0.170880000
H	2.374538000	4.245230000	3.407860000	C	-5.067701000	-2.470674000	0.024209000
H	5.741100000	2.403310000	-1.921410000	C	-4.915692000	-3.512905000	0.943079000
H	5.729392000	4.138036000	-1.581369000	C	-4.062235000	-3.365441000	2.037068000
H	4.593228000	3.458773000	-2.755001000	H	-2.690622000	-2.041155000	3.049309000
H	2.287260000	1.528457000	-2.650851000	H	-2.942506000	-0.224772000	1.404272000
H	3.949695000	0.983914000	-2.441927000	H	-5.741250000	-2.590911000	-0.820083000
H	3.956057000	-0.194433000	0.015082000	H	-5.468964000	-4.436865000	0.804869000
H	5.197923000	-0.676707000	-1.936230000	H	-3.944739000	-4.172703000	2.752929000
H	5.312848000	-2.071162000	-0.904507000	C	-4.476862000	-0.164661000	-0.850730000
H	4.912845000	-2.697315000	-3.312344000	H	-3.503538000	-0.026948000	-1.337347000
H	3.591127000	-3.266336000	-2.302609000	H	-5.176359000	-0.463375000	-1.638705000
H	2.620592000	-2.154429000	-4.291336000	C	-4.904808000	1.190819000	-0.270650000
H	3.597108000	-0.718729000	-4.018734000	H	-4.230216000	1.468934000	0.543334000
H	1.262071000	-0.386064000	-3.171082000	H	-5.911173000	1.123634000	0.152943000
H	1.403055000	-1.855349000	-2.212344000	C	-4.854862000	2.280715000	-1.357866000
H	-2.384030000	-4.488991000	-0.883954000	H	-3.899264000	2.245759000	-1.884746000

H	-5.653794000	2.114171000	-2.088877000	H	5.261898000	-0.862509000	-1.671583000
C	-5.005335000	3.669224000	-0.797894000	H	5.307368000	-2.181575000	-0.539016000
O	-6.191374000	3.866243000	-0.195262000	H	5.040187000	-2.973364000	-2.916131000
H	-6.216845000	4.772509000	0.154460000	H	3.658338000	-3.465108000	-1.947457000
O	-4.160948000	4.547481000	-0.852032000	H	2.811330000	-2.493652000	-4.060476000
⁵ IM1				H	3.780778000	-1.045401000	-3.834853000
Mn	0.800338000	0.350961000	-0.170446000	H	1.402510000	-0.644768000	-3.140172000
N	2.191116000	1.857079000	0.115469000	H	1.483589000	-2.046731000	-2.078477000
N	2.511610000	-0.343449000	-1.388959000	H	-2.376917000	-4.543695000	-0.923287000
N	-0.353553000	-1.334662000	-0.457271000	H	-1.127127000	-0.651379000	-2.243896000
N	1.733938000	-1.168118000	1.256231000	H	-3.711384000	-3.123524000	-2.750232000
C	3.154580000	1.951616000	-0.827854000	H	-2.264650000	-3.540098000	-3.675067000
C	4.128938000	2.953851000	-0.768249000	H	-2.779091000	-1.849226000	-3.558912000
C	4.066715000	3.843603000	0.306119000	H	0.036200000	-4.983051000	1.488280000
C	3.080392000	3.739513000	1.293263000	H	-1.659059000	-5.366543000	1.155945000
C	2.150830000	2.715963000	1.151859000	H	-1.251683000	-4.169645000	2.388698000
C	3.019779000	4.685017000	2.460440000	H	-0.004934000	-1.397446000	2.403935000
C	5.199437000	3.066195000	-1.821083000	H	0.889487000	-2.898693000	2.182990000
C	3.078666000	0.930348000	-1.923256000	H	2.084514000	-2.625234000	-0.200486000
C	3.495614000	-1.029823000	-0.454908000	H	2.876647000	-3.693307000	1.735200000
C	4.653077000	-1.664933000	-1.243867000	H	4.258911000	-3.458810000	0.704090000
C	4.176914000	-2.592510000	-2.363745000	H	4.763597000	-2.914243000	3.107962000
C	3.235660000	-1.831006000	-3.300761000	H	4.973282000	-1.484626000	2.106503000
C	2.068652000	-1.236780000	-2.511196000	H	3.644094000	-0.853462000	4.105490000
C	-0.296111000	-2.295830000	0.491930000	H	2.503502000	-2.157666000	3.803827000
C	-1.023337000	-3.483131000	0.354979000	H	1.596224000	0.028233000	2.965938000
C	-1.801528000	-3.632831000	-0.793812000	H	3.063395000	0.267370000	2.024136000
C	-1.869522000	-2.634319000	-1.769711000	O	0.110472000	1.088510000	-1.659569000
C	-1.124747000	-1.482408000	-1.549317000	O	-0.534112000	3.182319000	-1.532957000
C	-2.703708000	-2.789737000	-3.009522000	H	0.292032000	3.609902000	-1.266453000
C	-0.970188000	-4.558802000	1.406757000	O	-0.260288000	0.925210000	1.273198000
C	0.567992000	-1.985299000	1.681629000	C	-1.268927000	1.740268000	1.516576000
C	2.700631000	-1.992673000	0.439589000	O	-1.766587000	2.492754000	0.683575000
C	3.541252000	-2.923959000	1.329223000	H	-1.021916000	2.936291000	-0.698588000
C	4.226177000	-2.193107000	2.485995000	C	-1.736069000	1.708427000	2.950014000
C	3.176721000	-1.445604000	3.313305000	H	-1.092412000	2.379551000	3.529348000
C	2.385916000	-0.489950000	2.420177000	H	-2.762512000	2.069941000	3.012758000
H	4.810418000	4.631500000	0.379321000	H	-1.648433000	0.708476000	3.376149000
H	1.362171000	2.561071000	1.874546000	C	-3.598758000	-2.290339000	2.048984000
H	2.914253000	5.717176000	2.113076000	C	-3.478709000	-1.155884000	1.247671000
H	3.941242000	4.627894000	3.047824000	C	-4.155195000	-1.057099000	0.024725000
H	2.178200000	4.454292000	3.116298000	C	-4.966768000	-2.126370000	-0.373066000
H	5.840194000	2.178347000	-1.828397000	C	-5.078052000	-3.273337000	0.415876000
H	5.831244000	3.934799000	-1.630288000	C	-4.393794000	-3.359547000	1.630363000
H	4.766402000	3.172372000	-2.820073000	H	-3.063971000	-2.342556000	2.992680000
H	2.406259000	1.285201000	-2.709046000	H	-2.847786000	-0.337331000	1.572132000
H	4.056349000	0.755125000	-2.371118000	H	-5.507900000	-2.062168000	-1.313165000
H	3.913666000	-0.238296000	0.168162000	H	-5.700621000	-4.098214000	0.082697000

H	-4.478376000	-4.250851000	2.244002000	H	1.944645000	5.491785000	2.202716000
C	-4.028665000	0.187480000	-0.820934000	H	3.536905000	4.862531000	2.638711000
H	-2.983753000	0.515394000	-0.846521000	H	2.071401000	4.088339000	3.273491000
H	-4.317911000	-0.035155000	-1.854000000	H	4.693303000	2.659891000	-2.510825000
C	-4.887374000	1.346674000	-0.290832000	H	4.438205000	4.386479000	-2.233586000
H	-4.597044000	1.570321000	0.741211000	H	3.285235000	3.466538000	-3.210808000
H	-5.940913000	1.047988000	-0.273207000	H	1.351103000	1.202800000	-2.725729000
C	-4.712852000	2.610591000	-1.155167000	H	3.099055000	0.962378000	-2.719634000
H	-3.660113000	2.898323000	-1.176724000	H	3.566835000	-0.019267000	-0.181566000
H	-5.049380000	2.411375000	-2.176615000	H	4.698415000	-0.423370000	-2.207203000
C	-5.493226000	3.765161000	-0.584072000	H	5.141588000	-1.705185000	-1.117713000
O	-6.793811000	3.743169000	-0.958265000	H	4.656508000	-2.552208000	-3.440695000
H	-7.250124000	4.482517000	-0.523831000	H	3.537244000	-3.262252000	-2.285155000
O	-5.051043000	4.615329000	0.161392000	H	2.231900000	-2.457171000	-4.230489000
³ TS2				H	2.968283000	-0.865467000	-4.118727000
Mn	0.395958000	0.040365000	0.006010000	H	0.684217000	-0.884056000	-3.066671000
N	1.614589000	1.719536000	0.118565000	H	1.174979000	-2.243234000	-2.060327000
N	1.973773000	-0.380056000	-1.496446000	H	-1.915895000	-5.367937000	-0.141628000
N	-0.421612000	-1.849841000	-0.105974000	H	-1.400805000	-1.479334000	-1.883660000
N	1.818172000	-1.253774000	1.256971000	H	-3.397793000	-4.532595000	-2.131549000
C	2.330671000	1.986503000	-0.994135000	H	-1.885129000	-4.596012000	-3.042210000
C	3.140734000	3.123545000	-1.083095000	H	-2.838763000	-3.105645000	-3.022593000
C	3.189148000	3.963196000	0.031148000	H	0.680471000	-5.211462000	2.085797000
C	2.471261000	3.676360000	1.195440000	H	-0.963615000	-5.849035000	1.961294000
C	1.688672000	2.527473000	1.189323000	H	-0.620472000	-4.483614000	3.034208000
C	2.509669000	4.574748000	2.399674000	H	0.359700000	-1.674512000	2.702027000
C	3.931272000	3.425129000	-2.328961000	H	1.413393000	-3.045059000	2.356066000
C	2.210093000	0.970076000	-2.089372000	H	2.099054000	-2.662090000	-0.265241000
C	3.194858000	-0.877644000	-0.740314000	H	3.372398000	-3.592152000	1.473355000
C	4.308735000	-1.314975000	-1.706001000	H	4.494604000	-3.173368000	0.210108000
C	3.834598000	-2.318215000	-2.758577000	H	5.353706000	-2.544579000	2.491287000
C	2.648930000	-1.730352000	-3.527295000	H	5.172372000	-1.108247000	1.493065000
C	1.531949000	-1.342990000	-2.557025000	H	4.161467000	-0.649951000	3.710671000
C	-0.114675000	-2.706492000	0.891194000	H	3.176649000	-2.102740000	3.603678000
C	-0.675044000	-3.988839000	0.933021000	H	1.843401000	-0.065395000	2.977069000
C	-1.491467000	-4.368500000	-0.134546000	H	3.067478000	0.353154000	1.784882000
C	-1.746208000	-3.508895000	-1.206971000	O	-0.617767000	0.670447000	-1.185441000
C	-1.220640000	-2.224823000	-1.121813000	O	-0.422906000	4.611220000	-0.164784000
C	-2.516582000	-3.954755000	-2.417725000	H	-1.311223000	4.983929000	-0.299342000
C	-0.378965000	-4.933884000	2.066983000	O	-0.478780000	0.390528000	1.622486000
C	0.878842000	-2.209191000	1.902275000	C	-1.233115000	1.397649000	2.048357000
C	2.723780000	-1.943520000	0.266103000	O	-1.444075000	2.415397000	1.408286000
C	3.836933000	-2.739914000	0.966297000	H	-0.589930000	3.807102000	0.349805000
C	4.615186000	-1.911811000	1.991264000	C	-1.759893000	1.173371000	3.446706000
C	3.642203000	-1.309048000	3.008667000	H	-0.978436000	1.471306000	4.154318000
C	2.578760000	-0.481904000	2.287002000	H	-2.640148000	1.794241000	3.614054000
H	3.810752000	4.852840000	-0.006510000	H	-1.985735000	0.120799000	3.623563000
H	1.122633000	2.237096000	2.060562000	C	-4.050722000	-2.168944000	1.528662000

C	-3.622974000	-0.993103000	0.933157000	C	-0.031455000	-4.888863000	1.820514000
C	-3.898394000	-0.726790000	-0.428027000	C	1.108497000	-2.105068000	1.816518000
C	-4.636754000	-1.679349000	-1.163857000	C	2.963523000	-1.695589000	0.217627000
C	-5.101686000	-2.838386000	-0.556843000	C	4.103509000	-2.455394000	0.915588000
C	-4.794681000	-3.097578000	0.785281000	C	4.827744000	-1.616468000	1.970425000
H	-3.809701000	-2.371093000	2.566694000	C	3.816047000	-1.088614000	2.991258000
H	-3.048494000	-0.279574000	1.506854000	C	2.717536000	-0.295930000	2.282885000
H	-4.852078000	-1.486126000	-2.209836000	H	3.700320000	5.203435000	0.060690000
H	-5.687883000	-3.551356000	-1.126531000	H	1.066626000	2.469363000	2.050640000
H	-5.130826000	-4.018463000	1.249977000	H	1.960270000	5.845563000	2.175282000
C	-3.425222000	0.516704000	-1.076657000	H	3.375787000	5.010261000	2.819050000
H	-2.277053000	0.570576000	-0.982320000	H	1.748917000	4.438892000	3.233444000
H	-3.604384000	0.480075000	-2.156102000	H	4.767538000	3.057490000	-2.410407000
C	-3.967102000	1.829245000	-0.493874000	H	4.415062000	4.768790000	-2.143993000
H	-3.731813000	1.906232000	0.569709000	H	3.339165000	3.789780000	-3.151564000
H	-5.058042000	1.814538000	-0.586512000	H	1.480462000	1.459590000	-2.712684000
C	-3.390703000	3.035462000	-1.246069000	H	3.235900000	1.294903000	-2.689744000
H	-2.301723000	3.038820000	-1.192815000	H	3.731826000	0.275190000	-0.171054000
H	-3.675436000	2.977793000	-2.304022000	H	4.883601000	-0.037616000	-2.206387000
C	-3.885820000	4.361187000	-0.727569000	H	5.372509000	-1.326709000	-1.146214000
O	-5.226345000	4.426079000	-0.651857000	H	4.921321000	-2.135949000	-3.489337000
H	-5.477535000	5.304839000	-0.321794000	H	3.831066000	-2.916072000	-2.351901000
O	-3.180645000	5.304671000	-0.414699000	H	2.495883000	-2.120728000	-4.279987000
⁵ TS2				H	3.167832000	-0.503757000	-4.133340000
Mn	0.570132000	0.205444000	0.032420000	H	0.885969000	-0.634613000	-3.084662000
N	1.662509000	1.964045000	0.132126000	H	1.428474000	-1.995391000	-2.106443000
N	2.157554000	-0.114868000	-1.503695000	H	-1.593371000	-5.243870000	-0.385830000
N	-0.199266000	-1.693201000	-0.177507000	H	-1.241314000	-1.249630000	-1.906460000
N	2.012761000	-1.082076000	1.221146000	H	-3.161606000	-4.348286000	-2.247161000
C	2.403054000	2.261007000	-0.961462000	H	-1.713006000	-4.243567000	-3.259410000
C	3.154418000	3.439398000	-1.029296000	H	-2.740574000	-2.818527000	-3.033186000
C	3.124203000	4.283310000	0.083720000	H	1.041092000	-5.109364000	1.839236000
C	2.383099000	3.967152000	1.227797000	H	-0.564540000	-5.825733000	1.651930000
C	1.655611000	2.783135000	1.202120000	H	-0.310407000	-4.511082000	2.808667000
C	2.362059000	4.861577000	2.435422000	H	0.562044000	-1.626909000	2.633569000
C	3.962243000	3.782399000	-2.252595000	H	1.679098000	-2.933012000	2.238737000
C	2.340986000	1.253425000	-2.069552000	H	2.379513000	-2.429218000	-0.338789000
C	3.395689000	-0.582938000	-0.753548000	H	3.673797000	-3.342094000	1.393078000
C	4.526636000	-0.954329000	-1.727310000	H	4.790107000	-2.836431000	0.157010000
C	4.090678000	-1.950438000	-2.803076000	H	5.589293000	-2.226071000	2.464344000
C	2.883303000	-1.393206000	-3.560977000	H	5.352329000	-0.775355000	1.499929000
C	1.750531000	-1.072309000	-2.584209000	H	4.293644000	-0.421611000	3.714823000
C	0.145291000	-2.594205000	0.772471000	H	3.383352000	-1.918202000	3.561290000
C	-0.367340000	-3.893235000	0.742306000	H	1.951935000	0.057227000	2.974701000
C	-1.195824000	-4.235209000	-0.330670000	H	3.162657000	0.579199000	1.808396000
C	-1.510612000	-3.321045000	-1.338041000	O	-0.654577000	0.777048000	-1.177395000
C	-1.011159000	-2.031719000	-1.193989000	O	-1.063506000	2.982451000	-1.031773000
C	-2.332185000	-3.700609000	-2.536953000	H	-0.218738000	3.450692000	-1.041361000

O	-0.308225000	0.513297000	1.673054000	C	-3.793087000	-1.792193000	3.288368000
C	-1.245720000	1.341568000	2.100521000	C	-2.781527000	-0.772546000	3.821328000
O	-1.682829000	2.285762000	1.449436000	C	-1.684898000	-0.528427000	2.786035000
H	-1.272549000	2.766029000	-0.085086000	C	0.478633000	-2.687547000	0.059395000
C	-1.695089000	1.048424000	3.508989000	C	1.329789000	-3.758721000	0.372810000
H	-0.906872000	1.372161000	4.196781000	C	2.288957000	-3.547693000	1.364597000
H	-2.611847000	1.594790000	3.727807000	C	2.386221000	-2.324538000	2.037630000
H	-1.839273000	-0.023896000	3.653123000	C	1.487670000	-1.329483000	1.668238000
C	-3.471550000	-2.538608000	1.641436000	C	3.433983000	-2.071115000	3.086018000
C	-3.278793000	-1.340147000	0.958769000	C	1.224559000	-5.076700000	-0.348267000
C	-3.880876000	-1.104543000	-0.286352000	C	-0.555597000	-2.761984000	-1.033969000
C	-4.710799000	-2.100593000	-0.815472000	C	-2.543861000	-2.257951000	0.339188000
C	-4.910494000	-3.305002000	-0.137143000	C	-3.463648000	-3.410742000	-0.094943000
C	-4.285163000	-3.532452000	1.090096000	C	-4.259507000	-3.093018000	-1.364098000
H	-2.978427000	-2.702840000	2.594891000	C	-3.298812000	-2.698229000	-2.490670000
H	-2.633325000	-0.583312000	1.383389000	C	-2.421101000	-1.528608000	-2.047044000
H	-5.191410000	-1.936241000	-1.776033000	H	-4.461633000	4.174749000	-1.749861000
H	-5.548845000	-4.068493000	-0.571839000	H	-1.240231000	1.504050000	-2.688504000
H	-4.430739000	-4.472576000	1.612833000	H	-2.658497000	4.516656000	-3.850305000
C	-3.660329000	0.198087000	-1.019528000	H	-3.789813000	3.251110000	-4.330643000
H	-2.590050000	0.472695000	-1.015503000	H	-2.044952000	2.956034000	-4.423184000
H	-3.953471000	0.071609000	-2.068838000	H	-5.407210000	2.633890000	1.215730000
C	-4.485358000	1.342072000	-0.403976000	H	-5.364850000	4.216479000	0.427845000
H	-4.114884000	1.554895000	0.604182000	H	-4.227062000	3.842099000	1.729768000
H	-5.531186000	1.030647000	-0.305530000	H	-2.009642000	1.892788000	2.120182000
C	-4.409140000	2.621342000	-1.262395000	H	-3.683885000	1.346463000	2.051577000
H	-3.367589000	2.909703000	-1.412690000	H	-3.726219000	-0.484365000	0.080692000
H	-4.870933000	2.438155000	-2.236634000	H	-4.924702000	-0.387031000	2.112749000
C	-5.110393000	3.763325000	-0.577123000	H	-5.066029000	-2.019954000	1.527462000
O	-6.436776000	3.795761000	-0.847355000	H	-4.609973000	-1.935548000	4.001607000
H	-6.834251000	4.523091000	-0.340741000	H	-3.304178000	-2.767337000	3.167499000
O	-4.587916000	4.562101000	0.174187000	H	-2.307212000	-1.130684000	4.740246000
³ IM2				H	-3.290072000	0.165394000	4.072847000
Mn	-0.614392000	0.057140000	-0.027493000	H	-0.966499000	0.226372000	3.108867000
N	-1.956684000	1.449204000	-0.754981000	H	-1.130208000	-1.453735000	2.627853000
N	-2.201155000	-0.081649000	1.454365000	H	2.972612000	-4.353035000	1.617401000
N	0.578577000	-1.506400000	0.695856000	H	1.484094000	-0.351841000	2.134975000
N	-1.656076000	-1.794968000	-0.790367000	H	4.427781000	-2.026837000	2.627496000
C	-2.837290000	1.910495000	0.156286000	H	3.450029000	-2.873780000	3.828719000
C	-3.768238000	2.907544000	-0.164568000	H	3.257205000	-1.124362000	3.601021000
C	-3.752095000	3.401163000	-1.469797000	H	0.248679000	-5.544294000	-0.178066000
C	-2.850088000	2.918091000	-2.423960000	H	1.994829000	-5.766805000	0.000232000
C	-1.963098000	1.931951000	-2.008170000	H	1.343799000	-4.951714000	-1.429214000
C	-2.830919000	3.435979000	-3.836115000	H	-0.084807000	-2.489385000	-1.982277000
C	-4.743950000	3.428705000	0.858030000	H	-0.935857000	-3.780070000	-1.136113000
C	-2.725061000	1.310037000	1.532887000	H	-1.869633000	-2.645094000	1.105038000
C	-3.259076000	-1.018933000	0.909411000	H	-2.842847000	-4.295065000	-0.274668000
C	-4.354095000	-1.307244000	1.949004000	H	-4.119518000	-3.679201000	0.735900000

H	-4.857109000	-3.962371000	-1.653412000	C	1.440573000	-3.995922000	-0.494915000
H	-4.964806000	-2.272890000	-1.177914000	C	2.044768000	-4.407147000	0.696312000
H	-3.846911000	-2.392943000	-3.387373000	C	1.842587000	-3.712807000	1.898602000
H	-2.679506000	-3.556970000	-2.775052000	C	1.019596000	-2.591456000	1.840050000
H	-1.688590000	-1.247891000	-2.805678000	C	2.484186000	-4.151596000	3.185998000
H	-3.052216000	-0.656241000	-1.871176000	C	1.667764000	-4.728126000	-1.790381000
O	0.303213000	1.279597000	0.949404000	C	-0.021488000	-2.280106000	-1.670615000
O	0.430884000	3.707627000	-0.340437000	C	-2.343030000	-2.068645000	-0.834413000
H	1.163590000	4.230769000	0.022721000	C	-3.075370000	-2.830450000	-1.949930000
O	0.479740000	-0.048338000	-1.733591000	C	-3.416604000	-1.942551000	-3.149748000
C	1.179755000	0.767005000	-2.445534000	C	-2.143256000	-1.273603000	-3.676816000
O	1.513296000	1.917885000	-2.103540000	C	-1.443891000	-0.501366000	-2.558087000
H	0.806261000	3.162639000	-1.065443000	C	-2.663520000	1.889389000	0.556916000
C	1.636641000	0.201797000	-3.776997000	C	-3.499421000	3.006648000	0.416799000
H	0.793481000	-0.255847000	-4.300561000	C	-3.135610000	3.947630000	-0.548274000
H	2.087532000	0.979371000	-4.393231000	C	-1.990105000	3.787890000	-1.337647000
H	2.375039000	-0.586381000	-3.596831000	C	-1.222279000	2.649827000	-1.104984000
C	6.354559000	-0.912176000	-1.336262000	C	-1.612152000	4.791644000	-2.392788000
C	5.609206000	0.112730000	-0.791611000	C	-4.733914000	3.183210000	1.261308000
C	4.195749000	-0.038533000	-0.641800000	C	-2.904448000	0.798194000	1.567745000
C	3.574538000	-1.255648000	-1.067176000	C	-3.203132000	-1.045093000	-0.069280000
C	4.332484000	-2.270909000	-1.613735000	C	-4.570789000	-1.558195000	0.406680000
C	5.719087000	-2.098595000	-1.744023000	C	-4.463279000	-2.574338000	1.546152000
H	7.427426000	-0.809526000	-1.447675000	C	-3.669374000	-1.966207000	2.706319000
H	6.094979000	1.024155000	-0.466872000	C	-2.301100000	-1.488634000	2.222152000
H	2.501172000	-1.353891000	-0.971091000	H	2.685768000	-5.284371000	0.687333000
H	3.865335000	-3.193248000	-1.937555000	H	0.815827000	-1.997956000	2.724465000
H	6.316238000	-2.899603000	-2.167754000	H	3.572010000	-4.206137000	3.079793000
C	3.385640000	0.944258000	-0.078475000	H	2.133474000	-5.147810000	3.474407000
H	0.256032000	2.196144000	0.593632000	H	2.252734000	-3.459258000	3.998280000
H	2.328353000	0.719904000	0.049721000	H	0.728563000	-5.122973000	-2.192394000
C	3.771045000	2.287244000	0.376310000	H	2.351578000	-5.566110000	-1.644253000
H	3.260255000	2.964295000	-0.327162000	H	2.097176000	-4.062396000	-2.545727000
H	4.839013000	2.491629000	0.306254000	H	0.739795000	-1.727148000	-2.227454000
C	3.232911000	2.583237000	1.792676000	H	-0.370349000	-3.087799000	-2.317434000
H	2.238559000	2.134086000	1.916662000	H	-1.965210000	-2.803530000	-0.122851000
H	3.886612000	2.161405000	2.556700000	H	-2.433985000	-3.653361000	-2.281942000
C	3.052721000	4.067389000	2.012301000	H	-3.965735000	-3.305794000	-1.532735000
O	3.371093000	4.447399000	3.255169000	H	-3.888158000	-2.543791000	-3.932406000
H	3.184099000	5.396817000	3.353096000	H	-4.144637000	-1.173712000	-2.861382000
O	2.630479000	4.842365000	1.173816000	H	-2.373426000	-0.567500000	-4.480591000
⁵ IM2				H	-1.470564000	-2.027225000	-4.102067000
Mn	-0.451495000	-0.107983000	0.301710000	H	-0.506315000	-0.057504000	-2.896470000
N	0.436196000	-2.180373000	0.706406000	H	-2.088835000	0.314062000	-2.230992000
N	-1.124042000	-1.339390000	-1.356439000	H	-3.764939000	4.821315000	-0.694527000
N	-1.560949000	1.735045000	-0.188338000	H	-0.319085000	2.442800000	-1.667458000
N	-2.372150000	-0.510759000	1.083249000	H	-1.387641000	5.765841000	-1.945427000
C	0.625687000	-2.849709000	-0.433546000	H	-2.437320000	4.943657000	-3.095261000

H	-0.739623000	4.463687000	-2.962006000	H	3.332259000	-2.495953000	-0.129595000
H	-5.451928000	2.374082000	1.089284000	O	3.359093000	-1.500446000	-2.234578000
H	-5.228913000	4.126859000	1.024901000	³ TS3			
H	-4.491741000	3.184946000	2.328706000	Mn	-0.389366000	-0.077038000	-0.290756000
H	-2.367065000	1.038707000	2.489713000	N	-2.138171000	1.052237000	-0.521280000
H	-3.962710000	0.717064000	1.815651000	N	-1.409056000	-0.362150000	1.648785000
H	-3.381463000	-0.189374000	-0.721249000	N	1.140989000	-1.426727000	0.136535000
H	-5.163620000	-0.701388000	0.742595000	N	-1.333187000	-2.063142000	-0.682801000
H	-5.111112000	-1.967371000	-0.449372000	C	-2.687685000	1.474169000	0.634770000
H	-5.464155000	-2.866587000	1.876389000	C	-3.794296000	2.332835000	0.655195000
H	-3.966393000	-3.488300000	1.197198000	C	-4.323276000	2.723646000	-0.575012000
H	-3.503705000	-2.702416000	3.498718000	C	-3.782941000	2.262419000	-1.779644000
H	-4.231570000	-1.140401000	3.156545000	C	-2.679329000	1.422507000	-1.693065000
H	-1.726991000	-1.003602000	3.012448000	C	-4.357530000	2.653607000	-3.113638000
H	-1.723025000	-2.345334000	1.878841000	C	-4.387923000	2.817223000	1.952260000
O	1.082428000	0.387041000	-0.576092000	C	-2.035607000	0.965323000	1.890241000
O	1.904768000	0.886822000	-3.081794000	C	-2.459310000	-1.431877000	1.416541000
H	2.426575000	0.093124000	-3.265429000	C	-3.181236000	-1.815454000	2.717619000
O	0.114246000	0.530757000	2.095157000	C	-2.220549000	-2.191460000	3.848483000
C	1.324477000	0.755872000	2.507967000	C	-1.227574000	-1.048582000	4.081622000
O	2.338018000	0.560377000	1.815766000	C	-0.497766000	-0.713525000	2.781069000
H	1.550720000	0.722532000	-2.176514000	C	1.022292000	-2.658323000	-0.394156000
C	1.427552000	1.293776000	3.916783000	C	1.965039000	-3.660885000	-0.130329000
H	0.875473000	0.648056000	4.604747000	C	3.000017000	-3.348972000	0.753797000
H	2.469628000	1.368980000	4.226707000	C	3.094844000	-2.088855000	1.352696000
H	0.962484000	2.283852000	3.953871000	C	2.142660000	-1.144593000	0.984674000
C	2.576116000	4.161537000	1.872586000	C	4.154282000	-1.769201000	2.371470000
C	3.321106000	3.204950000	1.215373000	C	1.855666000	-5.026947000	-0.755628000
C	3.149826000	3.017874000	-0.192882000	C	-0.207227000	-2.868634000	-1.236583000
C	2.213300000	3.836050000	-0.901946000	C	-1.781685000	-2.592132000	0.661567000
C	1.466385000	4.778918000	-0.227454000	C	-2.612578000	-3.877580000	0.523292000
C	1.645771000	4.935119000	1.156634000	C	-3.775530000	-3.739014000	-0.462071000
H	2.698963000	4.314855000	2.938015000	C	-3.240301000	-3.281977000	-1.822276000
H	4.031132000	2.596310000	1.758225000	C	-2.457155000	-1.979259000	-1.666194000
H	2.096518000	3.686160000	-1.969844000	H	-5.181085000	3.390050000	-0.593800000
H	0.750801000	5.397541000	-0.754272000	H	-2.220051000	1.022278000	-2.583675000
H	1.054651000	5.675136000	1.686531000	H	-4.337153000	3.740574000	-3.240085000
C	3.836819000	2.050399000	-0.916239000	H	-5.401050000	2.333994000	-3.196689000
H	1.755881000	0.448796000	0.138106000	H	-3.794992000	2.203353000	-3.934410000
H	3.625120000	2.010628000	-1.984476000	H	-4.789716000	1.986172000	2.541942000
C	4.816978000	1.080602000	-0.387080000	H	-5.202913000	3.517557000	1.761170000
H	4.536561000	0.742145000	0.615636000	H	-3.640391000	3.325927000	2.568769000
H	5.748818000	1.656479000	-0.253588000	H	-1.237966000	1.650432000	2.193960000
C	5.125246000	-0.103173000	-1.326196000	H	-2.756888000	0.923410000	2.707646000
H	5.241762000	0.235815000	-2.356462000	H	-3.200005000	-0.982863000	0.753924000
H	6.067716000	-0.556296000	-1.007905000	H	-3.791954000	-0.963473000	3.034442000
C	4.072339000	-1.190712000	-1.299821000	H	-3.889966000	-2.619100000	2.506282000
O	4.017986000	-1.803587000	-0.108450000	H	-2.786580000	-2.403465000	4.760149000

H	-1.673034000	-3.108559000	3.596104000	H	1.910598000	1.886169000	-1.689479000
H	-0.476180000	-1.325402000	4.827498000	C	2.910236000	3.251062000	-0.294231000
H	-1.750175000	-0.168204000	4.472479000	H	2.209032000	3.958352000	-0.732692000
H	0.192651000	0.123174000	2.899541000	H	3.916668000	3.601347000	-0.552280000
H	0.090983000	-1.577993000	2.477301000	C	2.748681000	3.274010000	1.243690000
H	3.736418000	-4.110761000	0.993091000	H	2.083636000	2.462637000	1.558791000
H	2.152554000	-0.136244000	1.375652000	H	3.695891000	3.143106000	1.767700000
H	5.137010000	-2.114304000	2.040075000	C	2.089838000	4.552482000	1.711948000
H	3.931651000	-2.270331000	3.319676000	O	2.406979000	4.839946000	2.983434000
H	4.212059000	-0.695729000	2.561875000	H	1.916075000	5.632884000	3.257926000
H	0.951359000	-5.546499000	-0.420721000	O	1.326588000	5.236216000	1.056997000
H	2.715237000	-5.641768000	-0.482854000	⁵ TS3			
H	1.814103000	-4.965044000	-1.847226000	Mn	0.029280000	0.235222000	0.244861000
H	-0.025172000	-2.511549000	-2.253258000	N	-2.241921000	0.299967000	0.765128000
H	-0.467066000	-3.926750000	-1.291442000	N	-0.884095000	1.598076000	-1.193412000
H	-0.868466000	-2.855316000	1.196494000	N	2.086453000	0.619722000	-0.503807000
H	-1.947525000	-4.676744000	0.178537000	N	0.573059000	2.014621000	1.236487000
H	-2.955410000	-4.188824000	1.512383000	C	-2.958787000	0.511206000	-0.343267000
H	-4.299274000	-4.694945000	-0.553615000	C	-4.335467000	0.228862000	-0.409433000
H	-4.508085000	-3.010874000	-0.090835000	C	-4.931584000	-0.282000000	0.745849000
H	-4.056624000	-3.102963000	-2.528766000	C	-4.194694000	-0.479278000	1.922550000
H	-2.608299000	-4.063242000	-2.260119000	C	-2.839804000	-0.166049000	1.870879000
H	-2.022704000	-1.642932000	-2.608683000	C	-4.830901000	-1.004473000	3.179855000
H	-3.136778000	-1.198188000	-1.324221000	C	-5.121532000	0.457879000	-1.672343000
O	0.650314000	1.326394000	0.290277000	C	-2.214849000	1.036663000	-1.541914000
O	-0.505181000	3.640141000	-0.559822000	C	-1.016365000	2.899758000	-0.418691000
H	0.064516000	4.395076000	-0.350048000	C	-1.530278000	4.047283000	-1.300846000
O	0.080235000	-0.055999000	-2.243156000	C	-0.694980000	4.244809000	-2.567531000
C	0.141810000	0.903500000	-3.112837000	C	-0.623201000	2.927804000	-3.344042000
O	0.148299000	2.116799000	-2.842428000	C	-0.088479000	1.805047000	-2.453912000
H	-0.319272000	3.339251000	-1.469799000	C	2.794950000	1.342801000	0.374063000
C	0.225913000	0.427816000	-4.550263000	C	4.164624000	1.589375000	0.195858000
H	1.046688000	-0.286155000	-4.661646000	C	4.755567000	1.067659000	-0.955927000
H	-0.697718000	-0.099083000	-4.810420000	C	4.013978000	0.344203000	-1.897923000
H	0.368979000	1.269274000	-5.227686000	C	2.666509000	0.144147000	-1.613800000
C	5.679762000	-0.190967000	-0.211800000	C	4.638920000	-0.213649000	-3.147281000
C	4.789135000	0.862752000	-0.137310000	C	4.958238000	2.386429000	1.196639000
C	3.604251000	0.849754000	-0.925787000	C	2.022965000	1.863627000	1.560002000
C	3.349754000	-0.263873000	-1.777415000	C	0.336955000	3.156093000	0.265008000
C	4.245979000	-1.315500000	-1.840393000	C	0.492618000	4.525475000	0.943675000
C	5.407506000	-1.277865000	-1.059021000	C	-0.363618000	4.671821000	2.202294000
H	6.586564000	-0.181865000	0.381385000	C	-0.032859000	3.537648000	3.174918000
H	5.003614000	1.706598000	0.507035000	C	-0.226598000	2.180524000	2.499930000
H	2.433885000	-0.285110000	-2.353811000	H	-5.991618000	-0.519967000	0.732091000
H	4.048839000	-2.165020000	-2.483426000	H	-2.209622000	-0.293349000	2.742412000
H	6.110561000	-2.103074000	-1.106790000	H	-5.335749000	-1.956714000	2.990888000
C	2.706857000	1.931355000	-0.958073000	H	-5.583691000	-0.304108000	3.555917000
H	0.215037000	2.193295000	0.103210000	H	-4.086790000	-1.159934000	3.964004000

H	-5.124254000	1.517721000	-1.949704000	C	4.150753000	-2.723512000	0.301290000
H	-6.157714000	0.140693000	-1.542636000	C	4.049483000	-3.286513000	1.578105000
H	-4.691997000	-0.103490000	-2.507662000	H	2.807728000	-4.358414000	2.981485000
H	-2.059690000	0.220913000	-2.252461000	H	0.841238000	-4.396762000	1.492721000
H	-2.823462000	1.783505000	-2.055526000	H	3.127349000	-2.363118000	-1.549625000
H	-1.764909000	2.714991000	0.350668000	H	5.079094000	-2.268836000	-0.025066000
H	-2.566824000	3.831590000	-1.578797000	H	4.903341000	-3.257500000	2.247106000
H	-1.575533000	4.957436000	-0.698805000	C	0.734785000	-3.319320000	-1.029014000
H	-1.136235000	5.033628000	-3.183364000	H	-0.803913000	-1.890459000	0.074221000
H	0.318812000	4.575897000	-2.308958000	H	0.938144000	-2.928886000	-2.021316000
H	0.049250000	3.013301000	-4.203117000	C	-0.448249000	-4.213463000	-0.898293000
H	-1.610190000	2.669647000	-3.743673000	H	-0.867478000	-4.179159000	0.110515000
H	-0.066322000	0.851571000	-2.980903000	H	-0.014860000	-5.220816000	-1.000073000
H	0.932410000	2.042434000	-2.163118000	C	-1.537700000	-4.068435000	-1.972708000
H	5.813469000	1.242465000	-1.130835000	H	-1.100387000	-3.944236000	-2.963769000
H	2.022049000	-0.395267000	-2.299976000	H	-2.121245000	-4.995310000	-1.986064000
H	5.347625000	-1.012105000	-2.901915000	C	-2.535614000	-2.951622000	-1.759482000
H	5.193425000	0.560065000	-3.686044000	O	-3.067053000	-2.967718000	-0.524972000
H	3.882402000	-0.625704000	-3.819027000	H	-3.707433000	-2.238762000	-0.441580000
H	4.589758000	3.415916000	1.265309000	O	-2.865908000	-2.144702000	-2.605712000
H	6.010290000	2.425133000	0.908811000	³ PC			
H	4.895161000	1.948078000	2.197669000	Mn	-0.830488000	-0.219517000	-0.301822000
H	2.096144000	1.154366000	2.388490000	N	-1.797407000	1.562983000	-0.422114000
H	2.434365000	2.813782000	1.902653000	N	-1.747814000	-0.196923000	1.561890000
H	1.125801000	3.073652000	-0.481324000	N	0.264867000	-1.886436000	-0.136762000
H	1.546916000	4.659774000	1.206850000	N	-2.250356000	-1.544980000	-0.845538000
H	0.273597000	5.304137000	0.210109000	C	-2.164655000	2.087368000	0.758703000
H	-0.176369000	5.644314000	2.666133000	C	-2.729070000	3.368606000	0.851961000
H	-1.430532000	4.642362000	1.947606000	C	-2.898308000	4.078141000	-0.333478000
H	-0.686388000	3.564040000	4.051999000	C	-2.523078000	3.535856000	-1.571765000
H	0.993776000	3.642463000	3.543104000	C	-1.967797000	2.262458000	-1.563280000
H	0.050827000	1.355079000	3.153714000	C	-2.722812000	4.289066000	-2.858449000
H	-1.276127000	2.056338000	2.236453000	C	-3.117106000	3.945562000	2.186123000
O	-0.324891000	-1.432941000	-0.656747000	C	-1.878622000	1.238559000	1.959859000
O	-0.124431000	-1.342996000	-3.418035000	C	-3.119345000	-0.805378000	1.324596000
H	-0.940919000	-1.560473000	-3.884734000	C	-3.879523000	-1.054576000	2.635226000
O	0.520122000	-0.654624000	1.898629000	C	-3.064850000	-1.841476000	3.664221000
C	0.000153000	-1.743164000	2.399209000	C	-1.734964000	-1.128011000	3.920633000
O	-0.829063000	-2.441620000	1.803618000	C	-0.969144000	-0.949474000	2.611876000
H	-0.374606000	-1.358802000	-2.475729000	C	-0.232431000	-2.938110000	-0.812395000
C	0.462989000	-2.065532000	3.799204000	C	0.458358000	-4.152220000	-0.885694000
H	-0.033591000	-1.381241000	4.495673000	C	1.692406000	-4.218702000	-0.234515000
H	0.201056000	-3.090451000	4.061145000	C	2.221675000	-3.122680000	0.458512000
H	1.539177000	-1.908777000	3.890061000	C	1.459240000	-1.960649000	0.477746000
C	2.862873000	-3.905565000	1.998195000	C	3.555973000	-3.179855000	1.148602000
C	1.760142000	-3.932392000	1.160585000	C	-0.103211000	-5.324392000	-1.645111000
C	1.832547000	-3.334502000	-0.122464000	C	-1.529563000	-2.671394000	-1.517954000
C	3.054609000	-2.758498000	-0.545664000	C	-2.901951000	-2.037393000	0.439948000

C	-4.146777000	-2.891066000	0.157377000	H	1.483603000	1.642847000	2.034576000
C	-5.145317000	-2.210610000	-0.780301000	C	0.988084000	-0.046544000	-4.089632000
C	-4.441949000	-1.818617000	-2.081788000	H	0.340225000	0.717204000	-4.528551000
C	-3.245891000	-0.917077000	-1.783976000	H	2.011345000	0.084437000	-4.439510000
H	-3.333228000	5.072699000	-0.297481000	H	0.607397000	-1.021276000	-4.408772000
H	-1.659521000	1.763803000	-2.473407000	C	5.882074000	-1.163672000	-0.835848000
H	-2.232631000	5.266223000	-2.815930000	C	4.938839000	-0.144104000	-0.709157000
H	-3.788311000	4.464127000	-3.037902000	C	4.789212000	0.536442000	0.507743000
H	-2.318732000	3.736278000	-3.708960000	C	5.599601000	0.174534000	1.589703000
H	-3.890282000	3.339332000	2.670331000	C	6.547306000	-0.843650000	1.463277000
H	-3.505239000	4.958466000	2.068513000	C	6.691283000	-1.514522000	0.248160000
H	-2.258441000	3.984974000	2.863927000	H	5.986685000	-1.684878000	-1.782713000
H	-0.925083000	1.550846000	2.404243000	H	4.309055000	0.112265000	-1.554097000
H	-2.653212000	1.354554000	2.718446000	H	5.488644000	0.695075000	2.537160000
H	-3.675898000	-0.059216000	0.755504000	H	7.169319000	-1.111211000	2.312004000
H	-4.158798000	-0.085697000	3.060759000	H	7.426073000	-2.307224000	0.146182000
H	-4.823563000	-1.550360000	2.400251000	C	3.765198000	1.642953000	0.673800000
H	-3.636998000	-1.933715000	4.591300000	H	2.225167000	0.808765000	-0.295946000
H	-2.874634000	-2.861383000	3.307551000	H	3.856800000	2.042762000	1.688785000
H	-1.099429000	-1.706734000	4.597202000	C	3.943469000	2.796243000	-0.319649000
H	-1.908313000	-0.158739000	4.400804000	H	3.773818000	2.439896000	-1.340719000
H	-0.036185000	-0.403582000	2.758404000	H	4.981574000	3.138310000	-0.268607000
H	-0.723164000	-1.928931000	2.203780000	C	3.028900000	3.996612000	-0.014005000
H	2.257232000	-5.145781000	-0.273945000	H	3.146442000	4.315287000	1.024076000
H	1.805108000	-1.060669000	0.973228000	H	3.322989000	4.835246000	-0.655150000
H	4.339347000	-3.485826000	0.450487000	C	1.555036000	3.774294000	-0.253010000
H	3.536281000	-3.907631000	1.966273000	O	1.278522000	3.427376000	-1.524440000
H	3.835001000	-2.206442000	1.555342000	H	0.314572000	3.327825000	-1.607387000
H	-1.072090000	-5.632324000	-1.237764000	O	0.672244000	3.934909000	0.570637000
H	0.573811000	-6.178203000	-1.588447000	⁵ PC			
H	-0.253433000	-5.078997000	-2.701350000	Mn	0.805910000	-0.136679000	0.344303000
H	-1.330685000	-2.367563000	-2.548796000	N	1.677204000	1.693598000	0.404325000
H	-2.157939000	-3.561610000	-1.551640000	N	1.775590000	-0.158386000	-1.520219000
H	-2.159309000	-2.681577000	0.912582000	N	-0.226642000	-1.896437000	0.172187000
H	-3.822933000	-3.838454000	-0.284341000	N	2.376093000	-1.588812000	0.898126000
H	-4.603961000	-3.157760000	1.112319000	C	2.086610000	2.171660000	-0.784918000
H	-5.978276000	-2.889227000	-0.982488000	C	2.648121000	3.451319000	-0.898955000
H	-5.571180000	-1.317699000	-0.306499000	C	2.776110000	4.196683000	0.270862000
H	-5.113093000	-1.263956000	-2.743869000	C	2.368129000	3.694465000	1.515940000
H	-4.125107000	-2.713070000	-2.629191000	C	1.813281000	2.422048000	1.532188000
H	-2.693700000	-0.645697000	-2.683426000	C	2.529808000	4.490916000	2.781301000
H	-3.596212000	0.002977000	-1.318764000	C	3.082126000	3.989516000	-2.235367000
O	2.417439000	1.132337000	0.611782000	C	1.848874000	1.273321000	-1.957417000
O	1.052876000	2.137753000	2.760358000	C	3.172375000	-0.715175000	-1.253774000
H	0.881389000	2.996749000	2.344850000	C	3.956951000	-0.901085000	-2.561215000
O	-0.284967000	-0.039243000	-2.096100000	C	3.201505000	-1.738664000	-3.595769000
C	0.931806000	0.044586000	-2.585897000	C	1.827753000	-1.117719000	-3.864135000
O	1.937923000	0.184025000	-1.892610000	C	1.043165000	-0.966215000	-2.561927000

C	0.329008000	-2.957684000	0.788053000	H	4.324795000	-2.726341000	2.617747000
C	-0.316586000	-4.201422000	0.794324000	H	2.773884000	-0.762349000	2.776857000
C	-1.549053000	-4.288106000	0.143926000	H	3.621686000	0.013148000	1.449435000
C	-2.129116000	-3.183364000	-0.490606000	O	-2.465900000	1.093469000	-0.580959000
C	-1.419529000	-1.989857000	-0.445397000	O	-1.081997000	2.107088000	-2.714970000
C	-3.456217000	-3.267027000	-1.191146000	H	-0.952975000	2.978655000	-2.309933000
C	0.291777000	-5.394059000	1.483627000	O	0.279815000	0.007883000	2.156660000
C	1.637475000	-2.718911000	1.502934000	C	-0.941461000	0.054090000	2.646182000
C	3.023951000	-1.988287000	-0.398012000	O	-1.946629000	0.173133000	1.949772000
C	4.315155000	-2.790515000	-0.168576000	H	-1.510539000	1.607711000	-1.991142000
C	5.290896000	-2.093290000	0.783194000	C	-0.995584000	-0.057154000	4.148471000
C	4.586944000	-1.790719000	2.109741000	H	-0.381133000	0.728266000	4.597040000
C	3.331718000	-0.957545000	1.859723000	H	-2.024262000	0.027527000	4.496623000
H	3.209667000	5.191030000	0.216833000	H	-0.574436000	-1.018645000	4.456102000
H	1.479076000	1.946893000	2.446006000	C	-5.809777000	-1.369212000	0.846499000
H	2.026320000	5.458423000	2.695451000	C	-4.909813000	-0.314150000	0.697299000
H	3.588551000	4.687622000	2.976825000	C	-4.806171000	0.360979000	-0.527315000
H	2.114964000	3.960279000	3.640559000	C	-5.618448000	-0.041152000	-1.593533000
H	3.882770000	3.378865000	-2.666224000	C	-6.523795000	-1.094126000	-1.443853000
H	3.451522000	5.011248000	-2.135871000	C	-6.621781000	-1.760186000	-0.221597000
H	2.251276000	3.994033000	-2.947719000	H	-5.878400000	-1.886864000	1.798555000
H	0.883710000	1.534029000	-2.411968000	H	-4.279376000	-0.025151000	1.531342000
H	2.620954000	1.401537000	-2.715450000	H	-5.542014000	0.474644000	-2.546940000
H	3.680416000	0.049250000	-0.662681000	H	-7.147376000	-1.393480000	-2.280702000
H	4.178403000	0.084400000	-2.981829000	H	-7.322528000	-2.580748000	-0.102044000
H	4.928499000	-1.336818000	-2.320840000	C	-3.838825000	1.513554000	-0.714121000
H	3.783355000	-1.793177000	-4.519885000	H	-2.277275000	0.813857000	0.340649000
H	3.078472000	-2.768716000	-3.239244000	H	-3.914760000	1.857395000	-1.750580000
H	1.234025000	-1.747449000	-4.533183000	C	-4.124293000	2.701063000	0.211609000
H	1.938442000	-0.147396000	-4.360185000	H	-3.994348000	2.400312000	1.256321000
H	0.083468000	-0.473081000	-2.722866000	H	-5.173172000	2.988020000	0.090334000
H	0.845522000	-1.950771000	-2.141110000	C	-3.249427000	3.927510000	-0.105806000
H	-2.070407000	-5.241070000	0.132987000	H	-3.322389000	4.190266000	-1.163493000
H	-1.803379000	-1.081569000	-0.895976000	H	-3.614716000	4.781943000	0.475149000
H	-4.229475000	-3.635031000	-0.511926000	C	-1.783576000	3.784161000	0.224687000
H	-3.400881000	-3.958814000	-2.037903000	O	-1.569892000	3.483322000	1.519848000
H	-3.773950000	-2.290395000	-1.559376000	H	-0.610240000	3.431618000	1.662968000
H	1.264818000	-5.649303000	1.050873000	O	-0.860538000	3.965748000	-0.549078000
H	-0.359481000	-6.264119000	1.386163000	Part IV Alcohol oxidation of 4-OH-PBA by the			
H	0.446093000	-5.202828000	2.550287000	Mn^{IV}(O)(AcO•) species 2 via the gem-diol mechanism.			
H	1.426414000	-2.463424000	2.545917000	³ RC			
H	2.236207000	-3.632245000	1.510818000	Mn	0.835080000	0.121887000	-0.338841000
H	2.313206000	-2.651506000	-0.894685000	N	-0.892500000	-1.012141000	-0.467901000
H	4.034693000	-3.759601000	0.258101000	N	0.839340000	-0.961678000	1.593128000
H	4.778634000	-3.016987000	-1.130821000	N	2.731690000	0.969458000	-0.206391000
H	6.163525000	-2.731774000	0.947172000	N	2.257411000	-1.626320000	-0.848576000
H	5.661459000	-1.160494000	0.339267000	C	-1.374508000	-1.497928000	0.697741000
H	5.240673000	-1.232691000	2.786777000	C	-2.498436000	-2.328892000	0.722196000

C	-3.094658000	-2.635241000	-0.502544000	H	6.368373000	-0.814251000	-1.084419000
C	-2.605062000	-2.122452000	-1.707454000	H	7.085738000	0.756697000	-1.463137000
C	-1.488726000	-1.296520000	-1.638881000	H	5.951814000	0.004946000	-2.593809000
C	-3.239533000	-2.454529000	-3.027928000	H	3.053849000	-0.710648000	-2.557395000
C	-3.034867000	-2.882195000	2.015191000	H	4.249895000	-1.602721000	-1.623562000
C	-0.616559000	-1.074397000	1.922155000	H	3.337389000	-1.427165000	0.933957000
C	1.439788000	-2.340235000	1.360653000	H	4.489158000	-3.180235000	-0.143220000
C	1.646622000	-3.078936000	2.694477000	H	3.788093000	-3.859003000	1.296490000
C	2.440169000	-2.265042000	3.717646000	H	3.514547000	-5.371660000	-0.696210000
C	1.743441000	-0.923215000	3.954316000	H	1.941314000	-4.889734000	-0.078770000
C	1.579852000	-0.170753000	2.633930000	H	1.931322000	-4.608716000	-2.541676000
C	3.743726000	0.329364000	-0.831298000	H	3.403580000	-3.649437000	-2.477218000
C	5.036414000	0.867086000	-0.837133000	H	1.391147000	-2.166644000	-2.676202000
C	5.229497000	2.081542000	-0.175429000	H	0.677893000	-2.950549000	-1.274338000
C	4.179367000	2.747643000	0.465604000	O	0.099975000	1.502546000	0.287087000
C	2.927305000	2.146614000	0.415778000	O	0.717439000	0.661516000	-2.146694000
C	4.382757000	4.055662000	1.178773000	C	0.281343000	1.868290000	-2.454800000
C	6.172020000	0.164742000	-1.534071000	O	-0.114011000	2.673975000	-1.609777000
C	3.382688000	-0.946557000	-1.540325000	C	0.294688000	2.189876000	-3.924340000
C	2.694672000	-2.186244000	0.485586000	H	-0.079191000	3.197660000	-4.095994000
C	3.534391000	-3.462539000	0.311476000	H	1.318885000	2.093728000	-4.293927000
C	2.849545000	-4.513511000	-0.566243000	H	-0.326216000	1.459193000	-4.449482000
C	2.491822000	-3.901033000	-1.923938000	O	-2.473391000	1.882812000	1.171728000
C	1.624240000	-2.657659000	-1.729642000	C	-5.652921000	-0.839214000	1.147102000
H	-3.966942000	-3.279682000	-0.514524000	C	-4.677119000	0.159450000	1.161483000
H	-1.042908000	-0.862521000	-2.524031000	C	-4.265293000	0.763854000	-0.030016000
H	-4.314590000	-2.262770000	-2.990385000	C	-4.848976000	0.357213000	-1.236227000
H	-3.098422000	-3.514220000	-3.263612000	C	-5.829156000	-0.634933000	-1.251884000
H	-2.807962000	-1.862991000	-3.837587000	C	-6.230180000	-1.241709000	-0.058637000
H	-2.322158000	-3.576787000	2.472382000	H	-5.959850000	-1.305334000	2.078398000
H	-3.966126000	-3.421060000	1.837459000	H	-4.219802000	0.467862000	2.094721000
H	-3.239395000	-2.085680000	2.735008000	H	-4.529606000	0.815602000	-2.168659000
H	-0.969511000	-0.093063000	2.252239000	H	-6.277208000	-0.937186000	-2.193662000
H	-0.764035000	-1.772858000	2.745019000	H	-6.987575000	-2.019331000	-0.069620000
H	0.688883000	-2.890084000	0.793349000	C	-3.248642000	1.887839000	-0.032609000
H	0.664086000	-3.320804000	3.110894000	H	-1.537367000	1.848449000	0.913914000
H	2.117571000	-4.040860000	2.484572000	H	-2.575681000	1.751249000	-0.888556000
H	2.515660000	-2.826676000	4.652627000	C	-3.944081000	3.250076000	-0.183073000
H	3.465459000	-2.095019000	3.366770000	H	-4.665324000	3.373462000	0.630665000
H	2.326588000	-0.284026000	4.623374000	H	-4.510274000	3.252445000	-1.119520000
H	0.769545000	-1.077674000	4.431384000	C	-2.951726000	4.422371000	-0.199940000
H	1.041193000	0.769691000	2.758768000	H	-2.152408000	4.247957000	-0.923472000
H	2.564255000	0.061646000	2.228562000	H	-3.482580000	5.334126000	-0.498109000
H	6.223516000	2.518823000	-0.160600000	C	-2.302181000	4.722136000	1.130158000
H	2.052176000	2.594274000	0.869264000	O	-3.209026000	4.914524000	2.115690000
H	4.789065000	4.807662000	0.495740000	H	-2.726445000	5.120547000	2.932290000
H	5.096238000	3.937786000	2.000326000	O	-1.109955000	4.851477000	1.322657000
H	3.444799000	4.433723000	1.589932000	⁵ RC			

Mn	-0.613594000	0.187445000	-0.030726000	H	-1.083106000	-0.722201000	-3.014619000
N	0.826247000	-1.193272000	0.621966000	H	-2.648502000	-0.635576000	-2.222810000
N	-1.160085000	-1.650524000	-1.142149000	H	-5.040384000	3.660911000	-1.637262000
N	-2.162445000	1.348108000	-0.645552000	H	-1.149918000	1.958582000	-2.326406000
N	-2.374419000	-0.593474000	1.226744000	H	-3.053657000	4.796067000	-3.241403000
C	0.993142000	-2.281376000	-0.146599000	H	-3.782223000	3.466655000	-4.144069000
C	1.961244000	-3.273023000	0.177416000	H	-2.022366000	3.539568000	-3.947760000
C	2.801051000	-3.014589000	1.264517000	H	-6.041375000	1.400707000	0.798205000
C	2.694061000	-1.835263000	1.998874000	H	-6.245696000	3.086656000	0.303968000
C	1.648384000	-0.951153000	1.649699000	H	-5.264630000	2.689817000	1.721660000
C	3.566202000	-1.532177000	3.179648000	H	-2.747284000	1.215221000	2.213817000
C	2.011111000	-4.584211000	-0.554170000	H	-4.214885000	0.367344000	1.748463000
C	0.131818000	-2.338268000	-1.373839000	H	-3.597676000	-1.036702000	-0.405045000
C	-2.047945000	-2.512258000	-0.263937000	H	-4.986819000	-1.612224000	1.415080000
C	-2.602999000	-3.719863000	-1.037209000	H	-4.666191000	-3.088296000	0.550178000
C	-3.294444000	-3.323692000	-2.344235000	H	-4.499400000	-3.397041000	3.041653000
C	-2.329319000	-2.514191000	-3.215863000	H	-2.949430000	-3.734581000	2.284068000
C	-1.813671000	-1.299631000	-2.445967000	H	-2.561924000	-2.258929000	4.241365000
C	-3.245600000	1.431069000	0.153628000	H	-3.757307000	-1.109191000	3.654694000
C	-4.320062000	2.267487000	-0.176107000	H	-1.442693000	-0.333735000	3.077027000
C	-4.220202000	3.006440000	-1.355806000	H	-1.117174000	-1.879043000	2.312072000
C	-3.092248000	2.926113000	-2.180165000	O	0.463479000	0.738959000	-1.193956000
C	-2.072058000	2.076742000	-1.771739000	O	-0.254813000	1.306215000	1.444775000
C	-2.976332000	3.724463000	-3.449771000	C	-0.082344000	2.609630000	1.525809000
C	-5.533412000	2.367089000	0.711108000	O	-0.283353000	3.390244000	0.597928000
C	-3.204050000	0.616808000	1.420051000	C	0.402058000	3.057012000	2.883830000
C	-3.102891000	-1.604552000	0.385392000	H	0.066330000	4.075042000	3.083855000
C	-4.196124000	-2.333955000	1.184369000	H	0.069018000	2.377065000	3.668868000
C	-3.673712000	-2.936302000	2.491798000	H	1.495844000	3.056279000	2.852412000
C	-3.008020000	-1.842190000	3.333148000	O	2.521302000	1.528051000	0.471337000
C	-1.905785000	-1.155031000	2.528229000	C	3.661045000	-1.909346000	-1.897373000
H	3.554729000	-3.746521000	1.534054000	C	3.363968000	-0.626478000	-1.450105000
H	1.448240000	-0.049206000	2.212384000	C	4.141106000	-0.049956000	-0.444573000
H	4.507658000	-2.080968000	3.124601000	C	5.253171000	-0.776309000	0.076220000
H	3.055384000	-1.827715000	4.103592000	C	5.553117000	-2.064289000	-0.371228000
H	3.777386000	-0.462604000	3.250429000	C	4.765215000	-2.635295000	-1.359606000
H	1.129028000	-5.182085000	-0.296785000	H	3.072104000	-2.359864000	-2.688821000
H	2.897562000	-5.149751000	-0.265684000	H	2.509632000	-0.094023000	-1.855057000
H	2.015954000	-4.464164000	-1.639270000	H	5.869432000	-0.311167000	0.839008000
H	0.650935000	-1.798987000	-2.172647000	H	6.395024000	-2.603435000	0.046222000
H	-0.013278000	-3.363742000	-1.712731000	H	4.982175000	-3.628797000	-1.735166000
H	-1.396249000	-2.894974000	0.524030000	C	3.860243000	1.346726000	0.055698000
H	-1.777368000	-4.403656000	-1.259239000	H	1.874223000	1.343163000	-0.251901000
H	-3.271783000	-4.279365000	-0.380470000	H	4.468754000	1.533039000	0.946195000
H	-3.627766000	-4.221737000	-2.871751000	C	4.260436000	2.373715000	-1.039444000
H	-4.191682000	-2.727463000	-2.136333000	H	3.578622000	2.252380000	-1.887070000
H	-2.824760000	-2.150985000	-4.121163000	H	5.268261000	2.143441000	-1.396205000
H	-1.496054000	-3.145576000	-3.544528000	C	4.238078000	3.822848000	-0.529871000

H	4.997708000	3.973988000	0.239799000	H	0.893757000	-1.728296000	2.292066000
H	4.473763000	4.486112000	-1.369932000	H	0.849927000	-0.578240000	4.353057000
C	2.907298000	4.250648000	0.049167000	H	2.419695000	-1.314182000	4.225068000
O	1.896082000	4.128649000	-0.826599000	H	2.541682000	1.046925000	5.090112000
H	1.045052000	4.130054000	-0.327705000	H	3.417821000	0.907514000	3.572101000
O	2.760149000	4.678908000	1.177277000	H	1.972914000	2.921558000	3.457253000
³ TS1				H	0.560709000	1.981965000	3.918144000
Mn	0.614581000	-0.160344000	-0.513199000	H	0.608152000	2.347717000	1.454892000
N	-0.917221000	-1.313615000	0.235439000	H	2.245476000	1.683494000	1.381679000
N	0.718691000	0.262604000	1.669408000	H	5.516921000	2.608722000	-2.244227000
N	2.331863000	0.859330000	-1.061900000	H	1.344819000	2.664438000	-1.221367000
N	2.319074000	-1.579613000	0.119770000	H	3.681625000	4.526648000	-3.100745000
C	-1.396152000	-0.963513000	1.449648000	H	4.073982000	4.878187000	-1.416390000
C	-2.487937000	-1.632847000	2.009632000	H	2.379453000	4.732574000	-1.915308000
C	-3.045782000	-2.677818000	1.270259000	H	6.233449000	-0.499749000	-0.854823000
C	-2.542491000	-3.048646000	0.019878000	H	6.726594000	0.590483000	-2.156923000
C	-1.470650000	-2.313741000	-0.472596000	H	5.786895000	-0.862633000	-2.524907000
C	-3.117409000	-4.193118000	-0.766054000	H	3.051179000	-1.856222000	-1.823172000
C	-3.052992000	-1.218290000	3.340367000	H	4.322020000	-1.739672000	-0.609807000
C	-0.703793000	0.189953000	2.116545000	H	3.286350000	-0.152123000	1.304830000
C	1.529667000	-0.842919000	2.326926000	H	4.727098000	-2.008748000	1.497054000
C	1.797078000	-0.520555000	3.808025000	H	4.081470000	-1.715318000	3.085569000
C	2.417369000	0.861527000	4.019645000	H	4.111600000	-4.165476000	2.512990000
C	1.519016000	1.928518000	3.390036000	H	2.461305000	-3.626468000	2.787096000
C	1.292984000	1.630407000	1.907992000	H	2.506040000	-4.969801000	0.704745000
C	3.465072000	0.138394000	-1.203107000	H	3.816339000	-3.992890000	0.056483000
C	4.650841000	0.744857000	-1.635537000	H	1.618178000	-3.262539000	-0.904793000
C	4.609890000	2.113023000	-1.910701000	H	0.971456000	-3.078207000	0.718427000
C	3.434067000	2.858119000	-1.769608000	O	-0.382179000	1.121599000	-0.939505000
C	2.301759000	2.174810000	-1.343876000	O	0.590197000	-1.042775000	-2.164778000
C	3.383598000	4.331518000	-2.066144000	C	0.277493000	-0.445400000	-3.317564000
C	5.918448000	-0.051144000	-1.802594000	O	0.045947000	0.748773000	-3.412206000
C	3.356145000	-1.332890000	-0.912000000	C	0.225041000	-1.409860000	-4.476146000
C	2.781026000	-1.104272000	1.475280000	H	0.102027000	-0.864952000	-5.411062000
C	3.808559000	-2.069684000	2.089671000	H	1.134955000	-2.013542000	-4.499448000
C	3.322489000	-3.521335000	2.115258000	H	-0.623045000	-2.085342000	-4.327230000
C	2.930706000	-3.961618000	0.701123000	O	-3.402630000	1.496416000	1.257879000
C	1.882920000	-3.010528000	0.123487000	C	-5.476084000	-1.390196000	-1.028948000
H	-3.897381000	-3.212903000	1.679243000	C	-4.870649000	-0.353497000	-0.317763000
H	-1.029488000	-2.515797000	-1.439199000	C	-3.801061000	0.354769000	-0.875460000
H	-4.207064000	-4.200083000	-0.695533000	C	-3.327684000	-0.009966000	-2.147471000
H	-2.747869000	-5.147132000	-0.374500000	C	-3.923917000	-1.053421000	-2.851282000
H	-2.840811000	-4.126984000	-1.819988000	C	-5.006005000	-1.743298000	-2.295796000
H	-2.306350000	-1.303306000	4.136875000	H	-6.310494000	-1.927942000	-0.589567000
H	-3.903481000	-1.847738000	3.606979000	H	-5.222162000	-0.099479000	0.675730000
H	-3.389087000	-0.178169000	3.301419000	H	-2.482326000	0.519191000	-2.576085000
H	-1.200730000	1.128590000	1.861101000	H	-3.544892000	-1.329824000	-3.830262000
H	-0.752964000	0.093882000	3.201176000	H	-5.472576000	-2.556351000	-2.842698000

C	-3.111427000	1.477901000	-0.138385000	H	-2.714384000	-5.070171000	-0.841946000
H	-4.212267000	1.998200000	1.416333000	H	-2.874682000	-3.918954000	-2.178462000
H	-2.022599000	1.269890000	-0.210834000	H	-2.245177000	-1.653742000	4.000712000
C	-3.311669000	2.860202000	-0.774128000	H	-3.847134000	-2.163106000	3.450569000
H	-4.329323000	3.209712000	-0.561420000	H	-3.354216000	-0.466639000	3.292878000
H	-3.231056000	2.769376000	-1.860141000	H	-1.171884000	0.998347000	1.914811000
C	-2.265786000	3.886636000	-0.303714000	H	-0.742472000	-0.138629000	3.174437000
H	-1.270921000	3.581218000	-0.631798000	H	0.882020000	-1.907118000	2.111630000
H	-2.491730000	4.859359000	-0.752900000	H	0.854921000	-0.938919000	4.261811000
C	-2.203208000	4.076618000	1.192644000	H	2.415109000	-1.682085000	4.073306000
O	-3.368931000	4.532998000	1.703138000	H	2.570041000	0.593755000	5.134963000
H	-3.265665000	4.632477000	2.663764000	H	3.442217000	0.575116000	3.608372000
O	-1.227130000	3.875923000	1.886299000	H	2.024455000	2.609915000	3.673398000
⁵ TS1				H	0.599956000	1.652871000	4.052199000
Mn	0.645223000	-0.118825000	-0.546580000	H	0.649339000	2.224999000	1.625871000
N	-0.917893000	-1.296479000	0.095986000	H	2.279053000	1.552353000	1.496164000
N	0.736355000	0.132226000	1.661637000	H	5.609591000	2.693144000	-2.017003000
N	2.379040000	0.912039000	-1.019695000	H	1.428819000	2.740811000	-1.015723000
N	2.315829000	-1.617118000	-0.041013000	H	3.822492000	4.720230000	-2.706447000
C	-1.384769000	-1.057830000	1.343265000	H	4.208690000	4.908161000	-0.994792000
C	-2.463412000	-1.783971000	1.856085000	H	2.515504000	4.845172000	-1.515034000
C	-3.025371000	-2.763848000	1.034207000	H	6.264403000	-0.522519000	-0.901759000
C	-2.540680000	-3.015171000	-0.252219000	H	6.772560000	0.649699000	-2.124120000
C	-1.479870000	-2.231299000	-0.691396000	H	5.808715000	-0.757975000	-2.592492000
C	-3.116607000	-4.092202000	-1.128192000	H	3.035564000	-1.742108000	-2.004560000
C	-3.007704000	-1.501828000	3.229551000	H	4.312745000	-1.760242000	-0.793011000
C	-0.688109000	0.036761000	2.100008000	H	3.298654000	-0.295675000	1.251847000
C	1.532207000	-1.038385000	2.221425000	H	4.711873000	-2.185320000	1.295713000
C	1.803736000	-0.847918000	3.724054000	H	4.074768000	-2.002205000	2.904097000
C	2.441695000	0.503288000	4.052765000	H	4.064707000	-4.401985000	2.150052000
C	1.556975000	1.632932000	3.519518000	H	2.422732000	-3.860278000	2.465354000
C	1.326251000	1.465848000	2.018174000	H	2.446372000	-5.043673000	0.288607000
C	3.499598000	0.183718000	-1.217099000	H	3.773642000	-4.043762000	-0.285626000
C	4.700988000	0.800335000	-1.585748000	H	1.589732000	-3.207690000	-1.190317000
C	4.689648000	2.188631000	-1.736128000	H	0.943027000	-3.134222000	0.442198000
C	3.528648000	2.942794000	-1.534651000	O	-0.382395000	1.295375000	-0.795694000
C	2.378725000	2.248212000	-1.178895000	O	0.536825000	-0.821287000	-2.335611000
C	3.512127000	4.437877000	-1.695809000	C	0.279803000	-0.013119000	-3.328064000
C	5.954648000	-0.002602000	-1.814340000	O	0.072225000	1.196979000	-3.167312000
C	3.356352000	-1.305179000	-1.053874000	C	0.241670000	-0.651177000	-4.692065000
C	2.780382000	-1.250961000	1.349445000	H	0.073727000	0.101435000	-5.460929000
C	3.793967000	-2.276051000	1.885347000	H	1.182164000	-1.177705000	-4.871487000
C	3.285524000	-3.717902000	1.802623000	H	-0.568390000	-1.386614000	-4.705522000
C	2.888026000	-4.045378000	0.359787000	O	-3.563003000	1.312002000	1.443286000
C	1.856463000	-3.036858000	-0.145750000	C	-5.522705000	-1.343469000	-1.209916000
H	-3.864372000	-3.342890000	1.407896000	C	-4.966471000	-0.377843000	-0.372473000
H	-1.052046000	-2.344116000	-1.678736000	C	-3.891349000	0.401506000	-0.812326000
H	-4.203023000	-4.132955000	-1.026594000	C	-3.363274000	0.178357000	-2.098126000

C	-3.913115000	-0.792188000	-2.931149000	C	4.749701000	-0.609654000	-0.739976000
C	-4.999733000	-1.553463000	-2.490986000	C	4.739612000	-1.969595000	-1.442643000
H	-6.361712000	-1.938614000	-0.863426000	C	3.629602000	-1.993355000	-2.497785000
H	-5.358588000	-0.236848000	0.628258000	C	2.283979000	-1.667980000	-1.852217000
H	-2.509259000	0.760997000	-2.429475000	H	-0.676756000	-5.638484000	1.210776000
H	-3.493043000	-0.959037000	-3.917926000	H	-0.825542000	-2.337098000	-1.545522000
H	-5.430285000	-2.312781000	-3.135695000	H	-2.271305000	-5.578028000	-1.014548000
C	-3.238727000	1.446354000	0.059427000	H	-0.644180000	-5.817865000	-1.647119000
H	-4.414148000	1.732256000	1.619458000	H	-1.645880000	-4.505152000	-2.281628000
H	-2.154380000	1.260088000	-0.003118000	H	1.498626000	-4.185608000	3.475753000
C	-3.447358000	2.888247000	-0.427879000	H	0.126019000	-5.298156000	3.406227000
H	-4.463881000	3.211873000	-0.173460000	H	-0.082394000	-3.670527000	4.068440000
H	-3.371371000	2.915346000	-1.517827000	H	0.162659000	-0.862364000	2.986475000
C	-2.396793000	3.857614000	0.143885000	H	1.580174000	-1.883155000	3.182425000
H	-1.406976000	3.586780000	-0.227430000	H	2.687876000	-2.041768000	0.778964000
H	-2.627683000	4.874805000	-0.188691000	H	3.699771000	-1.970721000	2.898787000
C	-2.319256000	3.870644000	1.651305000	H	4.948420000	-1.595538000	1.745889000
O	-3.459339000	4.317757000	2.222915000	H	5.032328000	-0.096854000	3.768205000
H	-3.348904000	4.292180000	3.187422000	H	4.748421000	0.850242000	2.313439000
O	-1.350499000	3.545436000	2.307973000	H	3.138912000	1.585257000	4.052106000
³ IM1				H	2.606930000	-0.070233000	4.310944000
Mn	0.460105000	-0.029017000	-0.033740000	H	1.004316000	1.168288000	2.807406000
N	-0.020352000	-1.974681000	0.308979000	H	2.342075000	1.584425000	1.749627000
N	1.696317000	-0.409373000	1.629817000	H	2.034177000	5.413331000	-1.528519000
N	1.029267000	1.886749000	-0.411531000	H	-0.081783000	2.739065000	1.089146000
N	2.260322000	-0.354625000	-1.130731000	H	0.032539000	6.222387000	-0.006278000
C	0.311265000	-2.428317000	1.533479000	H	1.177473000	5.870540000	1.288241000
C	0.069958000	-3.754465000	1.913923000	H	-0.442276000	5.152905000	1.324148000
C	-0.496088000	-4.597940000	0.955938000	H	4.159711000	3.021352000	-2.877141000
C	-0.822583000	-4.136939000	-0.323738000	H	3.338271000	4.529513000	-3.300018000
C	-0.585042000	-2.792610000	-0.593168000	H	2.776380000	2.991930000	-3.972402000
C	-1.381292000	-5.054827000	-1.376410000	H	1.654637000	0.517643000	-2.937747000
C	0.421034000	-4.253664000	3.291031000	H	3.322777000	0.880832000	-2.518968000
C	0.939193000	-1.404932000	2.440808000	H	3.431663000	0.819995000	0.142380000
C	2.968784000	-1.039215000	1.105421000	H	5.028241000	0.164106000	-1.463071000
C	4.036927000	-1.199260000	2.198545000	H	5.511447000	-0.565337000	0.041458000
C	4.305585000	0.092993000	2.973023000	H	5.714663000	-2.155594000	-1.902188000
C	2.990862000	0.622566000	3.553101000	H	4.574042000	-2.775240000	-0.715805000
C	1.969708000	0.823336000	2.435214000	H	3.550134000	-2.980025000	-2.964494000
C	1.863352000	2.042632000	-1.453334000	H	3.856765000	-1.282016000	-3.300084000
C	2.256346000	3.311747000	-1.898658000	H	1.470377000	-1.637202000	-2.577532000
C	1.752552000	4.414093000	-1.208042000	H	2.042714000	-2.447257000	-1.129539000
C	0.903100000	4.257357000	-0.107026000	O	-0.914682000	0.548321000	1.068971000
C	0.566498000	2.955877000	0.251027000	O	-0.450181000	-0.126486000	-1.750553000
C	0.383839000	5.437209000	0.669486000	C	-1.201593000	0.708617000	-2.407598000
C	3.181458000	3.472767000	-3.076284000	O	-1.683355000	1.748525000	-1.955483000
C	2.318553000	0.768367000	-2.107352000	C	-1.438031000	0.288716000	-3.851336000
C	3.389180000	-0.235396000	-0.131366000	H	-2.283022000	0.830880000	-4.278031000

H	-0.542238000	0.521966000	-4.437829000	C	3.086873000	3.898474000	-1.078516000
H	-1.604911000	-0.788266000	-3.920820000	C	2.225553000	4.000121000	0.021083000
O	-3.955245000	0.338002000	1.806625000	C	1.527006000	2.849016000	0.376020000
C	-4.083334000	-3.080744000	-0.414871000	C	2.071557000	5.281094000	0.795287000
C	-4.020244000	-1.928021000	0.347451000	C	4.173614000	2.590266000	-2.956950000
C	-4.029894000	-0.657796000	-0.283196000	C	2.543219000	0.261174000	-2.013420000
C	-4.087099000	-0.582855000	-1.693876000	C	3.157049000	-1.124575000	-0.054820000
C	-4.146667000	-1.746466000	-2.447455000	C	4.391486000	-1.813314000	-0.658337000
C	-4.153569000	-2.991424000	-1.811650000	C	4.039903000	-3.069365000	-1.459999000
H	-4.082900000	-4.049716000	0.070276000	C	3.009739000	-2.724409000	-2.540200000
H	-3.973533000	-1.989802000	1.427223000	C	1.781396000	-2.063324000	-1.916289000
H	-4.080265000	0.372732000	-2.198888000	H	-2.293937000	-5.469452000	0.994630000
H	-4.193742000	-1.686131000	-3.528403000	H	-1.509853000	-2.199866000	-1.687612000
H	-4.212613000	-3.897004000	-2.405821000	H	-3.854446000	-4.820798000	-1.228609000
C	-4.013821000	0.525931000	0.529486000	H	-2.394701000	-5.615846000	-1.812226000
H	-3.975542000	1.195573000	2.319663000	H	-2.868140000	-4.048049000	-2.483858000
H	-1.462626000	-0.168569000	1.404919000	H	0.183911000	-4.703077000	3.298110000
C	-4.111430000	1.925119000	0.004692000	H	-1.428031000	-5.421557000	3.190326000
H	-5.111263000	2.292300000	0.271337000	H	-1.217824000	-3.813751000	3.897239000
H	-4.048162000	1.913876000	-1.077876000	H	-0.279915000	-1.157988000	2.913678000
C	-3.005942000	2.880493000	0.511906000	H	0.836213000	-2.499163000	3.082100000
H	-2.069844000	2.311051000	0.565680000	H	1.975351000	-2.767557000	0.663346000
H	-2.856923000	3.668656000	-0.224547000	H	2.863247000	-3.098930000	2.825512000
C	-3.217227000	3.547063000	1.843119000	H	4.220784000	-2.982325000	1.743220000
O	-3.913774000	2.756370000	2.723824000	H	4.585062000	-1.680761000	3.867108000
H	-3.987878000	3.185110000	3.593033000	H	4.611978000	-0.603995000	2.477577000
O	-2.805492000	4.630530000	2.168067000	H	3.165688000	0.407251000	4.217269000
⁵ IMI				H	2.229407000	-1.074725000	4.354377000
Mn	0.380004000	-0.111244000	-0.085993000	H	1.031951000	0.600343000	2.908743000
N	-0.663464000	-2.103074000	0.182218000	H	2.464433000	0.751117000	1.908130000
N	1.372331000	-1.022632000	1.637399000	H	3.647662000	4.772620000	-1.398349000
N	1.663240000	1.693178000	-0.284829000	H	0.841157000	2.835594000	1.215668000
N	2.103201000	-0.838588000	-1.108033000	H	2.032962000	6.141351000	0.121053000
C	-0.481786000	-2.650199000	1.389653000	H	2.925105000	5.430188000	1.466251000
C	-1.066220000	-3.876733000	1.741228000	H	1.161433000	5.273616000	1.398430000
C	-1.834769000	-4.511930000	0.763715000	H	4.969979000	1.860749000	-2.772503000
C	-2.020457000	-3.949466000	-0.504561000	H	4.642049000	3.552948000	-3.169790000
C	-1.413107000	-2.718757000	-0.740096000	H	3.637802000	2.267290000	-3.855645000
C	-2.829147000	-4.641287000	-1.567792000	H	1.861028000	0.268013000	-2.867522000
C	-0.872410000	-4.485804000	3.105268000	H	3.542038000	0.062768000	-2.403913000
C	0.361082000	-1.843508000	2.350966000	H	3.469797000	-0.149611000	0.320880000
C	2.475311000	-1.895829000	1.087794000	H	4.903809000	-1.099039000	-1.310699000
C	3.417568000	-2.396330000	2.194803000	H	5.099956000	-2.032694000	0.143167000
C	3.964483000	-1.264322000	3.068382000	H	4.945455000	-3.485475000	-1.910767000
C	2.801218000	-0.456490000	3.652682000	H	3.633531000	-3.843788000	-0.797335000
C	1.899530000	0.057432000	2.531291000	H	2.674226000	-3.624338000	-3.064691000
C	2.498633000	1.601444000	-1.326197000	H	3.459108000	-2.069913000	-3.295436000
C	3.247917000	2.699489000	-1.774153000	H	1.047647000	-1.758112000	-2.662227000

H	1.289672000	-2.773960000	-1.253486000	C	-2.877223000	0.150698000	1.457148000
O	-0.845034000	0.743377000	0.999115000	C	-3.741395000	0.040130000	2.723242000
O	-0.468471000	0.046174000	-1.851254000	C	-3.435092000	-1.205018000	3.557390000
C	-0.997945000	1.054721000	-2.486967000	C	-1.944615000	-1.229812000	3.904658000
O	-1.148680000	2.182971000	-2.018529000	C	-1.110369000	-1.179933000	2.627063000
C	-1.400132000	0.721827000	-3.914414000	C	-1.304468000	-2.596072000	-1.238477000
H	-2.065934000	1.486345000	-4.316950000	C	-1.334575000	-3.949245000	-1.598951000
H	-0.497345000	0.680944000	-4.533621000	C	-0.397218000	-4.789374000	-0.997805000
H	-1.875757000	-0.259911000	-3.962419000	C	0.524645000	-4.301386000	-0.064801000
O	-3.667549000	1.489106000	1.860879000	C	0.475411000	-2.941606000	0.218909000
C	-4.695604000	-1.796124000	-0.329938000	C	1.539143000	-5.195823000	0.594815000
C	-4.329921000	-0.693428000	0.421619000	C	-2.340236000	-4.467816000	-2.592416000
C	-4.024106000	0.534150000	-0.219293000	C	-2.244300000	-1.574022000	-1.806609000
C	-4.091825000	0.617086000	-1.628600000	C	-3.209772000	-0.833936000	0.333073000
C	-4.464285000	-0.494736000	-2.371112000	C	-4.699374000	-0.958667000	-0.022976000
C	-4.769445000	-1.696339000	-1.725781000	C	-5.254579000	0.283547000	-0.723748000
H	-4.927790000	-2.732860000	0.162832000	C	-4.409566000	0.596409000	-1.962073000
H	-4.281560000	-0.761863000	1.501051000	C	-2.942365000	0.764314000	-1.571815000
H	-3.855254000	1.538397000	-2.141828000	H	-0.940386000	5.672049000	0.774777000
H	-4.521440000	-0.426340000	-3.451066000	H	-0.202207000	2.365386000	-1.874074000
H	-5.065353000	-2.559884000	-2.311646000	H	0.188142000	5.944942000	-1.656858000
C	-3.669773000	1.673144000	0.582461000	H	-1.478508000	5.557901000	-2.087668000
H	-3.417355000	2.315898000	2.363108000	H	-0.148359000	4.617054000	-2.782104000
H	-1.528667000	0.154140000	1.337021000	H	-2.144897000	3.803701000	3.431112000
C	-3.368902000	3.038247000	0.044209000	H	-1.230633000	5.277626000	3.088784000
H	-4.208763000	3.682079000	0.337317000	H	-0.407427000	3.854744000	3.742797000
H	-3.346501000	3.006129000	-1.039441000	H	0.044595000	1.080152000	2.880680000
C	-2.018277000	3.637082000	0.502456000	H	-1.590718000	1.579287000	3.191848000
H	-1.276305000	2.830964000	0.514969000	H	-2.998371000	1.163019000	1.070387000
H	-1.687694000	4.362145000	-0.240111000	H	-3.575577000	0.931704000	3.336692000
C	-1.972647000	4.322173000	1.841056000	H	-4.792624000	0.083201000	2.431572000
O	-2.851242000	3.779388000	2.745249000	H	-4.044438000	-1.200151000	4.465365000
H	-2.762018000	4.204530000	3.614887000	H	-3.699330000	-2.114124000	3.002598000
O	-1.235201000	5.222121000	2.149674000	H	-1.678025000	-2.145162000	4.441419000
³ TS ₂ ^{diol}				H	-1.694041000	-0.391667000	4.564925000
Mn	-0.427592000	-0.097430000	-0.123435000	H	-0.040252000	-1.172926000	2.839375000
N	-0.543528000	1.921792000	0.101666000	H	-1.313891000	-2.071055000	2.033913000
N	-1.393662000	0.007544000	1.753824000	H	-0.393201000	-5.845436000	-1.252292000
N	-0.408126000	-2.117737000	-0.359424000	H	1.143851000	-2.474654000	0.925450000
N	-2.368168000	-0.426950000	-0.860276000	H	2.327638000	-5.473205000	-0.113275000
C	-0.792468000	2.352004000	1.353472000	H	1.074488000	-6.121381000	0.945800000
C	-0.928074000	3.713138000	1.649485000	H	2.009603000	-4.702986000	1.448445000
C	-0.825562000	4.609039000	0.583150000	H	-3.364052000	-4.337707000	-2.224880000
C	-0.581273000	4.166762000	-0.719909000	H	-2.182708000	-5.531508000	-2.778838000
C	-0.424611000	2.796715000	-0.907348000	H	-2.265869000	-3.940028000	-3.548451000
C	-0.496220000	5.121239000	-1.878573000	H	-1.857360000	-1.185941000	-2.751250000
C	-1.190428000	4.187664000	3.054407000	H	-3.219474000	-2.013728000	-2.017800000
C	-0.916943000	1.270198000	2.392296000	H	-2.855573000	-1.824430000	0.622304000

H	-4.827649000	-1.828151000	-0.675463000	C	-4.161221000	-0.284518000	1.141074000
H	-5.258298000	-1.194420000	0.884964000	C	-4.912464000	-0.001030000	-0.002720000
H	-6.298694000	0.114560000	-1.001573000	C	-4.303267000	0.250970000	-1.235233000
H	-5.243833000	1.144344000	-0.043223000	C	-2.910460000	0.204766000	-1.270397000
H	-4.736066000	1.526160000	-2.437526000	C	-5.100698000	0.557604000	-2.472823000
H	-4.524289000	-0.196818000	-2.709235000	C	-4.821199000	-0.527392000	2.473015000
H	-2.301486000	0.948037000	-2.434375000	C	-1.820435000	-0.601854000	2.122298000
H	-2.848420000	1.623129000	-0.908851000	C	-0.973332000	-2.725920000	1.182742000
O	1.305802000	-0.134586000	0.763599000	C	-1.290461000	-3.647103000	2.369978000
O	0.122784000	0.159261000	-1.936869000	C	-0.174789000	-3.676912000	3.416086000
C	0.858157000	-0.516193000	-2.784181000	C	0.115068000	-2.251775000	3.893191000
O	1.586650000	-1.461334000	-2.489890000	C	0.450922000	-1.348392000	2.706478000
C	0.737609000	-0.000984000	-4.205963000	C	2.608445000	-1.756061000	-0.883216000
H	1.417299000	-0.537336000	-4.867800000	C	3.952102000	-2.015915000	-1.197939000
H	-0.291084000	-0.124693000	-4.558598000	C	4.916074000	-1.332048000	-0.458537000
H	0.960083000	1.069378000	-4.229154000	C	4.558675000	-0.441749000	0.563187000
O	3.498156000	0.744615000	1.689359000	C	3.198340000	-0.275520000	0.797517000
C	2.663706000	4.104553000	-0.462311000	C	5.587830000	0.309346000	1.362965000
C	2.774979000	2.935886000	0.280909000	C	4.328655000	-2.973801000	-2.296424000
C	2.956419000	1.701616000	-0.368038000	C	1.477917000	-2.380563000	-1.659470000
C	3.010138000	1.659014000	-1.769399000	C	0.135886000	-3.220475000	0.243260000
C	2.899438000	2.834220000	-2.508354000	C	0.009751000	-4.686006000	-0.202763000
C	2.734261000	4.057876000	-1.857786000	C	-1.161838000	-4.920038000	-1.159865000
H	2.523108000	5.052789000	0.044798000	C	-1.042182000	-3.981855000	-2.364528000
H	2.730438000	2.973832000	1.362255000	C	-0.953716000	-2.529258000	-1.899004000
H	3.161502000	0.720919000	-2.286534000	H	-5.995693000	0.033725000	0.074152000
H	2.957397000	2.794641000	-3.590722000	H	-2.352102000	0.402784000	-2.178400000
H	2.657889000	4.972802000	-2.435529000	H	-5.940895000	1.218895000	-2.244679000
C	3.184790000	0.486209000	0.435968000	H	-5.513395000	-0.360443000	-2.905544000
H	3.945679000	-0.001306000	2.151687000	H	-4.479264000	1.036893000	-3.232765000
H	1.275010000	0.318313000	1.613358000	H	-4.603890000	-1.532229000	2.851193000
C	3.690728000	-0.767598000	-0.229584000	H	-5.904950000	-0.429829000	2.386855000
H	4.645241000	-0.505381000	-0.702476000	H	-4.476136000	0.188752000	3.225630000
H	2.992402000	-1.015889000	-1.030872000	H	-1.493563000	0.341232000	2.570159000
C	3.855514000	-2.029395000	0.643634000	H	-2.308768000	-1.171725000	2.912276000
H	3.015698000	-2.116579000	1.334777000	H	-1.889862000	-2.611347000	0.604543000
H	3.852156000	-2.898349000	-0.013798000	H	-2.217228000	-3.301755000	2.838553000
C	5.134201000	-2.083343000	1.444855000	H	-1.514207000	-4.644906000	1.987407000
O	5.058348000	-1.254823000	2.530636000	H	-0.472060000	-4.309511000	4.257003000
H	5.900547000	-1.242147000	3.015814000	H	0.735963000	-4.119406000	2.993784000
O	6.113096000	-2.741302000	1.205983000	H	0.969834000	-2.229102000	4.575628000
⁵ TS _{2diol}				H	-0.742705000	-1.857085000	4.448753000
Mn	0.073050000	-0.306069000	-0.125623000	H	0.608389000	-0.319497000	3.035979000
N	-2.178651000	-0.086619000	-0.191937000	H	1.375323000	-1.687164000	2.241925000
N	-0.603889000	-1.320862000	1.637293000	H	5.967147000	-1.496972000	-0.679610000
N	2.256347000	-0.908249000	0.085549000	H	2.843748000	0.384171000	1.581805000
N	0.176672000	-2.274138000	-0.942522000	H	6.174037000	0.969253000	0.715242000
C	-2.769786000	-0.321469000	0.986388000	H	6.287334000	-0.378774000	1.847691000

H	5.118170000	0.922681000	2.135458000	³ IM2 _{dioI}			
H	3.966269000	-3.985702000	-2.083716000	Mn	0.194784000	0.317999000	0.195550000
H	5.412971000	-3.021796000	-2.411485000	N	-1.864762000	0.624906000	0.262115000
H	3.898843000	-2.669184000	-3.256556000	N	-0.142926000	1.519706000	-1.577198000
H	1.368369000	-1.868761000	-2.619559000	N	2.212455000	0.140474000	-0.020310000
H	1.702124000	-3.424126000	-1.886729000	N	0.817549000	2.135417000	1.023376000
H	1.096804000	-3.106366000	0.744610000	C	-2.441581000	1.071411000	-0.870335000
H	0.943057000	-4.978966000	-0.693760000	C	-3.803839000	1.380044000	-0.933438000
H	-0.060666000	-5.318292000	0.684720000	C	-4.550842000	1.197451000	0.231284000
H	-1.169707000	-5.964295000	-1.484493000	C	-3.966451000	0.708622000	1.402124000
H	-2.115728000	-4.741515000	-0.647749000	C	-2.603286000	0.431582000	1.364539000
H	-1.915055000	-4.068166000	-3.018549000	C	-4.768702000	0.463462000	2.648748000
H	-0.168080000	-4.249407000	-2.968457000	C	-4.444010000	1.861735000	-2.208412000
H	-0.824589000	-1.833158000	-2.727775000	C	-1.517131000	1.179893000	-2.047475000
H	-1.879824000	-2.259655000	-1.394378000	C	-0.127658000	2.962316000	-1.087340000
O	0.386308000	1.354603000	0.782274000	C	-0.171788000	3.967519000	-2.247361000
O	0.129489000	0.413686000	-1.887503000	C	0.899014000	3.710255000	-3.308984000
C	1.065806000	0.903402000	-2.673773000	C	0.769235000	2.275574000	-3.825634000
O	2.238807000	1.044411000	-2.352092000	C	0.867797000	1.287752000	-2.664988000
C	0.536737000	1.270322000	-4.046635000	C	2.927084000	0.909003000	0.823160000
H	1.295240000	1.805607000	-4.617568000	C	4.322372000	0.824000000	0.894615000
H	0.259132000	0.354809000	-4.578808000	C	4.947786000	-0.094231000	0.051322000
H	-0.367209000	1.877918000	-3.954400000	C	4.215034000	-0.887913000	-0.839874000
O	0.221993000	3.703053000	1.797307000	C	2.834881000	-0.729410000	-0.835813000
C	-3.666458000	3.258045000	0.594383000	C	4.878662000	-1.873033000	-1.762260000
C	-2.341700000	3.214478000	1.006744000	C	5.107031000	1.679121000	1.853262000
C	-1.302649000	3.340249000	0.066099000	C	2.117677000	1.826989000	1.692370000
C	-1.618369000	3.501691000	-1.292278000	C	1.059025000	3.101296000	-0.129830000
C	-2.949186000	3.568034000	-1.696641000	C	1.352210000	4.525593000	0.365948000
C	-3.972874000	3.446452000	-0.757135000	C	0.304430000	5.049495000	1.349871000
H	-4.461742000	3.147180000	1.323074000	C	0.173410000	4.076387000	2.524170000
H	-2.102367000	3.083642000	2.055126000	C	-0.173683000	2.679275000	2.015110000
H	-0.842010000	3.604553000	-2.038641000	H	-5.611900000	1.428732000	0.219321000
H	-3.183850000	3.708721000	-2.746011000	H	-2.070453000	0.050163000	2.225127000
H	-5.008892000	3.489240000	-1.076070000	H	-5.453565000	-0.377273000	2.498343000
C	0.090499000	3.366570000	0.538941000	H	-5.371443000	1.339346000	2.905137000
H	1.163254000	3.903183000	2.033863000	H	-4.122593000	0.225440000	3.496281000
H	0.417165000	1.331052000	1.746016000	H	-3.989153000	2.793372000	-2.561032000
C	1.220097000	3.631107000	-0.426915000	H	-5.508548000	2.045462000	-2.054034000
H	1.199932000	4.713885000	-0.609865000	H	-4.341701000	1.120195000	-3.007380000
H	0.964547000	3.153494000	-1.367610000	H	-1.475931000	0.225214000	-2.580550000
C	2.644493000	3.154219000	-0.096948000	H	-1.872023000	1.915198000	-2.768844000
H	2.593571000	2.119906000	0.249385000	H	-1.047383000	3.083614000	-0.514655000
H	3.213502000	3.136085000	-1.025345000	H	-1.160943000	3.915315000	-2.712938000
C	3.469636000	3.930262000	0.895961000	H	-0.100355000	4.975930000	-1.835269000
O	2.756415000	4.299147000	2.003753000	H	0.785487000	4.425419000	-4.128071000
H	3.320629000	4.771085000	2.638848000	H	1.901592000	3.863920000	-2.890582000
O	4.643283000	4.181851000	0.794805000	H	1.568973000	2.034064000	-4.531642000

H	-0.176673000	2.148299000	-4.363263000	C	1.542307000	-3.729340000	0.416667000
H	0.742398000	0.259710000	-3.010556000	H	1.987364000	-2.759724000	0.193859000
H	1.857015000	1.361552000	-2.215589000	H	1.899591000	-4.025760000	1.402545000
H	6.029160000	-0.190326000	0.085436000	C	2.097609000	-4.744076000	-0.551935000
H	2.202388000	-1.308850000	-1.494506000	O	1.916564000	-4.371396000	-1.855482000
H	5.515487000	-2.560962000	-1.198240000	H	2.296900000	-5.050481000	-2.438238000
H	5.515156000	-1.355140000	-2.486843000	O	2.667724000	-5.766462000	-0.261222000
H	4.140074000	-2.460238000	-2.311879000	⁵ IM2 _{dioI}			
H	4.983956000	2.743868000	1.627691000	Mn	0.399922000	0.146601000	0.232761000
H	6.170760000	1.443404000	1.794134000	N	-1.320438000	1.161103000	0.709090000
H	4.779998000	1.520969000	2.885705000	N	0.257726000	1.484058000	-1.421297000
H	1.903228000	1.340802000	2.646827000	N	2.145197000	-0.792292000	-0.331551000
H	2.664703000	2.742902000	1.914981000	N	1.972677000	1.636435000	0.879289000
H	1.955850000	2.738211000	-0.632975000	C	-1.892462000	1.841707000	-0.304493000
H	2.334422000	4.528703000	0.848577000	C	-3.038879000	2.616237000	-0.106059000
H	1.456159000	5.179254000	-0.502371000	C	-3.560786000	2.656755000	1.188732000
H	0.595952000	6.042491000	1.702561000	C	-2.975200000	1.946849000	2.241410000
H	-0.667405000	5.162357000	0.853259000	C	-1.840370000	1.199628000	1.946397000
H	-0.623860000	4.385218000	3.206579000	C	-3.554074000	1.959784000	3.628622000
H	1.099879000	4.058240000	3.108835000	C	-3.684091000	3.368909000	-1.238146000
H	-0.240269000	1.948768000	2.821484000	C	-1.209397000	1.688037000	-1.629910000
H	-1.144328000	2.709406000	1.522364000	C	0.894339000	2.802765000	-0.983517000
O	-0.104866000	-1.603989000	-0.919831000	C	0.950502000	3.812408000	-2.139771000
O	0.091940000	-0.517753000	1.857660000	C	1.635865000	3.251695000	-3.387144000
C	0.880670000	-1.146717000	2.725167000	C	0.936182000	1.961739000	-3.822650000
O	2.057791000	-1.396030000	2.530002000	C	0.903521000	0.955522000	-2.672866000
C	0.147611000	-1.511060000	3.997607000	C	3.275051000	-0.351530000	0.252133000
H	0.774679000	-2.141640000	4.627107000	C	4.502849000	-0.992827000	0.032254000
H	-0.107985000	-0.593549000	4.537145000	C	4.503941000	-2.119080000	-0.789170000
H	-0.790237000	-2.022095000	3.764957000	C	3.327263000	-2.595376000	-1.378890000
O	-0.717580000	-3.613165000	-1.844167000	C	2.163991000	-1.885900000	-1.116351000
C	-4.433283000	-2.031605000	-1.109841000	C	3.307650000	-3.815434000	-2.257494000
C	-3.074646000	-2.231187000	-1.338090000	C	5.768152000	-0.499333000	0.682694000
C	-2.237987000	-2.695223000	-0.312884000	C	3.147497000	0.807510000	1.206430000
C	-2.791835000	-2.961652000	0.942842000	C	2.247228000	2.485755000	-0.327803000
C	-4.157919000	-2.776744000	1.166729000	C	3.120501000	3.705942000	0.010037000
C	-4.981192000	-2.309821000	0.144558000	C	2.575187000	4.521500000	1.185453000
H	-5.064481000	-1.664552000	-1.912518000	C	2.398691000	3.610655000	2.404738000
H	-2.668100000	-2.047222000	-2.326958000	C	1.496186000	2.429940000	2.051123000
H	-2.180970000	-3.329346000	1.756833000	H	-4.449166000	3.252110000	1.377443000
H	-4.572035000	-2.996403000	2.145281000	H	-1.321121000	0.613663000	2.693169000
H	-6.041202000	-2.159168000	0.321912000	H	-4.505043000	1.416843000	3.649264000
C	-0.766185000	-2.927792000	-0.633265000	H	-3.753097000	2.983236000	3.958401000
H	0.201606000	-3.882575000	-2.031912000	H	-2.878461000	1.488049000	4.344890000
H	-0.288813000	-1.464734000	-1.859198000	H	-3.012268000	4.134398000	-1.640523000
C	0.008676000	-3.600702000	0.504143000	H	-4.593511000	3.865096000	-0.895897000
H	-0.443751000	-4.585517000	0.647647000	H	-3.954018000	2.694703000	-2.055436000
H	-0.188061000	-3.032727000	1.410928000	H	-1.612278000	0.815941000	-2.148712000

H	-1.391538000	2.547268000	-2.273431000	H	-6.415002000	0.960584000	-0.876075000
H	0.225891000	3.205763000	-0.221709000	C	-2.062025000	-2.256692000	-0.656498000
H	-0.068346000	4.121204000	-2.392209000	H	-1.498356000	-3.824747000	-1.692575000
H	1.443521000	4.717356000	-1.780016000	H	-0.862601000	-1.340258000	-1.917053000
H	1.604521000	3.992414000	-4.190693000	C	-1.795243000	-2.928612000	0.693022000
H	2.694704000	3.048678000	-3.185310000	H	-2.672811000	-3.531325000	0.940195000
H	1.462229000	1.487784000	-4.656327000	H	-1.721929000	-2.141420000	1.443464000
H	-0.079022000	2.177755000	-4.172649000	C	-0.508024000	-3.772332000	0.829775000
H	0.365408000	0.052436000	-2.964337000	H	0.345278000	-3.241981000	0.403683000
H	1.919642000	0.658583000	-2.418563000	H	-0.316757000	-3.915853000	1.893255000
H	5.439417000	-2.641123000	-0.968380000	C	-0.567897000	-5.159734000	0.235129000
H	1.217560000	-2.199103000	-1.532553000	O	-0.393366000	-5.146165000	-1.118778000
H	3.767276000	-4.666351000	-1.746234000	H	-0.458598000	-6.053559000	-1.461981000
H	3.875022000	-3.638824000	-3.176930000	O	-0.742401000	-6.185501000	0.845440000
H	2.286462000	-4.088865000	-2.531639000	³ TS3			
H	6.000386000	0.525652000	0.375016000	Mn	-0.420169000	-0.116368000	0.246377000
H	6.611551000	-1.134032000	0.406121000	N	1.371740000	-1.136838000	0.670392000
H	5.683075000	-0.504232000	1.773972000	N	-0.228360000	-1.487915000	-1.467954000
H	3.020590000	0.405728000	2.216198000	N	-2.196513000	0.768274000	-0.275768000
H	4.067805000	1.395320000	1.214574000	N	-1.818706000	-1.626334000	0.894726000
H	2.819802000	1.857134000	-1.012067000	C	1.952294000	-1.770051000	-0.365583000
H	4.122319000	3.342541000	0.262980000	C	3.163801000	-2.457585000	-0.218459000
H	3.250649000	4.319095000	-0.883880000	C	3.754643000	-2.445740000	1.045070000
H	3.260862000	5.342440000	1.413532000	C	3.161722000	-1.780009000	2.121898000
H	1.612529000	4.978837000	0.922674000	C	1.952486000	-1.137206000	1.880449000
H	1.945144000	4.152238000	3.240323000	C	3.810111000	-1.726498000	3.477387000
H	3.375564000	3.251879000	2.749713000	C	3.806085000	-3.170676000	-1.378132000
H	1.387066000	1.734087000	2.884928000	C	1.236005000	-1.651914000	-1.681976000
H	0.496583000	2.801966000	1.816120000	C	-0.832704000	-2.807749000	-1.028351000
O	-0.865297000	-1.409339000	-0.952347000	C	-0.937960000	-3.802370000	-2.195221000
O	0.286169000	-0.734695000	1.883908000	C	-1.652548000	-3.218130000	-3.416079000
C	1.004880000	-1.534602000	2.668953000	C	-0.950257000	-1.930449000	-3.856478000
O	2.052662000	-2.061791000	2.341465000	C	-0.889822000	-0.937170000	-2.697015000
C	0.367544000	-1.712433000	4.029955000	C	-3.286960000	0.270220000	0.343565000
H	0.898945000	-2.475217000	4.598313000	C	-4.554786000	0.831205000	0.157062000
H	0.406667000	-0.760767000	4.569525000	C	-4.645036000	1.943101000	-0.683091000
H	-0.686093000	-1.983687000	3.924823000	C	-3.518489000	2.474044000	-1.318400000
O	-2.188860000	-3.137874000	-1.728006000	C	-2.304214000	1.840373000	-1.076232000
C	-4.857832000	-0.039845000	-1.984948000	C	-3.592266000	3.665092000	-2.234078000
C	-3.743750000	-0.872834000	-1.911833000	C	-5.767488000	0.274507000	0.855205000
C	-3.294209000	-1.357909000	-0.673932000	C	-3.035913000	-0.864666000	1.297879000
C	-3.986319000	-0.999434000	0.485912000	C	-2.148763000	-2.492320000	-0.309655000
C	-5.109087000	-0.171758000	0.409741000	C	-2.999087000	-3.712613000	0.078906000
C	-5.546437000	0.312500000	-0.821296000	C	-2.393184000	-4.525059000	1.225278000
H	-5.193301000	0.325411000	-2.950303000	C	-2.161220000	-3.612251000	2.432416000
H	-3.235320000	-1.168645000	-2.823348000	C	-1.277231000	-2.430259000	2.039760000
H	-3.671214000	-1.358540000	1.457386000	H	4.699282000	-2.961789000	1.189878000
H	-5.637669000	0.094052000	1.319232000	H	1.422394000	-0.596942000	2.654231000

H	4.717856000	-1.114394000	3.441038000	C	4.053920000	1.211933000	0.524486000
H	4.102199000	-2.725782000	3.812781000	C	5.274219000	0.551219000	0.375182000
H	3.138849000	-1.292780000	4.221643000	C	5.659547000	0.055854000	-0.869265000
H	3.170749000	-3.983494000	-1.746224000	H	5.105255000	-0.164924000	-2.943681000
H	4.763800000	-3.599883000	-1.078992000	H	2.937722000	0.948135000	-2.684095000
H	3.988510000	-2.488109000	-2.212707000	H	3.778432000	1.592589000	1.499780000
H	1.593678000	-0.765669000	-2.207473000	H	5.922701000	0.428978000	1.236193000
H	1.440116000	-2.512171000	-2.319386000	H	6.611142000	-0.452526000	-0.983097000
H	-0.132534000	-3.222091000	-0.301438000	C	1.864092000	2.061878000	-0.426248000
H	0.073221000	-4.107997000	-2.482118000	H	2.377682000	3.042426000	-2.278762000
H	-1.424836000	-4.712184000	-1.838473000	H	0.834130000	2.183084000	-1.776736000
H	-1.654892000	-3.951286000	-4.227445000	C	1.672095000	2.905915000	0.821735000
H	-2.702661000	-3.004045000	-3.180635000	H	2.542265000	3.552749000	0.947676000
H	-1.486179000	-1.449784000	-4.680271000	H	1.646341000	2.214284000	1.666299000
H	0.057680000	-2.155208000	-4.223035000	C	0.381646000	3.734125000	0.834008000
H	-0.347307000	-0.029736000	-2.966102000	H	-0.492664000	3.119333000	0.631438000
H	-1.902830000	-0.642628000	-2.422286000	H	0.258526000	4.149051000	1.840328000
H	-5.613877000	2.408533000	-0.839844000	C	0.343031000	4.907336000	-0.118063000
H	-1.389174000	2.197499000	-1.526022000	O	1.447842000	5.677892000	-0.036198000
H	-4.413267000	4.326320000	-1.946874000	H	1.351446000	6.419349000	-0.655877000
H	-3.769337000	3.345211000	-3.267059000	O	-0.587881000	5.175190000	-0.847490000
H	-2.659355000	4.232940000	-2.208933000	⁵ TS3			
H	-5.943052000	-0.769690000	0.575759000	Mn	-0.392295000	-0.116360000	0.245350000
H	-6.657802000	0.847790000	0.591567000	N	1.290524000	-1.222417000	0.687889000
H	-5.651760000	0.309133000	1.943216000	N	-0.323297000	-1.417024000	-1.439239000
H	-2.868799000	-0.457454000	2.297953000	N	-2.142346000	0.867880000	-0.250979000
H	-3.902002000	-1.523430000	1.361184000	N	-2.017112000	-1.605356000	0.864757000
H	-2.755086000	-1.862973000	-0.962684000	C	1.833774000	-1.872533000	-0.359127000
H	-3.994256000	-3.363975000	0.372453000	C	2.991966000	-2.643917000	-0.215208000
H	-3.158631000	-4.324219000	-0.811286000	C	3.565286000	-2.697234000	1.056397000
H	-3.063526000	-5.348301000	1.487546000	C	3.008100000	-2.016718000	2.144150000
H	-1.442761000	-4.977616000	0.915395000	C	1.849908000	-1.285632000	1.906687000
H	-1.660483000	-4.148857000	3.243773000	C	3.642860000	-2.043104000	3.506571000
H	-3.119944000	-3.260306000	2.829959000	C	3.595549000	-3.378691000	-1.381639000
H	-1.126035000	-1.736045000	2.866906000	C	1.131083000	-1.665707000	-1.666456000
H	-0.294342000	-2.796076000	1.742796000	C	-1.013121000	-2.722626000	-1.066865000
O	0.747677000	1.298362000	-0.810091000	C	-1.128605000	-3.663361000	-2.277105000
O	-0.341324000	0.671397000	1.951168000	C	-1.786098000	-2.998891000	-3.488714000
C	-1.037825000	1.474320000	2.746206000	C	-1.016501000	-1.728355000	-3.859276000
O	-2.071363000	2.040451000	2.428834000	C	-0.936655000	-0.786490000	-2.658635000
C	-0.403897000	1.607159000	4.115098000	C	-3.270745000	0.441417000	0.345658000
H	-0.945961000	2.339104000	4.713240000	C	-4.484224000	1.119041000	0.167722000
H	-0.422259000	0.635356000	4.618114000	C	-4.472681000	2.261554000	-0.633293000
H	0.644313000	1.903316000	4.020116000	C	-3.299741000	2.715609000	-1.244527000
O	1.637336000	3.009958000	-1.648523000	C	-2.147850000	1.972761000	-1.014955000
C	4.813758000	0.213399000	-1.969702000	C	-3.265481000	3.935403000	-2.123794000
C	3.586628000	0.853348000	-1.818862000	C	-5.749361000	0.645647000	0.834023000
C	3.197919000	1.366034000	-0.570792000	C	-3.151407000	-0.751818000	1.258616000

C	-2.342804000	-2.384450000	-0.373857000	H	-0.883619000	2.262340000	4.760264000
C	-3.256329000	-3.585605000	-0.076778000	H	-0.427444000	0.541333000	4.615794000
C	-2.718714000	-4.476704000	1.046765000	H	0.707752000	1.786476000	4.097481000
C	-2.480420000	-3.633400000	2.303975000	O	1.877540000	2.981102000	-1.646174000
C	-1.544268000	-2.468581000	1.984880000	C	4.831715000	-0.070712000	-1.932006000
H	4.469922000	-3.280743000	1.200087000	C	3.659320000	0.668358000	-1.799278000
H	1.346874000	-0.723674000	2.682790000	C	3.291156000	1.205293000	-0.554942000
H	4.594182000	-1.500474000	3.492733000	C	4.110677000	0.973340000	0.554685000
H	3.854854000	-3.069383000	3.819507000	C	5.274244000	0.213478000	0.423358000
H	2.997271000	-1.577890000	4.254208000	C	5.640187000	-0.305681000	-0.817252000
H	2.907766000	-4.137722000	-1.769320000	H	5.109391000	-0.466181000	-2.903271000
H	4.517217000	-3.879594000	-1.081220000	H	3.037515000	0.822795000	-2.675903000
H	3.834374000	-2.695129000	-2.200715000	H	3.850128000	1.370269000	1.527607000
H	1.543252000	-0.783180000	-2.156732000	H	5.893620000	0.032295000	1.295360000
H	1.279890000	-2.511575000	-2.336139000	H	6.547457000	-0.892041000	-0.917184000
H	-0.354693000	-3.197242000	-0.337796000	C	2.005440000	1.991827000	-0.427773000
H	-0.127978000	-4.009427000	-2.553965000	H	2.644361000	2.995543000	-2.244456000
H	-1.667785000	-4.560308000	-1.966861000	H	1.047152000	2.184767000	-1.810082000
H	-1.801213000	-3.697355000	-4.329964000	C	1.847227000	2.824720000	0.832853000
H	-2.830724000	-2.746796000	-3.267741000	H	2.754666000	3.411558000	0.986523000
H	-1.513096000	-1.187241000	-4.670100000	H	1.763395000	2.120422000	1.663430000
H	-0.013134000	-1.982699000	-4.218303000	C	0.612921000	3.733299000	0.846904000
H	-0.348276000	0.104629000	-2.880498000	H	-0.297071000	3.181644000	0.620280000
H	-1.940941000	-0.461810000	-2.390778000	H	0.501790000	4.132422000	1.861098000
H	-5.397349000	2.812094000	-0.780538000	C	0.668139000	4.927693000	-0.077431000
H	-1.200102000	2.260610000	-1.445887000	O	1.823873000	5.615610000	0.035071000
H	-4.026561000	4.656811000	-1.816674000	H	1.788100000	6.376595000	-0.567110000
H	-3.468052000	3.662952000	-3.165657000	O	-0.232175000	5.279738000	-0.809452000
H	-2.286928000	4.418633000	-2.080638000	³ PC			
H	-6.023839000	-0.359922000	0.497458000	Mn	-0.646363000	0.029791000	0.328867000
H	-6.577690000	1.316726000	0.600662000	N	-0.210912000	-1.884918000	0.946169000
H	-5.638285000	0.609164000	1.922330000	N	-1.025307000	-1.055047000	-1.435574000
H	-2.976658000	-0.391331000	2.276963000	N	-1.045671000	1.857483000	-0.369117000
H	-4.092421000	-1.306549000	1.279234000	N	-2.709678000	-0.000185000	0.540605000
H	-2.899542000	-1.703410000	-1.020488000	C	0.086529000	-2.741619000	-0.046003000
H	-4.237859000	-3.197506000	0.216108000	C	0.530889000	-4.044522000	0.211989000
H	-3.428444000	-4.150883000	-0.994952000	C	0.650547000	-4.422534000	1.549563000
H	-3.430119000	-5.281979000	1.251452000	C	0.334897000	-3.539055000	2.588015000
H	-1.780022000	-4.956205000	0.740245000	C	-0.094228000	-2.265215000	2.229126000
H	-2.029399000	-4.232165000	3.101263000	C	0.451049000	-3.938152000	4.033628000
H	-3.435723000	-3.257421000	2.689080000	C	0.872336000	-4.985623000	-0.912346000
H	-1.391584000	-1.817286000	2.847577000	C	-0.057038000	-2.187203000	-1.433914000
H	-0.563244000	-2.862698000	1.709913000	C	-2.441100000	-1.587768000	-1.302482000
O	0.863505000	1.304973000	-0.845744000	C	-2.931201000	-2.264533000	-2.591310000
O	-0.278740000	0.645551000	1.967392000	C	-2.758910000	-1.388453000	-3.834419000
C	-0.945218000	1.476410000	2.758629000	C	-1.297414000	-0.947790000	-3.954887000
O	-1.919027000	2.127161000	2.418060000	C	-0.857294000	-0.230350000	-2.680717000
C	-0.353988000	1.529710000	4.151965000	C	-2.249974000	2.340864000	-0.012717000

C	-2.647235000	3.639519000	-0.347917000	H	-2.731582000	-0.490496000	2.574418000
C	-1.734145000	4.416296000	-1.062296000	H	-2.684346000	-1.873196000	1.494281000
C	-0.473134000	3.924420000	-1.419523000	O	1.258158000	0.112373000	-0.251058000
C	-0.166609000	2.622541000	-1.036504000	O	-0.435669000	0.602254000	2.104992000
C	0.514929000	4.759687000	-2.187484000	C	-0.321368000	1.742553000	2.767920000
C	-3.995276000	4.173578000	0.058198000	O	-0.196647000	2.840987000	2.248111000
C	-3.091572000	1.414310000	0.817219000	C	-0.355851000	1.536407000	4.268260000
C	-3.294327000	-0.422951000	-0.795540000	H	-0.250166000	2.489823000	4.785002000
C	-4.807057000	-0.680098000	-0.718540000	H	-1.298883000	1.060460000	4.552684000
C	-5.204221000	-1.626665000	0.415572000	H	0.450788000	0.860524000	4.567765000
C	-4.664696000	-1.084081000	1.741226000	O	3.091219000	2.591903000	-1.133350000
C	-3.151077000	-0.902407000	1.656661000	C	4.070952000	-0.759518000	-3.162342000
H	0.995979000	-5.424842000	1.786333000	C	3.161515000	-0.337234000	-2.203121000
H	-0.343491000	-1.512756000	2.966171000	C	3.417579000	-0.556789000	-0.830052000
H	1.447665000	-4.335501000	4.247699000	C	4.603806000	-1.208832000	-0.448197000
H	-0.273417000	-4.722218000	4.277078000	C	5.502789000	-1.645811000	-1.417160000
H	0.268590000	-3.088634000	4.695133000	C	5.241296000	-1.420991000	-2.770209000
H	-0.006830000	-5.199440000	-1.530118000	H	3.874408000	-0.573287000	-4.212585000
H	1.247138000	-5.932457000	-0.520140000	H	2.267236000	0.201816000	-2.500144000
H	1.639046000	-4.561019000	-1.568107000	H	4.820684000	-1.393673000	0.595177000
H	0.905843000	-1.811217000	-1.785376000	H	6.408773000	-2.160050000	-1.115556000
H	-0.370006000	-2.962253000	-2.133938000	H	5.949747000	-1.756035000	-3.520802000
H	-2.396177000	-2.351314000	-0.525016000	C	2.414466000	-0.139761000	0.153636000
H	-2.373714000	-3.196678000	-2.726927000	H	3.831357000	2.349664000	-1.701840000
H	-3.971086000	-2.567184000	-2.451796000	H	3.368178000	3.395489000	-0.673943000
H	-3.067565000	-1.945775000	-4.723093000	C	2.724661000	0.010029000	1.620575000
H	-3.406710000	-0.504932000	-3.774603000	H	3.601317000	-0.563137000	1.912533000
H	-1.161938000	-0.253383000	-4.789283000	H	1.866296000	-0.368262000	2.176369000
H	-0.654025000	-1.811613000	-4.155456000	C	2.912629000	1.494668000	1.998923000
H	0.189507000	0.066959000	-2.720279000	H	2.106027000	2.110529000	1.599957000
H	-1.445674000	0.677718000	-2.559850000	H	2.862248000	1.577169000	3.091111000
H	-2.009160000	5.429708000	-1.341330000	C	4.216990000	2.147946000	1.600656000
H	0.802793000	2.190203000	-1.250053000	O	5.231573000	1.277271000	1.446372000
H	0.113523000	5.020572000	-3.172316000	H	6.035377000	1.774255000	1.220879000
H	1.455090000	4.223016000	-2.325403000	O	4.360153000	3.347085000	1.474622000
H	0.722375000	5.696181000	-1.660802000	⁵ PC			
H	-4.805658000	3.585152000	-0.385442000	Mn	-0.572066000	-0.138428000	0.315578000
H	-4.112008000	5.208200000	-0.268804000	N	0.857321000	-1.558908000	0.705418000
H	-4.124191000	4.144286000	1.144860000	N	-0.685458000	-1.274733000	-1.461632000
H	-2.915930000	1.613559000	1.877873000	N	-1.924405000	1.290860000	-0.238052000
H	-4.154821000	1.576007000	0.636639000	N	-2.512369000	-1.162422000	0.748760000
H	-3.144882000	0.428223000	-1.461028000	C	1.321263000	-2.211000000	-0.377573000
H	-5.313052000	0.280012000	-0.576160000	C	2.374391000	-3.127570000	-0.282328000
H	-5.146971000	-1.045712000	-1.689716000	C	2.932773000	-3.322912000	0.981299000
H	-6.292980000	-1.722224000	0.450493000	C	2.454781000	-2.646266000	2.109856000
H	-4.803412000	-2.632361000	0.236776000	C	1.395434000	-1.767165000	1.920330000
H	-4.870999000	-1.773662000	2.565157000	C	3.076774000	-2.831201000	3.465639000
H	-5.155354000	-0.136475000	1.990816000	C	2.885848000	-3.856857000	-1.495011000

C	0.683924000	-1.830615000	-1.678167000	H	-3.279034000	-0.982623000	-1.181422000
C	-1.673484000	-2.406804000	-1.191739000	H	-4.993237000	-2.167529000	-0.096249000
C	-1.929969000	-3.237997000	-2.458869000	H	-4.351927000	-3.239106000	-1.309478000
C	-2.351558000	-2.385040000	-3.657997000	H	-4.757441000	-4.420590000	0.871876000
C	-1.305028000	-1.297708000	-3.917764000	H	-3.046027000	-4.469338000	0.472963000
C	-1.090325000	-0.457326000	-2.660229000	H	-3.283197000	-3.788612000	2.849719000
C	-3.161046000	1.161536000	0.274566000	H	-4.395453000	-2.499348000	2.403209000
C	-4.135682000	2.145618000	0.060364000	H	-2.089988000	-1.583956000	2.753087000
C	-3.768955000	3.256971000	-0.698637000	H	-1.448403000	-2.753094000	1.614000000
C	-2.481855000	3.392122000	-1.233169000	O	1.184054000	1.115364000	-0.516061000
C	-1.582251000	2.368845000	-0.965635000	O	-0.369068000	0.497427000	2.071891000
C	-2.080922000	4.587863000	-2.051951000	C	-0.819174000	1.483566000	2.842222000
C	-5.520593000	2.011992000	0.635772000	O	-1.441733000	2.447167000	2.429446000
C	-3.425529000	-0.062238000	1.117514000	C	-0.459003000	1.280054000	4.297434000
C	-2.931187000	-1.798693000	-0.545814000	H	-0.832296000	2.109164000	4.897594000
C	-4.112226000	-2.764363000	-0.355982000	H	-0.887151000	0.338523000	4.653411000
C	-3.868072000	-3.796164000	0.748620000	H	0.627274000	1.204793000	4.402552000
C	-3.528971000	-3.075391000	2.057177000	O	5.284004000	3.097750000	-1.129212000
C	-2.329512000	-2.151937000	1.852729000	C	4.708937000	-0.793026000	-1.865823000
H	3.762814000	-4.015044000	1.087522000	C	3.620571000	0.013803000	-1.549032000
H	0.963771000	-1.192322000	2.729243000	C	3.419969000	0.433937000	-0.221768000
H	4.105440000	-2.455545000	3.463819000	C	4.319403000	0.037810000	0.781141000
H	3.113979000	-3.890104000	3.737123000	C	5.378754000	-0.809141000	0.465209000
H	2.518647000	-2.294684000	4.235395000	C	5.577724000	-1.219500000	-0.855045000
H	2.116521000	-4.516612000	-1.910453000	H	4.879441000	-1.092361000	-2.894238000
H	3.752480000	-4.467164000	-1.236566000	H	2.947213000	0.363881000	-2.323666000
H	3.186192000	-3.159347000	-2.281487000	H	4.173143000	0.356974000	1.806724000
H	1.283545000	-1.052529000	-2.153752000	H	6.052859000	-1.141813000	1.246826000
H	0.653297000	-2.675295000	-2.365124000	H	6.414299000	-1.865272000	-1.100018000
H	-1.181540000	-3.050860000	-0.460501000	C	2.251597000	1.272308000	0.100004000
H	-1.020068000	-3.792349000	-2.708701000	H	5.237899000	2.197533000	-1.469884000
H	-2.675360000	-4.000348000	-2.225421000	H	4.362832000	3.402327000	-1.088710000
H	-2.468237000	-3.022000000	-4.538968000	C	2.359758000	2.294183000	1.207143000
H	-3.327616000	-1.920096000	-3.472697000	H	3.394030000	2.633194000	1.289057000
H	-1.628775000	-0.620620000	-4.713585000	H	2.124631000	1.772942000	2.143883000
H	-0.362509000	-1.746185000	-4.249707000	C	1.407544000	3.472928000	1.038733000
H	-0.317207000	0.299992000	-2.800267000	H	0.361884000	3.157012000	1.011566000
H	-2.016132000	0.057887000	-2.412447000	H	1.492281000	4.149962000	1.894114000
H	-4.505351000	4.033678000	-0.883653000	C	1.689123000	4.265439000	-0.212680000
H	-0.566892000	2.389418000	-1.339716000	O	0.835568000	5.287734000	-0.362817000
H	-1.959444000	5.467341000	-1.411380000	H	1.059203000	5.770470000	-1.176142000
H	-2.846954000	4.822735000	-2.796002000	O	2.570158000	4.027994000	-1.018776000
H	-1.135715000	4.414302000	-2.570204000	Part V. Alcohol oxidation of 4-OH-PBA by the			
H	-6.029283000	1.123499000	0.246940000	Mn^{IV}(O)(AcO•) species 2 via the DHA and R-DHA			
H	-6.124765000	2.884573000	0.382394000	mechanisms.			
H	-5.491803000	1.923660000	1.726347000	³ TS _{DHA}			
H	-3.255688000	0.189532000	2.169025000	Mn	0.626855000	0.053406000	-0.106534000
H	-4.473390000	-0.359382000	1.032140000	N	0.585280000	2.056350000	-0.434882000

N	2.471539000	0.281761000	-1.101742000	H	0.507929000	-5.622146000	1.310204000
N	0.691629000	-1.941184000	0.261207000	H	0.104187000	-2.502068000	-1.624234000
N	1.856496000	0.009278000	1.632183000	H	-0.949779000	-5.887523000	-0.949775000
C	1.435044000	2.494540000	-1.381979000	H	0.690334000	-5.888228000	-1.598142000
C	1.479446000	3.843289000	-1.760350000	H	-0.512946000	-4.759624000	-2.247903000
C	0.601137000	4.714710000	-1.114439000	H	2.330022000	-3.742824000	3.608289000
C	-0.288070000	4.263204000	-0.131881000	H	1.165863000	-5.071771000	3.520297000
C	-0.256805000	2.906996000	0.174482000	H	0.651669000	-3.474645000	4.082878000
C	-1.242578000	5.194993000	0.564565000	H	0.486688000	-0.822043000	2.987656000
C	2.431023000	4.326899000	-2.822644000	H	2.110125000	-1.460600000	3.166707000
C	2.283503000	1.432082000	-2.029684000	H	3.268865000	-1.293762000	0.808656000
C	3.501288000	0.654403000	-0.055326000	H	4.149304000	-0.975868000	2.976985000
C	4.931932000	0.661115000	-0.617970000	H	5.297738000	-0.284911000	1.868379000
C	5.294254000	-0.629304000	-1.356786000	H	4.911441000	1.180387000	3.881618000
C	4.264284000	-0.893444000	-2.458860000	H	4.449427000	2.022722000	2.408865000
C	2.861082000	-0.951059000	-1.859681000	H	2.639650000	2.316438000	4.078353000
C	1.003801000	-2.289331000	1.519857000	H	2.544932000	0.580083000	4.335988000
C	0.953175000	-3.622857000	1.947993000	H	0.730258000	1.348851000	2.773215000
C	0.564775000	-4.579521000	1.009736000	H	1.939497000	2.108022000	1.753604000
C	0.252590000	-4.222564000	-0.307242000	O	-0.261865000	-0.253616000	-1.708264000
C	0.333318000	-2.873053000	-0.633900000	O	-0.865079000	0.258305000	1.142757000
C	-0.154817000	-5.242488000	-1.336207000	C	-1.864675000	-0.481746000	1.506669000
C	1.292557000	-3.998674000	3.366381000	O	-2.293837000	-1.459380000	0.882997000
C	1.367156000	-1.149308000	2.430719000	C	-2.501529000	-0.059534000	2.820199000
C	3.265513000	-0.258117000	1.152829000	H	-3.547875000	-0.364984000	2.852263000
C	4.298465000	-0.140897000	2.284714000	H	-1.974777000	-0.562403000	3.639567000
C	4.191950000	1.175932000	3.057789000	H	-2.415002000	1.016859000	2.974430000
C	2.764026000	1.347701000	3.584732000	O	-2.938555000	0.690106000	-1.476622000
C	1.763312000	1.273828000	2.433240000	C	-4.954407000	2.490483000	1.553983000
H	0.610732000	5.767452000	-1.382764000	C	-4.274962000	1.886649000	0.508868000
H	-0.903169000	2.462201000	0.920394000	C	-4.611806000	0.571448000	0.107093000
H	-1.937346000	5.644853000	-0.151927000	C	-5.647152000	-0.114792000	0.777224000
H	-0.702356000	6.012070000	1.052775000	C	-6.325148000	0.501553000	1.820612000
H	-1.827072000	4.669330000	1.323110000	C	-5.979458000	1.799002000	2.211237000
H	3.472484000	4.153736000	-2.530777000	H	-4.690210000	3.496222000	1.860814000
H	2.303300000	5.397059000	-2.994549000	H	-3.480893000	2.414138000	-0.003407000
H	2.266466000	3.808288000	-3.772489000	H	-5.920798000	-1.123103000	0.496111000
H	1.792427000	1.059979000	-2.933939000	H	-7.118934000	-0.028772000	2.334047000
H	3.241713000	1.844100000	-2.349028000	H	-6.508450000	2.272654000	3.031687000
H	3.261880000	1.677840000	0.238481000	C	-3.864220000	-0.040284000	-0.964000000
H	5.030526000	1.506399000	-1.306954000	H	-2.452145000	0.244445000	-2.212694000
H	5.628842000	0.869508000	0.196499000	H	-0.229160000	0.496903000	-2.311074000
H	6.300173000	-0.543857000	-1.777705000	C	-4.167969000	-1.386197000	-1.550178000
H	5.313237000	-1.477243000	-0.660333000	H	-4.794502000	-1.191466000	-2.432332000
H	4.457340000	-1.847286000	-2.959308000	H	-4.786819000	-1.941823000	-0.851267000
H	4.326153000	-0.114768000	-3.228130000	C	-2.961484000	-2.277039000	-1.911329000
H	2.089231000	-1.106632000	-2.614318000	H	-2.225962000	-2.208510000	-1.102099000
H	2.804138000	-1.789502000	-1.165549000	H	-3.296096000	-3.315130000	-1.951697000

C	-2.231618000	-2.010773000	-3.200159000	H	5.553312000	-1.342362000	-0.430430000
O	-2.431552000	-0.744538000	-3.669211000	H	6.466248000	-0.071144000	1.538781000
H	-1.891155000	-0.600557000	-4.464050000	H	5.485650000	0.988924000	0.536170000
O	-1.516451000	-2.797646000	-3.769318000	H	4.826661000	1.319678000	2.905121000
⁵ TS _{DHA}				H	4.578520000	-0.410408000	3.112991000
Mn	0.545114000	-0.000291000	0.144486000	H	2.386803000	0.746324000	2.727396000
N	0.408052000	-2.102202000	0.458693000	H	3.021839000	1.468365000	1.263489000
N	2.562347000	-0.573106000	1.116462000	H	1.073636000	5.720345000	-1.156818000
N	0.850089000	2.035201000	-0.170457000	H	0.324928000	2.618839000	1.728906000
N	1.786987000	-0.028403000	-1.597268000	H	-0.277628000	6.163253000	1.078793000
C	1.261605000	-2.660329000	1.330854000	H	1.294739000	5.859033000	1.818876000
C	1.181140000	-4.022655000	1.659238000	H	-0.121338000	4.935454000	2.351755000
C	0.178179000	-4.771316000	1.042144000	H	2.667579000	3.682565000	-3.497961000
C	-0.713921000	-4.191649000	0.132720000	H	1.680381000	5.145091000	-3.371982000
C	-0.554377000	-2.834963000	-0.126730000	H	0.966493000	3.639579000	-3.967647000
C	-1.805878000	-4.985664000	-0.532028000	H	0.469239000	0.979576000	-2.881592000
C	2.135322000	-4.651217000	2.640648000	H	2.146366000	1.435895000	-3.117939000
C	2.280429000	-1.741258000	1.968629000	H	3.352736000	1.072089000	-0.748896000
C	3.463426000	-0.948954000	-0.021363000	H	4.092129000	0.804477000	-2.992193000
C	4.925242000	-1.108300000	0.431617000	H	5.225571000	-0.032627000	-1.975191000
C	5.443624000	0.113023000	1.196511000	H	4.621884000	-1.364463000	-4.028503000
C	4.520514000	0.407083000	2.384156000	H	4.163754000	-2.232642000	-2.570033000
C	3.081064000	0.583227000	1.900804000	H	2.256153000	-2.311390000	-4.143114000
C	1.193453000	2.360027000	-1.427351000	H	2.298899000	-0.567458000	-4.349630000
C	1.293424000	3.697030000	-1.832802000	H	0.494080000	-1.219123000	-2.729539000
C	1.014254000	4.673013000	-0.873708000	H	1.667578000	-2.120820000	-1.787485000
C	0.661001000	4.336132000	0.438479000	O	-0.251956000	0.351587000	1.770364000
C	0.594421000	2.980530000	0.744306000	O	-1.047112000	-0.140549000	-1.208596000
C	0.369078000	5.379113000	1.482709000	C	-1.954354000	0.685385000	-1.607769000
C	1.671550000	4.061281000	-3.244141000	O	-2.298675000	1.705910000	-0.990722000
C	1.402280000	1.197922000	-2.357868000	C	-2.607664000	0.320519000	-2.931320000
C	3.237376000	0.066223000	-1.155994000	H	-3.415136000	1.010449000	-3.175257000
C	4.199925000	-0.072972000	-2.346999000	H	-1.858684000	0.340049000	-3.729908000
C	3.946124000	-1.339254000	-3.168808000	H	-2.996583000	-0.699902000	-2.879055000
C	2.485747000	-1.372560000	-3.629861000	O	-2.947883000	-0.561983000	1.580744000
C	1.542198000	-1.252499000	-2.434000000	C	-5.000195000	-2.403303000	-1.404511000
H	0.094050000	-5.829934000	1.271829000	C	-4.316081000	-1.787646000	-0.369308000
H	-1.187998000	-2.295669000	-0.820189000	C	-4.551360000	-0.422798000	-0.073274000
H	-2.612396000	-5.204653000	0.176427000	C	-5.487707000	0.301569000	-0.842229000
H	-1.425958000	-5.942599000	-0.900419000	C	-6.169925000	-0.325633000	-1.875863000
H	-2.234725000	-4.438890000	-1.375093000	C	-5.928102000	-1.673217000	-2.158439000
H	3.168978000	-4.595356000	2.282278000	H	-4.819461000	-3.448985000	-1.626490000
H	1.888707000	-5.703314000	2.793857000	H	-3.602598000	-2.345546000	0.223020000
H	2.098837000	-4.149116000	3.612573000	H	-5.675254000	1.349091000	-0.648577000
H	1.891486000	-1.381577000	2.927854000	H	-6.885410000	0.234986000	-2.466290000
H	3.187624000	-2.302920000	2.205963000	H	-6.461709000	-2.157078000	-2.969866000
H	3.119346000	-1.926506000	-0.364482000	C	-3.815499000	0.191605000	1.003460000
H	4.984470000	-1.986752000	1.083303000	H	-2.489307000	-0.117108000	2.337711000

H	-0.107866000	-0.330725000	2.435978000	H	-2.408747000	-3.564097000	2.661826000
C	-4.068987000	1.573484000	1.525922000	H	-4.057190000	-3.338391000	2.059915000
H	-4.713159000	1.444239000	2.407320000	H	-3.245795000	-2.032307000	2.934056000
H	-4.655063000	2.124353000	0.796272000	H	-0.897621000	-0.283923000	2.486704000
C	-2.830073000	2.427820000	1.866458000	H	-0.661677000	-1.994828000	2.830313000
H	-2.095995000	2.311470000	1.061372000	H	0.759967000	-2.938966000	0.751460000
H	-3.126699000	3.478386000	1.871105000	H	0.812377000	-3.518750000	3.039924000
C	-2.122778000	2.178917000	3.170817000	H	2.270089000	-4.150216000	2.331317000
O	-2.394925000	0.946430000	3.695395000	H	2.689522000	-3.058594000	4.561633000
H	-1.872828000	0.810444000	4.503858000	H	3.585679000	-2.232372000	3.295020000
O	-1.373311000	2.950864000	3.714725000	H	2.451521000	-0.523035000	4.684058000
³ TS _{1OH}				H	0.905186000	-1.337491000	4.495416000
Mn	0.751743000	0.139762000	-0.194510000	H	1.080559000	0.605904000	2.911859000
N	-0.928803000	-1.072817000	-0.317164000	H	2.596647000	-0.036199000	2.300222000
N	0.873429000	-1.061781000	1.669039000	H	5.943587000	2.867103000	0.029960000
N	2.564018000	1.087352000	-0.056525000	H	1.777015000	2.610009000	1.077718000
N	2.244087000	-1.494744000	-0.827479000	H	4.375896000	5.024612000	0.782905000
C	-1.384004000	-1.565647000	0.852508000	H	4.723574000	4.123718000	2.259706000
C	-2.562661000	-2.319907000	0.906211000	H	3.048435000	4.530320000	1.848857000
C	-3.222829000	-2.565061000	-0.300919000	H	6.283913000	-0.425631000	-1.047321000
C	-2.735914000	-2.077305000	-1.516817000	H	6.921083000	1.201743000	-1.317636000
C	-1.575238000	-1.310151000	-1.470279000	H	5.834177000	0.466422000	-2.503812000
C	-3.415664000	-2.365138000	-2.826559000	H	2.987571000	-0.455971000	-2.485083000
C	-3.098146000	-2.841194000	2.212392000	H	4.235589000	-1.314810000	-1.590174000
C	-0.554578000	-1.230262000	2.060484000	H	3.359834000	-1.394752000	0.936272000
C	1.504161000	-2.399097000	1.338758000	H	4.545813000	-3.020911000	-0.289013000
C	1.774338000	-3.218782000	2.611854000	H	3.896819000	-3.832251000	1.106862000
C	2.574380000	-2.445770000	3.663168000	H	3.633896000	-5.197378000	-0.990109000
C	1.858856000	-1.132937000	3.995750000	H	2.057030000	-4.813689000	-0.313611000
C	1.632114000	-0.315976000	2.724473000	H	1.998218000	-4.346500000	-2.748699000
C	3.609992000	0.543796000	-0.712562000	H	3.435828000	-3.340525000	-2.627195000
C	4.864544000	1.166066000	-0.703375000	H	1.360117000	-1.922017000	-2.671900000
C	4.981036000	2.364242000	0.003993000	H	0.711924000	-2.844093000	-1.324711000
C	3.892371000	2.931988000	0.674720000	O	-0.058074000	1.388094000	0.631661000
C	2.683863000	2.249097000	0.609092000	O	0.569684000	0.593739000	-2.002300000
C	4.011340000	4.224759000	1.434557000	C	0.550895000	1.785806000	-2.603308000
C	6.039350000	0.569405000	-1.433699000	O	0.777154000	2.843475000	-2.045477000
C	3.327534000	-0.720041000	-1.478930000	C	0.204934000	1.660669000	-4.071841000
C	2.730575000	-2.139789000	0.446127000	H	0.319391000	2.624806000	-4.566657000
C	3.610059000	-3.368935000	0.160733000	H	0.842733000	0.912139000	-4.548252000
C	2.945080000	-4.373090000	-0.784502000	H	-0.831179000	1.320856000	-4.167593000
C	2.542179000	-3.668699000	-2.083909000	O	-2.401249000	1.560435000	1.051569000
C	1.635898000	-2.477843000	-1.774241000	C	-5.982263000	-0.595500000	1.105252000
H	-4.140967000	-3.144104000	-0.288613000	C	-4.864952000	0.221939000	1.125113000
H	-1.137423000	-0.867013000	-2.355679000	C	-4.348273000	0.733144000	-0.083476000
H	-4.497140000	-2.438309000	-2.696227000	C	-5.004399000	0.450327000	-1.304811000
H	-3.062450000	-3.317864000	-3.235894000	C	-6.120346000	-0.371371000	-1.319954000
H	-3.204131000	-1.586016000	-3.562373000	C	-6.612912000	-0.896906000	-0.116598000

H	-6.369709000	-1.010915000	2.028883000	C	3.982223000	-1.989051000	-2.477568000
H	-4.357978000	0.454492000	2.053665000	C	2.605882000	-1.418718000	-2.136896000
H	-4.611967000	0.853752000	-2.232700000	H	-2.470919000	-4.798656000	-1.134654000
H	-6.610892000	-0.606738000	-2.257652000	H	-0.646463000	-1.277040000	-2.791896000
H	-7.490133000	-1.534974000	-0.125810000	H	-3.240135000	-3.619732000	-3.491096000
C	-3.103170000	1.538887000	-0.102242000	H	-1.713479000	-4.419331000	-3.869913000
H	-1.283541000	1.536553000	0.844466000	H	-1.930953000	-2.705062000	-4.260903000
H	-2.472029000	1.270728000	-0.968479000	H	-0.719191000	-4.770866000	1.882342000
C	-3.511956000	3.086715000	-0.500569000	H	-2.269810000	-5.251868000	1.178782000
H	-4.269419000	3.399709000	0.216410000	H	-2.168642000	-3.816580000	2.208065000
H	-3.945453000	3.033811000	-1.498421000	H	-0.797511000	-1.248190000	2.097018000
C	-2.285914000	3.987164000	-0.483759000	H	0.206134000	-2.683453000	2.273640000
H	-1.436360000	3.550767000	-1.014060000	H	1.961464000	-2.567499000	0.238126000
H	-2.555193000	4.907013000	-1.021716000	H	2.204926000	-3.352375000	2.453664000
C	-1.801490000	4.429716000	0.879841000	H	3.811654000	-3.126634000	1.826617000
O	-2.809810000	4.631707000	1.754162000	H	3.577344000	-2.271579000	4.184137000
H	-2.430498000	4.946614000	2.590810000	H	4.019162000	-0.963879000	3.095339000
O	-0.643230000	4.649233000	1.159867000	H	2.161314000	-0.179269000	4.531397000
⁵ TS1 _{OH}				H	1.192486000	-1.586732000	4.120011000
Mn	0.505440000	0.215886000	-0.389124000	H	0.488538000	0.401431000	2.755784000
N	-0.383136000	-1.616248000	-0.777607000	H	2.148772000	0.622743000	2.229327000
N	1.136706000	-0.995794000	1.344875000	H	3.723290000	5.015334000	0.650475000
N	1.621666000	1.886085000	0.019921000	H	0.160877000	2.673350000	1.231641000
N	2.635384000	-0.404984000	-1.041450000	H	1.224187000	6.029836000	1.449665000
C	-0.609111000	-2.382518000	0.306826000	H	1.995989000	5.253671000	2.833453000
C	-1.369482000	-3.554143000	0.220265000	H	0.342391000	4.805220000	2.379158000
C	-1.872868000	-3.897269000	-1.036082000	H	5.651409000	2.476691000	-0.723668000
C	-1.625197000	-3.110696000	-2.166128000	H	5.425683000	4.230233000	-0.772920000
C	-0.869067000	-1.958117000	-1.980629000	H	4.883521000	3.227408000	-2.125687000
C	-2.155578000	-3.479283000	-3.524424000	H	2.834302000	1.083208000	-2.498379000
C	-1.646946000	-4.394434000	1.438627000	H	4.310511000	0.813009000	-1.578973000
C	-0.045697000	-1.864115000	1.599650000	H	3.502095000	-0.025406000	0.818200000
C	2.339163000	-1.826100000	0.943728000	H	5.364102000	-0.720845000	-0.442341000
C	2.921645000	-2.582789000	2.149396000	H	5.135476000	-1.923285000	0.795696000
C	3.218092000	-1.671446000	3.343370000	H	5.634407000	-2.953307000	-1.444646000
C	1.953871000	-0.899387000	3.734253000	H	4.044145000	-3.453792000	-0.886388000
C	1.416122000	-0.125342000	2.532150000	H	3.855870000	-2.746995000	-3.256647000
C	2.825691000	2.001026000	-0.577726000	H	4.627045000	-1.207452000	-2.896074000
C	3.624037000	3.133770000	-0.371989000	H	2.130887000	-0.942109000	-2.996103000
C	3.122486000	4.128581000	0.469409000	H	1.951130000	-2.231672000	-1.818187000
C	1.870161000	4.011688000	1.082527000	O	-0.862407000	0.753696000	0.445769000
C	1.144117000	2.857025000	0.817472000	O	0.193971000	0.786366000	-2.167262000
C	1.323416000	5.081717000	1.987361000	C	-0.450593000	1.833149000	-2.641501000
C	4.969113000	3.274547000	-1.035680000	O	-0.873601000	2.756080000	-1.948041000
C	3.223864000	0.875720000	-1.496968000	C	-0.653803000	1.790472000	-4.137890000
C	3.324299000	-0.906867000	0.199551000	H	-0.511209000	2.789150000	-4.555216000
C	4.695156000	-1.526453000	-0.121384000	H	0.013450000	1.074923000	-4.617976000
C	4.627610000	-2.587425000	-1.223378000	H	-1.694061000	1.497103000	-4.313852000

O	-3.082212000	0.036327000	-0.599868000	C	-2.178969000	2.084858000	-1.747129000
C	-2.253561000	0.764133000	3.579595000	C	-3.128370000	3.673874000	-3.455597000
C	-2.771543000	0.856431000	2.292423000	C	-5.683191000	2.272106000	0.693303000
C	-3.622160000	-0.181854000	1.768383000	C	-3.289793000	0.622831000	1.451361000
C	-4.021294000	-1.235158000	2.609529000	C	-3.116265000	-1.614873000	0.425625000
C	-3.496648000	-1.323089000	3.886066000	C	-4.195105000	-2.358203000	1.231359000
C	-2.610175000	-0.318253000	4.377913000	C	-3.667844000	-2.930418000	2.549479000
H	-1.612021000	1.547266000	3.965369000	C	-3.038320000	-1.810301000	3.383177000
H	-2.579217000	1.734475000	1.689652000	C	-1.941967000	-1.107815000	2.583030000
H	-4.679283000	-2.008234000	2.229392000	H	3.529932000	-3.545533000	1.685908000
H	-3.740652000	-2.169306000	4.518525000	H	1.273346000	0.049503000	2.361131000
H	-2.238123000	-0.394099000	5.393655000	H	4.436519000	-1.202712000	3.064572000
C	-4.088131000	-0.121663000	0.351334000	H	3.424605000	-2.235041000	4.076880000
H	-2.211603000	0.361986000	-0.202281000	H	3.044833000	-0.509067000	3.913776000
H	-4.653046000	-1.024278000	0.091833000	H	1.295241000	-5.029019000	-0.432094000
C	-5.123697000	1.091736000	0.257687000	H	3.042940000	-4.913243000	-0.175866000
H	-4.719612000	1.961776000	0.775882000	H	2.307934000	-4.148713000	-1.585656000
H	-6.041451000	0.785539000	0.763567000	H	0.669798000	-1.701592000	-2.100081000
C	-5.397258000	1.443049000	-1.206216000	H	0.058537000	-3.291410000	-1.644799000
H	-5.777692000	0.587496000	-1.767531000	H	-1.373977000	-2.860538000	0.588798000
H	-6.175464000	2.217305000	-1.219267000	H	-1.704607000	-4.395740000	-1.173685000
C	-4.194930000	1.988746000	-1.952984000	H	-3.208598000	-4.305024000	-0.305769000
O	-3.481614000	2.863425000	-1.226459000	H	-3.546255000	-4.289562000	-2.801570000
H	-2.601714000	3.006624000	-1.651882000	H	-4.165394000	-2.806857000	-2.089304000
O	-3.927381000	1.707953000	-3.105603000	H	-2.803378000	-2.206579000	-4.069515000
³ IM1 _{OH}				H	-1.446886000	-3.153554000	-3.475106000
Mn	-0.674459000	0.238175000	0.043700000	H	-1.111192000	-0.717587000	-2.974603000
N	0.769366000	-1.089546000	0.714949000	H	-2.685327000	-0.667378000	-2.188128000
N	-1.169798000	-1.636150000	-1.095270000	H	-5.208287000	3.553152000	-1.666917000
N	-2.260267000	1.367915000	-0.612281000	H	-1.248032000	1.998024000	-2.292588000
N	-2.422770000	-0.570494000	1.270363000	H	-3.281601000	4.740445000	-3.265865000
C	0.989489000	-2.175006000	-0.056985000	H	-3.897550000	3.352112000	-4.164630000
C	1.968852000	-3.115028000	0.283193000	H	-2.151851000	3.543865000	-3.925950000
C	2.747154000	-2.846126000	1.409796000	H	-6.150391000	1.286802000	0.792944000
C	2.545892000	-1.700935000	2.188205000	H	-6.419813000	2.952370000	0.263218000
C	1.518641000	-0.845800000	1.805366000	H	-5.439494000	2.626490000	1.699434000
C	3.405415000	-1.391147000	3.381229000	H	-2.850234000	1.240378000	2.240061000
C	2.164667000	-4.369391000	-0.526138000	H	-4.288021000	0.335278000	1.783568000
C	0.164370000	-2.260763000	-1.308000000	H	-3.619287000	-1.065311000	-0.371524000
C	-2.034144000	-2.505007000	-0.203405000	H	-5.007424000	-1.655718000	1.443424000
C	-2.552858000	-3.735765000	-0.967295000	H	-4.637071000	-3.131654000	0.600365000
C	-3.247015000	-3.374858000	-2.282571000	H	-4.487701000	-3.402062000	3.098144000
C	-2.302452000	-2.547000000	-3.158713000	H	-2.923739000	-3.714075000	2.359054000
C	-1.828199000	-1.306332000	-2.400723000	H	-2.585586000	-2.203857000	4.297947000
C	-3.356450000	1.417798000	0.176251000	H	-3.805911000	-1.091727000	3.692023000
C	-4.456270000	2.207416000	-0.177629000	H	-1.504855000	-0.268651000	3.125886000
C	-4.367609000	2.934400000	-1.366832000	H	-1.138583000	-1.815650000	2.375521000
C	-3.227819000	2.888952000	-2.176876000	O	0.411559000	0.809729000	-1.248802000

O	-0.313753000	1.428224000	1.437628000	C	-3.248329000	-3.373786000	-2.283727000
C	-0.080822000	2.742127000	1.431749000	C	-2.303092000	-2.546044000	-3.159263000
O	-0.117363000	3.425871000	0.420355000	C	-1.828550000	-1.305855000	-2.400667000
C	0.240904000	3.267545000	2.807232000	C	-3.356464000	1.417628000	0.177366000
H	0.146267000	4.352427000	2.819037000	C	-4.456110000	2.207447000	-0.176572000
H	-0.408415000	2.809435000	3.555481000	C	-4.367212000	2.934440000	-1.365757000
H	1.276530000	3.001788000	3.038945000	C	-3.227405000	2.888709000	-2.175767000
O	2.684835000	1.420508000	0.190930000	C	-2.178783000	2.084329000	-1.745984000
C	3.796776000	-1.812087000	-2.448717000	C	-3.127693000	3.673607000	-3.454485000
C	3.537400000	-0.590965000	-1.827086000	C	-5.683110000	2.272286000	0.694244000
C	4.245993000	-0.222259000	-0.678082000	C	-3.290107000	0.622442000	1.452351000
C	5.214833000	-1.084945000	-0.159457000	C	-3.117762000	-1.614872000	0.425306000
C	5.469295000	-2.311512000	-0.776681000	C	-4.197319000	-2.358063000	1.230194000
C	4.763906000	-2.674422000	-1.924477000	C	-3.670842000	-2.931383000	2.548151000
H	3.248299000	-2.088824000	-3.343818000	C	-3.040881000	-1.812160000	3.382753000
H	2.789442000	0.075668000	-2.244241000	C	-1.943835000	-1.109882000	2.583373000
H	5.767684000	-0.800098000	0.731286000	H	3.530289000	-3.547454000	1.683862000
H	6.216920000	-2.979498000	-0.361241000	H	1.273840000	0.047206000	2.361615000
H	4.962833000	-3.625490000	-2.407671000	H	4.437541000	-1.204802000	3.062562000
C	3.994129000	1.104994000	0.006086000	H	3.426550000	-2.237686000	4.075250000
H	1.284680000	1.091936000	-0.885726000	H	3.046326000	-0.511732000	3.913021000
H	4.541774000	1.172918000	0.960222000	H	1.293986000	-5.030196000	-0.433766000
C	4.572523000	2.302713000	-0.886558000	H	3.041775000	-4.914921000	-0.177814000
H	4.000532000	2.323402000	-1.815372000	H	2.306550000	-4.149482000	-1.587036000
H	5.599040000	2.004767000	-1.111850000	H	0.668829000	-1.702251000	-2.099468000
C	4.557365000	3.657283000	-0.180594000	H	0.056979000	-3.292080000	-1.644945000
H	5.202363000	3.650729000	0.699914000	H	-1.375896000	-2.861267000	0.588313000
H	4.953703000	4.404961000	-0.878404000	H	-1.706669000	-4.395690000	-1.174687000
C	3.182806000	4.111123000	0.260443000	H	-3.210961000	-4.304758000	-0.307277000
O	2.280162000	4.072284000	-0.735295000	H	-3.547828000	-4.288175000	-2.803129000
H	1.379356000	4.143467000	-0.347003000	H	-4.166499000	-2.805405000	-2.090570000
O	2.913209000	4.478764000	1.385721000	H	-2.803496000	-2.205137000	-4.070173000
⁵ IM _{OH}				H	-1.447678000	-3.152892000	-3.475500000
Mn	-0.674905000	0.236895000	0.044616000	H	-1.111085000	-0.717242000	-2.974126000
N	0.768729000	-1.091533000	0.715650000	H	-2.685440000	-0.666553000	-2.188189000
N	-1.170792000	-1.636383000	-1.095068000	H	-5.207751000	3.553364000	-1.665883000
N	-2.260272000	1.367509000	-0.611112000	H	-1.247837000	1.997209000	-2.291397000
N	-2.423934000	-0.571432000	1.270904000	H	-3.280582000	4.740230000	-3.264762000
C	0.988384000	-2.176719000	-0.056697000	H	-3.896956000	3.352098000	-4.163542000
C	1.968162000	-3.116700000	0.282418000	H	-2.151204000	3.543284000	-3.924811000
C	2.747254000	-2.848042000	1.408493000	H	-6.150394000	1.287025000	0.793905000
C	2.546440000	-1.703034000	2.187335000	H	-6.419644000	2.952591000	0.264072000
C	1.518785000	-0.847970000	1.805478000	H	-5.439461000	2.626695000	1.700378000
C	3.406700000	-1.393557000	3.379905000	H	-2.849858000	1.239500000	2.241069000
C	2.163537000	-4.370693000	-0.527585000	H	-4.288495000	0.335655000	1.784731000
C	0.163113000	-2.261613000	-1.307659000	H	-3.620125000	-1.064437000	-0.371653000
C	-2.035829000	-2.505229000	-0.203852000	H	-5.009288000	-1.655218000	1.442412000
C	-2.554769000	-3.735488000	-0.968347000	H	-4.639534000	-3.130888000	0.598610000

H	-4.491182000	-3.402880000	3.096222000	C	2.388377000	-1.050954000	3.180979000
H	-2.927136000	-3.715362000	2.357497000	C	1.420967000	-0.287192000	2.536851000
H	-2.588687000	-2.206540000	4.297436000	C	2.877114000	-0.686261000	4.554286000
H	-3.808155000	-1.093337000	3.691806000	C	2.936571000	-3.724746000	0.497679000
H	-1.506247000	-0.271377000	3.126888000	C	0.836125000	-1.936950000	-0.702105000
H	-1.140892000	-1.818138000	2.375578000	C	-1.467392000	-2.370614000	0.084933000
O	0.411094000	0.807079000	-1.247390000	C	-1.727565000	-3.691794000	-0.660238000
O	-0.310608000	1.427991000	1.436511000	C	-2.238002000	-3.491065000	-2.089017000
C	-0.077138000	2.741869000	1.430102000	C	-1.263355000	-2.605201000	-2.869909000
O	-0.114340000	3.425754000	0.418825000	C	-1.060124000	-1.278921000	-2.139255000
C	0.246107000	3.267160000	2.805276000	C	-3.271729000	1.364798000	0.024118000
H	0.153241000	4.352180000	2.816905000	C	-4.408046000	1.971236000	-0.523621000
H	-0.403642000	2.810256000	3.553902000	C	-4.266538000	2.596928000	-1.763818000
H	1.281364000	2.999680000	3.036668000	C	-3.042940000	2.621082000	-2.441058000
O	2.683001000	1.424867000	0.186382000	C	-1.964971000	2.001478000	-1.820191000
C	3.799491000	-1.812383000	-2.445843000	C	-2.886823000	3.287230000	-3.779859000
C	3.538385000	-0.590858000	-1.825782000	C	-5.730843000	1.947435000	0.195988000
C	4.245196000	-0.220547000	-0.676173000	C	-3.272307000	0.674570000	1.359012000
C	5.213895000	-1.082114000	-0.155381000	C	-2.718331000	-1.578966000	0.494409000
C	5.469844000	-2.309247000	-0.770906000	C	-3.823667000	-2.399851000	1.180628000
C	4.766333000	-2.673679000	-1.919345000	C	-3.446805000	-2.848640000	2.594358000
H	3.252463000	-2.090311000	-3.341467000	C	-3.070237000	-1.628867000	3.439982000
H	2.790552000	0.074889000	-2.244507000	C	-1.940198000	-0.849331000	2.766695000
H	5.765467000	-0.795959000	0.735735000	H	3.641051000	-2.784525000	2.961199000
H	6.217342000	-2.976332000	-0.353796000	H	0.989824000	0.598153000	2.986600000
H	4.966544000	-3.625064000	-2.401378000	H	3.943209000	-0.443488000	4.527016000
C	3.992279000	1.107660000	0.005691000	H	2.743163000	-1.525360000	5.243312000
H	1.284281000	1.090837000	-0.884622000	H	2.337783000	0.175722000	4.951716000
H	4.537478000	1.176753000	0.961127000	H	2.149825000	-4.476140000	0.371284000
C	4.573167000	2.304530000	-0.887358000	H	3.753262000	-4.182409000	1.057540000
H	4.002232000	2.324765000	-1.816830000	H	3.306408000	-3.461893000	-0.496566000
H	5.599585000	2.005138000	-1.111122000	H	1.395341000	-1.380010000	-1.455943000
C	4.558765000	3.659919000	-0.182771000	H	0.889516000	-2.990657000	-0.973870000
H	5.204202000	3.654162000	0.697412000	H	-0.900139000	-2.608300000	0.985497000
H	4.954889000	4.406673000	-0.881680000	H	-0.792309000	-4.259307000	-0.687391000
C	3.184518000	4.114518000	0.258602000	H	-2.415524000	-4.296065000	-0.065975000
O	2.281911000	4.077842000	-0.737258000	H	-2.347394000	-4.463401000	-2.576923000
H	1.381184000	4.147107000	-0.348325000	H	-3.232460000	-3.028156000	-2.080625000
O	2.915442000	4.481551000	1.384202000	H	-1.647152000	-2.376326000	-3.868311000
³ TS _{2CH}				H	-0.304702000	-3.116462000	-3.009901000
Mn	-0.468954000	0.515463000	0.344681000	H	-0.338040000	-0.638333000	-2.644310000
N	0.961842000	-0.612436000	1.314707000	H	-2.008242000	-0.744093000	-2.096919000
N	-0.573652000	-1.455721000	-0.732725000	H	-5.132927000	3.072440000	-2.214054000
N	-2.087122000	1.392413000	-0.626206000	H	-0.982163000	1.976171000	-2.272228000
N	-2.270525000	-0.425904000	1.368254000	H	-3.121845000	4.353594000	-3.707798000
C	1.428764000	-1.697773000	0.656358000	H	-3.573087000	2.847698000	-4.510001000
C	2.413903000	-2.514401000	1.223939000	H	-1.868198000	3.184214000	-4.158590000
C	2.881038000	-2.165879000	2.493495000	H	-6.094915000	0.922127000	0.319844000

H	-6.480232000	2.504301000	-0.368383000	N	0.683119000	1.769116000	0.046712000
H	-5.652827000	2.394682000	1.191359000	N	-0.293757000	-0.181733000	1.617077000
H	-2.991441000	1.386557000	2.140216000	N	-2.025452000	-1.187539000	-0.872487000
H	-4.265704000	0.296871000	1.602417000	N	-2.507449000	1.188270000	0.360721000
H	-3.150714000	-1.125991000	-0.398558000	C	1.419221000	1.510260000	1.151359000
H	-4.727455000	-1.784261000	1.227091000	C	2.394968000	2.410523000	1.588773000
H	-4.080627000	-3.245910000	0.540419000	C	2.573412000	3.575878000	0.837261000
H	-4.288027000	-3.382130000	3.045167000	C	1.809753000	3.843408000	-0.302587000
H	-2.606010000	-3.552927000	2.564365000	C	0.861322000	2.892882000	-0.665889000
H	-2.722308000	-1.926921000	4.433214000	C	2.016453000	5.080985000	-1.129491000
H	-3.944394000	-0.985443000	3.589275000	C	3.211687000	2.135902000	2.823437000
H	-1.676156000	0.055195000	3.316459000	C	1.129822000	0.203845000	1.832908000
H	-1.051135000	-1.478290000	2.721725000	C	-1.227873000	0.719006000	2.408267000
O	0.697381000	1.342984000	-0.791364000	C	-1.174853000	0.382531000	3.908109000
O	-0.459523000	1.861724000	1.649793000	C	-1.417922000	-1.099723000	4.199746000
C	-0.219509000	3.163319000	1.467797000	C	-0.419489000	-1.951279000	3.411893000
O	0.023070000	3.647695000	0.369291000	C	-0.510580000	-1.634133000	1.919345000
C	-0.261027000	3.950608000	2.747167000	C	-3.321693000	-0.805718000	-0.819856000
H	-0.264081000	5.017555000	2.526790000	C	-4.348707000	-1.724220000	-1.067114000
H	-1.135822000	3.675003000	3.339507000	C	-3.978848000	-3.037708000	-1.363796000
H	0.632913000	3.700336000	3.327251000	C	-2.637917000	-3.432680000	-1.416907000
O	2.708603000	2.452835000	-2.651316000	C	-1.682258000	-2.455958000	-1.165558000
C	1.950306000	-1.375628000	-4.242073000	C	-2.234967000	-4.846411000	-1.731881000
C	2.074516000	-0.137718000	-3.614086000	C	-5.795906000	-1.310183000	-1.015848000
C	3.048257000	0.070267000	-2.623274000	C	-3.576027000	0.645370000	-0.516537000
C	3.898001000	-0.990879000	-2.276775000	C	-2.620774000	0.643155000	1.762923000
C	3.775532000	-2.229758000	-2.911341000	C	-3.755314000	1.331144000	2.541887000
C	2.796828000	-2.430372000	-3.886581000	C	-3.667222000	2.858591000	2.507599000
H	1.191761000	-1.519602000	-5.004899000	C	-3.629349000	3.340536000	1.054688000
H	1.423804000	0.686354000	-3.885968000	C	-2.464147000	2.682792000	0.314677000
H	4.670068000	-0.861803000	-1.527836000	H	3.325733000	4.292447000	1.153227000
H	4.452836000	-3.035620000	-2.646882000	H	0.230329000	3.009594000	-1.537790000
H	2.698241000	-3.396664000	-4.370072000	H	2.967300000	5.018390000	-1.668785000
C	3.109154000	1.427562000	-1.940717000	H	2.051961000	5.971698000	-0.496361000
H	0.655804000	2.317043000	-0.574474000	H	1.218048000	5.206625000	-1.863442000
H	2.069988000	1.300704000	-1.227424000	H	2.580816000	2.138189000	3.718945000
C	4.303789000	1.699142000	-1.001161000	H	3.980017000	2.899880000	2.950500000
H	4.360656000	2.782795000	-0.884099000	H	3.703103000	1.161255000	2.767835000
H	5.209324000	1.391249000	-1.535208000	H	1.755180000	-0.582746000	1.405635000
C	4.307391000	1.034055000	0.385924000	H	1.360007000	0.253264000	2.897108000
H	3.808413000	0.058349000	0.374889000	H	-0.840061000	1.730408000	2.283172000
H	5.328690000	0.840535000	0.720608000	H	-0.191402000	0.671958000	4.291146000
C	3.613338000	1.867573000	1.436167000	H	-1.888829000	1.022079000	4.430622000
O	4.142801000	1.686136000	2.663682000	H	-1.313458000	-1.283497000	5.272520000
H	3.651577000	2.236905000	3.295779000	H	-2.442420000	-1.383130000	3.928958000
O	2.680404000	2.615716000	1.236090000	H	-0.623366000	-3.019005000	3.533732000
⁵ TS2CH				H	0.599061000	-1.782369000	3.775531000
Mn	-0.606122000	0.273656000	-0.547532000	H	0.225910000	-2.191012000	1.341161000

H	-1.498903000	-1.907712000	1.552466000	H	5.016397000	0.721457000	-1.899621000
H	-4.756452000	-3.771265000	-1.554982000	C	3.136933000	0.716146000	-2.847226000
H	-0.622187000	-2.672119000	-1.187346000	O	2.984015000	2.056152000	-2.779076000
H	-2.628160000	-5.149698000	-2.706886000	H	2.400392000	2.334968000	-3.503666000
H	-2.639482000	-5.536110000	-0.984709000	O	2.599082000	0.045033000	-3.700437000
H	-1.148919000	-4.955444000	-1.748840000	³ PC			
H	-6.074036000	-0.966287000	-0.014035000	Mn	-0.648969000	0.326800000	0.600849000
H	-6.441058000	-2.151003000	-1.274807000	N	0.767937000	-0.559375000	1.760750000
H	-6.002531000	-0.495020000	-1.715679000	N	-0.460740000	-1.489984000	-0.397615000
H	-3.566588000	1.218148000	-1.448248000	N	-2.006367000	1.178608000	-0.619571000
H	-4.558579000	0.779693000	-0.062311000	N	-2.361985000	-0.500227000	1.407100000
H	-2.892582000	-0.407146000	1.652517000	C	1.427350000	-1.568981000	1.163323000
H	-4.706665000	1.015641000	2.101343000	C	2.494389000	-2.223907000	1.788586000
H	-3.766039000	0.947485000	3.563829000	C	2.866607000	-1.765569000	3.054254000
H	-4.526178000	3.286517000	3.031761000	C	2.195454000	-0.706020000	3.674017000
H	-2.770035000	3.204868000	3.035901000	C	1.136353000	-0.130772000	2.977680000
H	-3.491779000	4.424269000	0.999493000	C	2.600322000	-0.196628000	5.029926000
H	-4.577889000	3.113978000	0.554741000	C	3.202113000	-3.376615000	1.125161000
H	-2.428933000	2.966306000	-0.738223000	C	0.965385000	-1.888853000	-0.228865000
H	-1.527006000	3.001503000	0.772065000	C	-1.367490000	-2.463058000	0.337233000
O	0.802359000	-0.769877000	-1.177541000	C	-1.468964000	-3.815520000	-0.383072000
O	-1.022298000	1.123967000	-2.173354000	C	-1.826879000	-3.687133000	-1.865723000
C	-0.908733000	0.607582000	-3.400210000	C	-0.826122000	-2.759432000	-2.559776000
O	-0.442453000	-0.502942000	-3.611033000	C	-0.797183000	-1.403174000	-1.860270000
C	-1.402609000	1.539790000	-4.473878000	C	-3.258336000	1.191744000	-0.122530000
H	-1.331396000	1.055385000	-5.446883000	C	-4.309659000	1.811313000	-0.808501000
H	-2.436105000	1.829936000	-4.268335000	C	-4.004654000	2.413081000	-2.030918000
H	-0.795331000	2.449688000	-4.464753000	C	-2.706143000	2.399787000	-2.553626000
O	2.841643000	-3.280298000	-1.689209000	C	-1.728186000	1.765316000	-1.796499000
C	2.668039000	-3.354766000	2.518183000	C	-2.373650000	3.026539000	-3.880054000
C	2.584058000	-3.234548000	1.132604000	C	-5.705768000	1.829820000	-0.245531000
C	3.361528000	-2.288031000	0.447689000	C	-3.419491000	0.536289000	1.219976000
C	4.224356000	-1.460995000	1.181670000	C	-2.690841000	-1.727546000	0.576306000
C	4.307855000	-1.582991000	2.570965000	C	-3.825392000	-2.560773000	1.191337000
C	3.525796000	-2.522597000	3.244366000	C	-3.601692000	-2.895397000	2.667570000
H	2.062501000	-4.094015000	3.032452000	C	-3.372739000	-1.602993000	3.455513000
H	1.922843000	-3.879694000	0.563913000	C	-2.196569000	-0.830801000	2.863181000
H	4.845595000	-0.726522000	0.683677000	H	3.695677000	-2.245429000	3.566078000
H	4.991902000	-0.947276000	3.124177000	H	0.564479000	0.694370000	3.383086000
H	3.587527000	-2.611041000	4.324047000	H	3.621074000	0.198203000	5.002781000
C	3.207769000	-2.170611000	-1.064272000	H	2.580825000	-1.002826000	5.769503000
H	0.640612000	-0.868258000	-2.149624000	H	1.934834000	0.599292000	5.370237000
H	2.180781000	-1.551748000	-1.125374000	H	2.523107000	-4.225435000	0.989792000
C	4.260512000	-1.313674000	-1.809667000	H	4.043958000	-3.710561000	1.733542000
H	4.252623000	-1.644650000	-2.849213000	H	3.586166000	-3.108432000	0.136303000
H	5.243930000	-1.561412000	-1.398435000	H	1.550716000	-1.325361000	-0.961849000
C	4.059744000	0.204826000	-1.764752000	H	1.104873000	-2.944900000	-0.460470000
H	3.673905000	0.556986000	-0.803406000	H	-0.890017000	-2.638795000	1.302120000

H	-0.507353000	-4.329996000	-0.287619000	H	0.621925000	2.169609000	-0.254012000
H	-2.186275000	-4.441124000	0.152191000	H	1.747250000	1.080577000	-0.030588000
H	-1.822709000	-4.676365000	-2.331490000	C	5.176596000	0.690036000	-1.542898000
H	-2.841433000	-3.286380000	-1.982401000	H	5.893856000	1.474507000	-1.293759000
H	-1.105391000	-2.586868000	-3.603078000	H	5.645800000	0.024367000	-2.270882000
H	0.171140000	-3.212165000	-2.573635000	C	4.858737000	-0.144760000	-0.275909000
H	-0.072848000	-0.724509000	-2.309275000	H	4.108675000	-0.904200000	-0.500556000
H	-1.779135000	-0.941205000	-1.948399000	H	5.767038000	-0.647143000	0.057821000
H	-4.797816000	2.902933000	-2.588341000	C	4.320926000	0.718378000	0.835926000
H	-0.700126000	1.706553000	-2.130340000	O	5.226136000	0.996855000	1.775828000
H	-2.895192000	3.979238000	-4.003011000	H	4.823741000	1.577285000	2.444900000
H	-2.683326000	2.372095000	-4.702183000	O	3.182423000	1.155836000	0.890829000
H	-1.300413000	3.205016000	-3.976961000	⁵ PC			
H	-6.098042000	0.813934000	-0.128232000	Mn	-0.893069000	0.130713000	-0.554366000
H	-6.378896000	2.377012000	-0.907432000	N	0.347856000	1.708199000	-0.161757000
H	-5.732308000	2.308275000	0.738508000	N	-0.730573000	-0.048014000	1.535711000
H	-3.295049000	1.283092000	2.008423000	N	-2.167346000	-1.465159000	-0.867450000
H	-4.414870000	0.105099000	1.330824000	N	-2.889844000	1.022913000	-0.026854000
H	-3.050832000	-1.345990000	-0.380405000	C	0.999802000	1.619534000	1.015639000
H	-4.758183000	-1.996645000	1.089656000	C	1.941023000	2.579353000	1.401806000
H	-3.963164000	-3.461240000	0.589111000	C	2.179654000	3.629169000	0.511638000
H	-4.468496000	-3.436976000	3.056239000	C	1.497151000	3.732182000	-0.705344000
H	-2.735254000	-3.558191000	2.785727000	C	0.572448000	2.736307000	-0.997093000
H	-3.138774000	-1.814560000	4.503089000	C	1.761286000	4.851580000	-1.672333000
H	-4.280850000	-0.989643000	3.451670000	C	2.656984000	2.487601000	2.723297000
H	-2.019790000	0.114509000	3.377366000	C	0.657196000	0.417957000	1.842368000
H	-1.292547000	-1.431461000	2.960145000	C	-1.759820000	0.902723000	2.143103000
O	0.840553000	1.198283000	-0.402110000	C	-1.808484000	0.770604000	3.672391000
O	-0.817235000	1.797750000	1.801639000	C	-2.025096000	-0.669952000	4.140419000
C	-0.563330000	3.056375000	1.550292000	C	-0.937862000	-1.571155000	3.549741000
O	-0.006144000	3.450340000	0.514776000	C	-0.919335000	-1.458380000	2.026117000
C	-1.013253000	4.009155000	2.626850000	C	-3.471747000	-1.156921000	-1.005338000
H	-0.666083000	5.019275000	2.413009000	C	-4.423150000	-2.150686000	-1.275336000
H	-2.106553000	3.998707000	2.677211000	C	-3.964388000	-3.462729000	-1.398331000
H	-0.637323000	3.675552000	3.597355000	C	-2.608540000	-3.782790000	-1.265370000
O	3.754420000	2.557344000	-1.924187000	C	-1.736928000	-2.733322000	-1.001827000
C	1.055038000	0.566120000	-4.432474000	C	-2.107538000	-5.194598000	-1.397301000
C	1.928577000	1.248882000	-3.592896000	C	-5.882929000	-1.814975000	-1.432997000
C	3.018904000	0.583244000	-3.005268000	C	-3.839677000	0.301987000	-0.897919000
C	3.202860000	-0.785443000	-3.261103000	C	-3.100566000	0.676626000	1.418639000
C	2.317527000	-1.472485000	-4.092456000	C	-4.310905000	1.410132000	2.019359000
C	1.250067000	-0.796759000	-4.685997000	C	-4.273036000	2.921735000	1.777978000
H	0.224542000	1.089609000	-4.894488000	C	-4.143096000	3.199654000	0.276871000
H	1.790679000	2.304314000	-3.388285000	C	-2.907291000	2.494834000	-0.280039000
H	4.037780000	-1.324187000	-2.828547000	H	2.909125000	4.388307000	0.778040000
H	2.468183000	-2.529569000	-4.283304000	H	-0.009273000	2.752934000	-1.908287000
H	0.569368000	-1.328740000	-5.342600000	H	2.755316000	4.738493000	-2.117241000
C	3.953780000	1.370274000	-2.147697000	H	1.734453000	5.819528000	-1.164416000

H	1.027008000	4.861382000	-2.480226000	O	0.862747000	-1.197194000	-0.935364000
H	1.955778000	2.601124000	3.556994000	O	-1.124704000	0.637270000	-2.381889000
H	3.408970000	3.273523000	2.805907000	C	-0.317642000	0.546318000	-3.402753000
H	3.157654000	1.523474000	2.843196000	O	0.832674000	0.088414000	-3.318420000
H	1.345640000	-0.398423000	1.614390000	C	-0.891730000	1.046736000	-4.701258000
H	0.766740000	0.626766000	2.906015000	H	-0.129150000	1.047338000	-5.478854000
H	-1.402490000	1.905623000	1.905824000	H	-1.719353000	0.393963000	-4.995544000
H	-0.871117000	1.152122000	4.089381000	H	-1.300055000	2.051360000	-4.565494000
H	-2.584516000	1.438765000	4.050137000	O	5.863621000	-2.493932000	-0.903387000
H	-2.001939000	-0.710274000	5.232688000	C	2.563409000	-3.167390000	1.641886000
H	-3.013828000	-1.030056000	3.831135000	C	3.461845000	-2.850309000	0.623636000
H	-1.113099000	-2.621823000	3.798753000	C	4.376771000	-1.797950000	0.788890000
H	0.037974000	-1.305970000	3.969412000	C	4.375990000	-1.063270000	1.981751000
H	-0.122920000	-2.058363000	1.584700000	C	3.501571000	-1.407246000	3.015610000
H	-1.863618000	-1.824159000	1.627708000	C	2.596799000	-2.457391000	2.848093000
H	-4.680510000	-4.253476000	-1.602930000	H	1.856886000	-3.980114000	1.506981000
H	-0.671186000	-2.886510000	-0.895151000	H	3.476265000	-3.418053000	-0.300577000
H	-2.369331000	-5.607738000	-2.376172000	H	5.083524000	-0.253581000	2.126554000
H	-2.562924000	-5.837631000	-0.637638000	H	3.529940000	-0.859235000	3.951680000
H	-1.022852000	-5.243312000	-1.282220000	H	1.923549000	-2.727901000	3.654331000
H	-6.289736000	-1.370157000	-0.518677000	C	5.389059000	-1.551284000	-0.288674000
H	-6.458702000	-2.714861000	-1.654937000	H	1.165626000	-0.914505000	-1.828240000
H	-6.042878000	-1.100277000	-2.246270000	H	1.634742000	-1.548268000	-0.468590000
H	-3.786798000	0.749925000	-1.895181000	C	5.854319000	-0.128127000	-0.562515000
H	-4.869754000	0.407804000	-0.551279000	H	6.531876000	-0.176140000	-1.417536000
H	-3.325683000	-0.391203000	1.442607000	H	6.440608000	0.217175000	0.297085000
H	-5.214054000	0.998734000	1.555871000	C	4.731361000	0.886284000	-0.823065000
H	-4.392269000	1.170708000	3.081617000	H	4.147277000	1.069564000	0.086405000
H	-5.181274000	3.381006000	2.178326000	H	5.144540000	1.851139000	-1.123748000
H	-3.428345000	3.375758000	2.312027000	C	3.742318000	0.402753000	-1.855606000
H	-4.045848000	4.271692000	0.080605000	O	3.116449000	1.388399000	-2.505246000
H	-5.043960000	2.859771000	-0.247388000	H	2.384134000	0.991813000	-3.031406000
H	-2.804856000	2.632337000	-1.358180000	O	3.489756000	-0.774372000	-2.045823000
H	-2.015653000	2.922709000	0.183723000				