

Electronic Supplementary Material (ESI) for

Theoretical Investigation of dioxygen activation and hydrocarbon oxidation catalysed by the bioinspired metal-organic frameworks

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Computational Methodology

Density functional theory (DFT) calculations were carried out using the Gaussian 16 suite of programs.^{S1} The spin-unrestricted B3LYP(BJ) functional^{S2-S5} corrected with Grimme 10's dispersion^{S6} using the Becke-Johnson damping scheme^{S7} was employed with two basis sets: (a) The def2-SVP basis set for all atoms. This basis set is denoted as B1 and was used to optimize transition states (TSs) and minima; (b) The def2-TZVPP basis set for all atoms, denoted as B2, which was used for single point energy (SPE) corrections. All calculations including optimization were performed in vacuum environment. The experimental reaction temperature of 298.15 K was adopted in the free energy calculations. The employed method has been extensively used in nonheme chemistry and proven to be reliable. Transition states were ascertained by vibrational frequency analysis to possess a single mode along the reaction coordinate with a sole imaginary frequency. The minimum energy crossing points (MECPs) were located by using the sobMECP program,^{S8} in which the methods developed by Harvey and Robb were employed. The energy values in the text are free energies calculated by the formula $G = G(\text{B1}) + \text{SPE}(\text{B2}) - \text{SPE}(\text{B1})$, in which B1 denotes the energy is calculated at the UB3LYP-D3(BJ)/def2-SVP level, B2 is the one at the UB3LYP-D3(BJ)/def2-TZVPP level.^{S9-S10} The images of optimized structure are drawn by the CYLview software.^{S11}

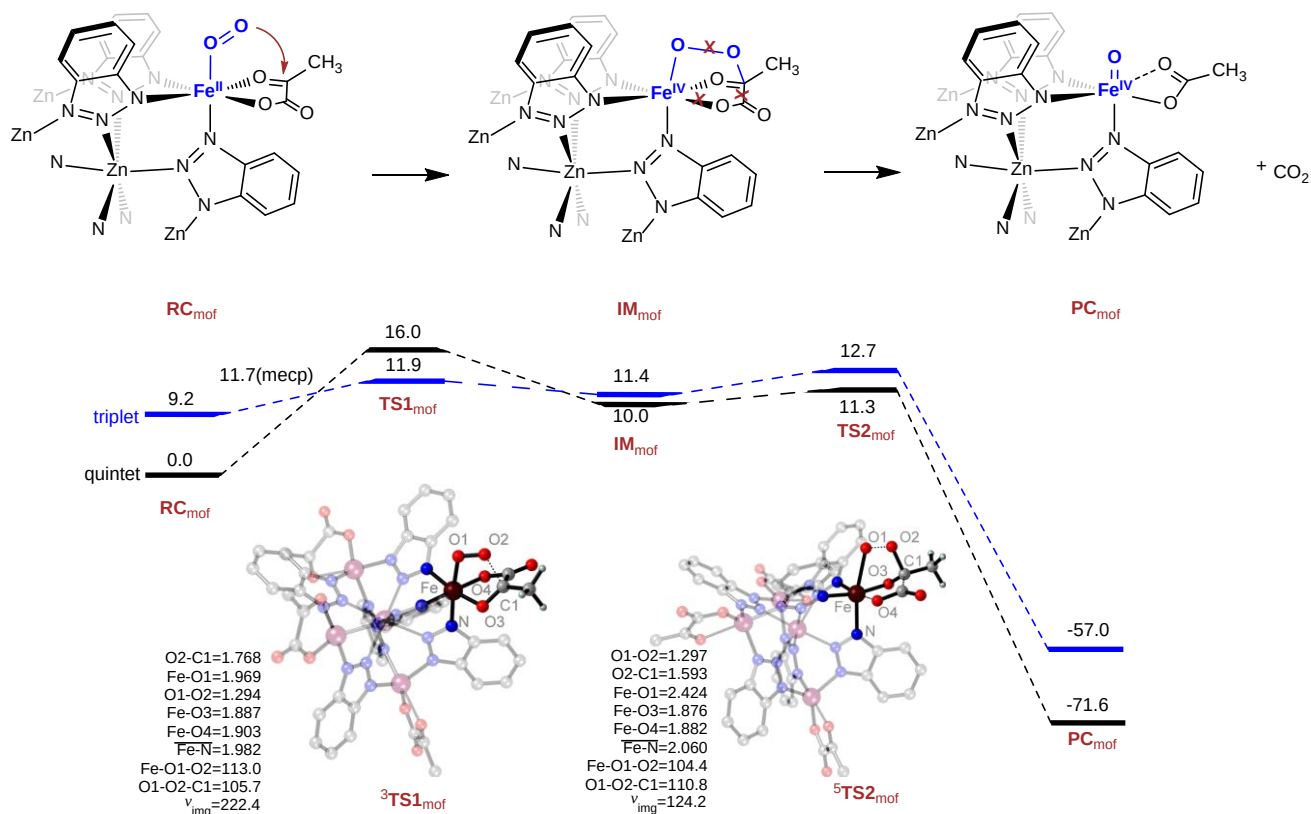
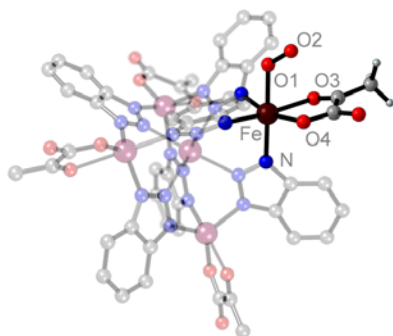


Figure S1. The energy profile (kcal mol⁻¹) for the O₂ activation by the model of the FeZn₄(prv)₄(btdd)₃ MOF. Values are Gibbs free energies calculated at the UB3LYP-D3(BJ)/B2 level. Hydrogen atoms of the supporting ligand are omitted for clarity. Lengths are in Å units, angles are in degree units and imaginary frequencies are in cm⁻¹ units.

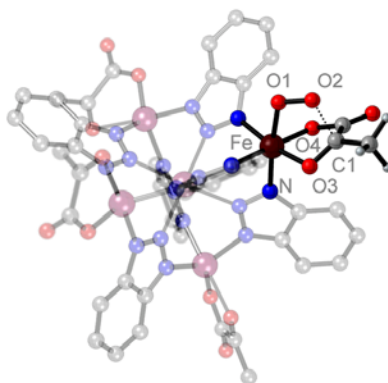
Table S1. Various SCF and Gibbs free energies of dioxygen activation by the FeZn₄(prv)₄(btdd)₃ MOF. Calculations were done at the UB3LYP-D3(BJ)/B2//B1 level in vacuum environment.

	OPT/B1+ZPE	ΔE	SPE/B2+ZPE	ΔE	G/B2	ΔG
³ RC _{mof}	-12266.881971 ^a	4.7	-12272.358650	5.3	-12272.480121	9.2
⁵ RC _{mof}	-12266.889468	0.0	-12272.367080	0.0	-12272.494807	0.0
³ TS1 _{mof}	-12266.879163	6.5	-12272.355943	7.0	-12272.475882	11.9
⁵ TS1 _{mof}	-12266.868675	13.0	-12272.346216	13.1	-12272.469361	16.0
³ IM _{mof}	-12266.880328	5.7	-12272.356408	6.7	-12272.476596	11.4
⁵ IM _{mof}	-12266.879044	6.5	-12272.356333	6.7	-12272.478831	10.0
³ TS2 _{mof}	-12266.879206	6.4	-12272.355228	7.4	-12272.474502	12.7
⁵ TS2 _{mof}	-12266.877915	7.2	-12272.355152	7.5	-12272.476793	11.3
³ PC _{mof}	-12266.980494	-57.1	-12272.461995	-59.6	-12272.585658	-57.0
⁵ PC _{mof}	-12266.996330	-67.1	-12272.480305	-71.0	-12272.608964	-71.6

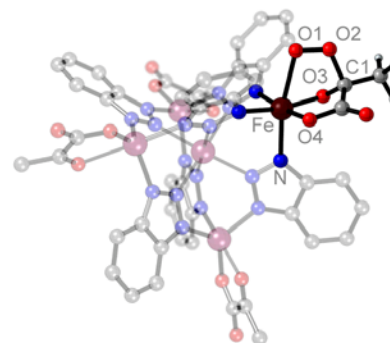
a. Absolute energies are in au units and the relative ones are in kcal mol⁻¹ units.

$^{3/5}\text{RC}_{\text{mof}}$ 

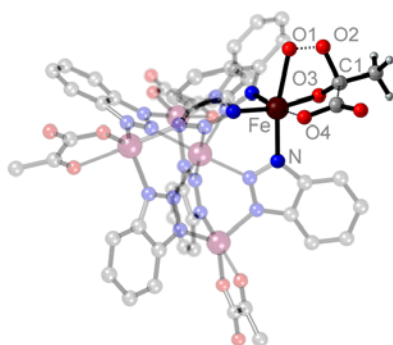
Fe-O1=1.959/2.070
 O1-O2=1.281/1.231
 O2-C1=2.279/3.116
 Fe-O3=1.954/2.274
 Fe-O4=1.877/1.969
 Fe-N=1.988/2.121
 Fe-O1-O2=117.2/125.6

 $^{3/5}\text{TS1}_{\text{mof}}$ 

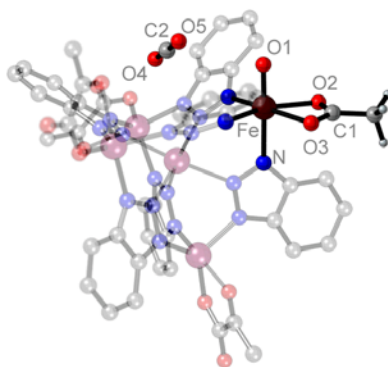
O2-C1=1.768/2.180
 Fe-O1=1.969/2.183
 O1-O2=1.294/1.270
 Fe-O3=1.887/2.109
 Fe-O4=1.903/1.881
 Fe-N=1.982/2.065
 Fe-O1-O2=113.0/116.0
 O1-O2-C1=105.7/102.8
 $\nu_{\text{img}}=i$ 222.4/61.81

 $^{3/5}\text{IM}_{\text{mof}}$ 

Fe-O1=1.852/2.424
 O1-O2=1.397/1.297
 O2-C1=1.413/1.593
 Fe-O3=1.895/1.876
 Fe-O4=1.961/1.882
 Fe-N=1.985/2.060
 Fe-O1-O2=109.4/104.4
 O1-O2-C1=109.8/110.8

 $^{3/5}\text{TS2}_{\text{mof}}$ 

O1-O2=1.397/1.297
 O2-C1=1.413/1.593
 Fe-O1=1.852/2.424
 Fe-O3=1.895/1.876
 Fe-O4=1.961/1.882
 Fe-N=1.985/2.060
 Fe-O1-O2=109.4/104.4
 O1-O2-C1=109.8/110.8
 $\nu_{\text{img}}=i$ 123.5/124.2

 $^{3/5}\text{PC}_{\text{mof}}$ 

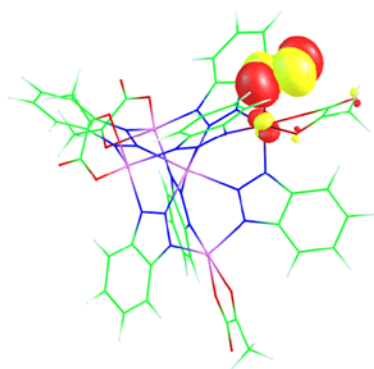
Fe-O1=1.608/1.611
 Fe-O2=3.175/2.087
 O1-O2=3.111/2.657
 O2-C1=1.228/1.278
 Fe-O3=1.918/2.239
 Fe-N=2.022/2.093
 Fe-O1-O2=77.4/51.8
 O1-O2-C1=77.9/94.0
 O4-C2-O5=172.4/179.6

Figure S2. Optimized structures of dioxygen activation by the $\text{FeZn}_4(\text{prv})_4(\text{btdd})_3$ MOF. Calculations were done at the UB3LYP-D3(BJ)/B1 level in vacuum environment. Hydrogen atoms of the L are omitted for clarity. Lengths are in Å units, angles are in degree units and imaginary frequencies are in cm^{-1} units.

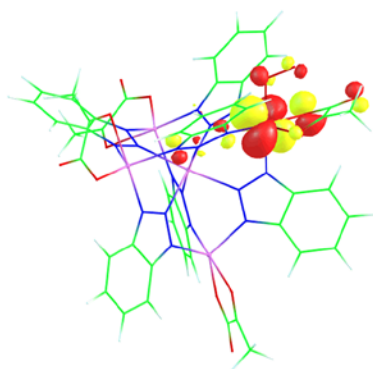
Table S2. Mulliken charges and spin densities of dioxygen activation by the FeZn₄(prv)₄(btdd)₃ MOF. Calculations were done at the UB3LYP-D3(BJ)/B1 level in vacuum environment.

spin							charge					
	Fe	O1	O2	L	prv		Fe	O1	O2	L	prv	
³ RC _{mof}	1.03	0.44	0.56	-0.02	-0.02		0.60	-0.15	-0.14	-0.32	0.01	
⁵ RC _{mof}	3.87	0.02	-0.14	0.12	0.13		0.85	-0.10	-0.03	-0.44	-0.29	
³ TS1 _{mof}	1.03	0.52	0.46	0.01	-0.01		0.59	-0.12	-0.12	-0.39	0.04	
⁵ TS1 _{mof}	2.90	0.53	0.56	-0.03	0.04		0.78	-0.16	-0.13	-0.39	-0.10	
³ IM _{mof}	0.97	0.21	0.21	0.63	-0.02		0.60	-0.23	-0.13	-0.25	0.01	
⁵ IM _{mof}	2.85	0.66	0.39	0.03	0.08		0.77	-0.14	-0.13	-0.42	-0.09	
³ TS2 _{mof}	0.97	0.21	0.21	0.63	-0.02		0.60	-0.23	-0.13	-0.25	0.01	
⁵ TS2 _{mof}	2.85	0.66	0.39	0.03	0.08		0.77	-0.14	-0.13	-0.42	-0.09	
	Fe	O1	O2	L	CO ₂	CH ₃ CO	Fe	O1	O2	L	CO ₂	CH ₃ CO
³ PC _{mof}	1.25	0.81	0.01	-0.05	0.00	-0.02	0.67	-0.33	-0.31	-0.01	0.06	-0.09
⁵ PC _{mof}	3.10	0.68	0.07	0.10	0.00	0.06	0.80	-0.33	-0.37	-0.15	0.01	0.05

$^3\text{RC}_{\text{mof}}$

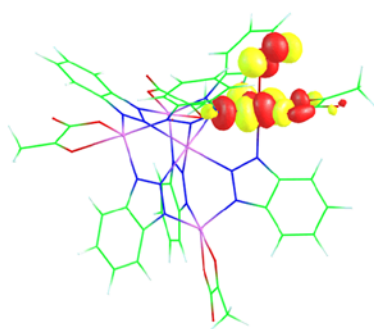


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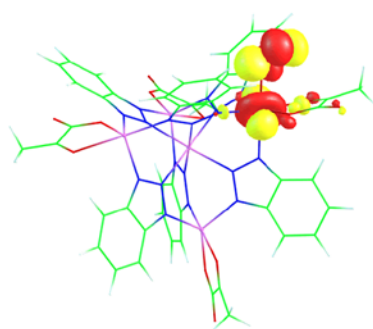


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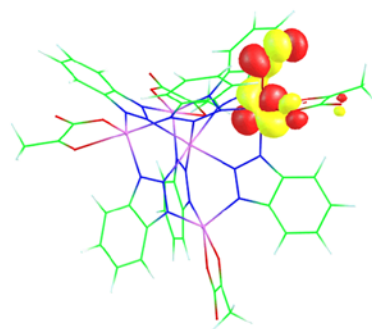
$^5\text{RC}_{\text{mof}}$



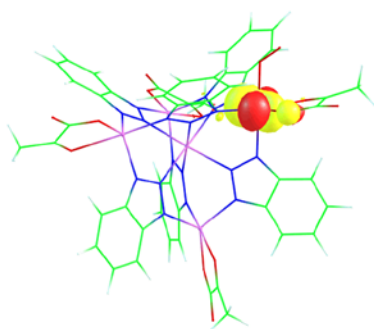
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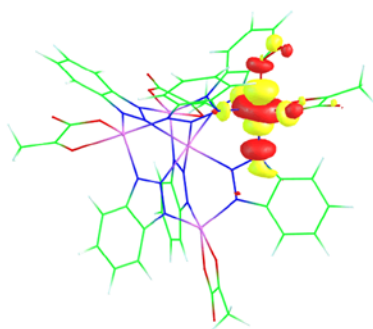
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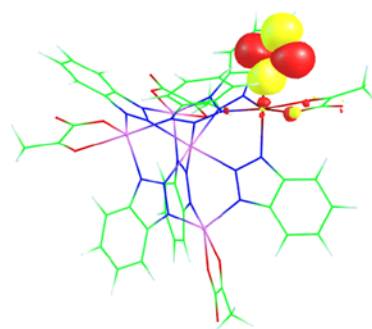
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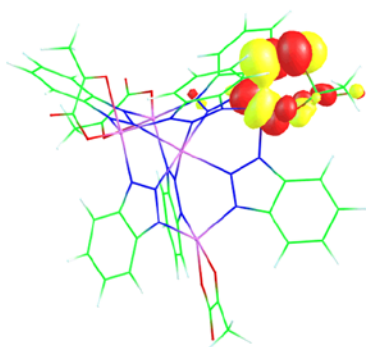
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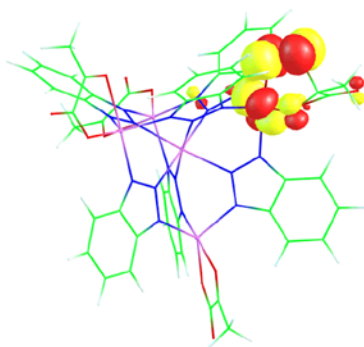
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Figure S3. Singly-occupied natural orbitals (SNOs) of dioxygen activation by the $\text{FeZn}_4(\text{prv})_4(\text{btdd})_3$ MOF. Calculations were done at the UB3LYP-D3(BJ)/B1 level in solvent. Positive values represent alpha-electron occupations. (To be continued)

$^3\text{TS1}_{\text{mof}}$

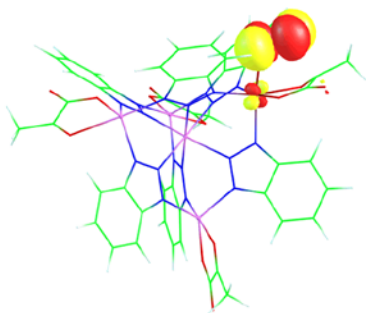


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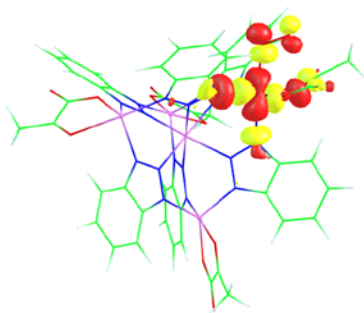


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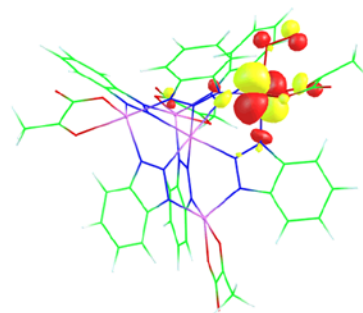
$^5\text{TS1}_{\text{mof}}$



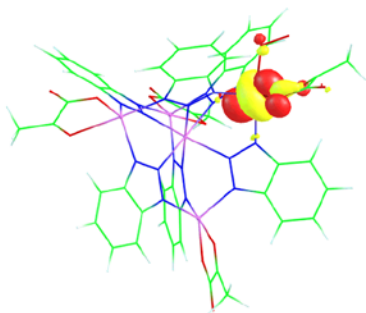
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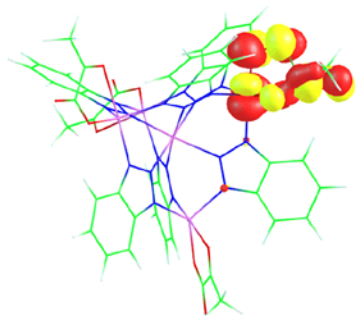
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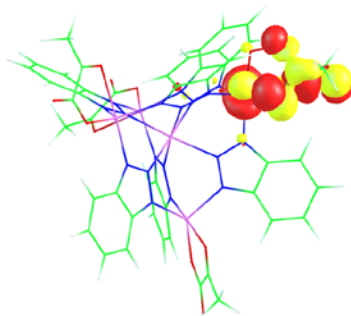
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Figure S3. Singly-occupied natural orbitals (SNOs) of dioxygen activation by the $\text{FeZn}_4(\text{prv})_4(\text{btdd})_3$ MOF. Calculations were done at the UB3LYP-D3(BJ)/B1 level in solvent. Positive values represent alpha-electron occupations. (To be continued)

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

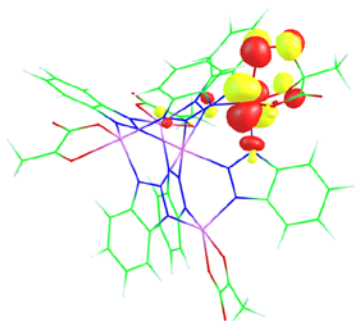


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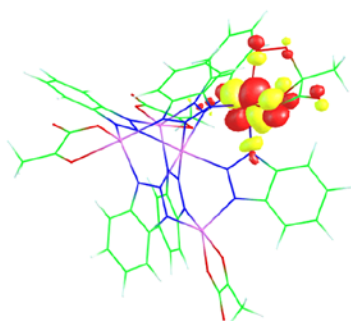


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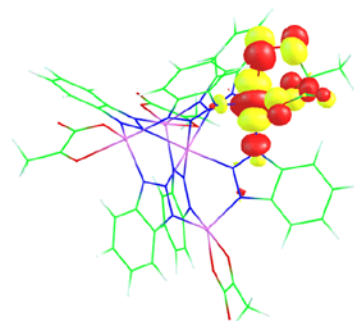
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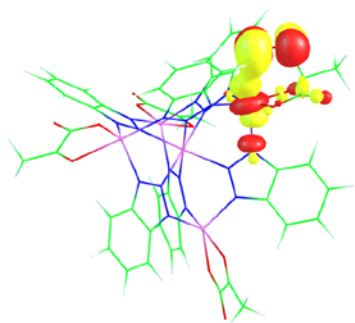
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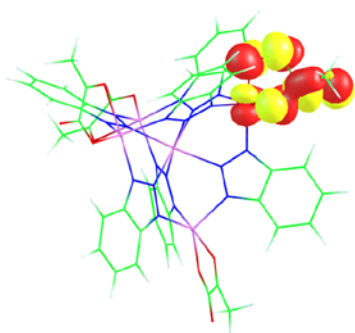
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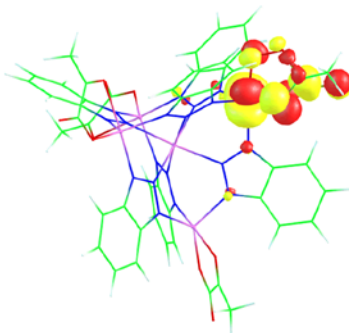
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Figure S3. Singly-occupied natural orbitals (SNOs) of dioxygen activation by the $\text{FeZn}_4(\text{prv})_4(\text{btdd})_3$ MOF. Calculations were done at the UB3LYP-D3(BJ)/B1 level in solvent. Positive values represent alpha-electron occupations. (To be continued)

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

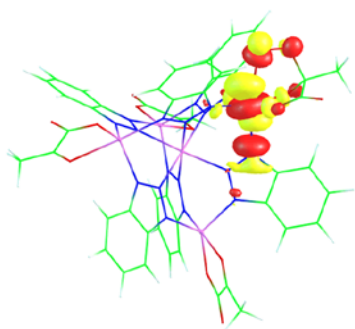


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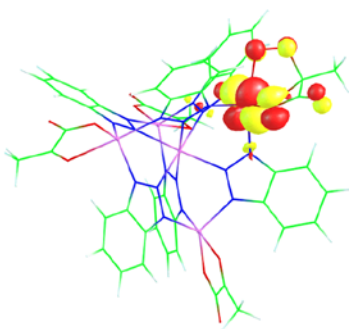


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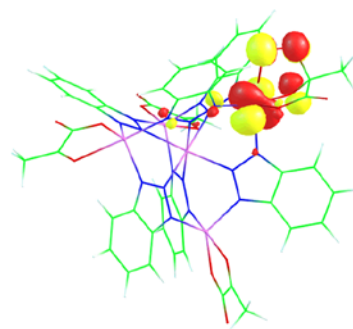
$^5\text{TS2}_{\text{mol}}$



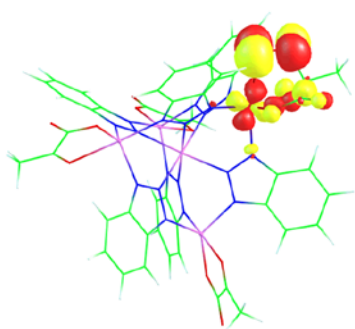
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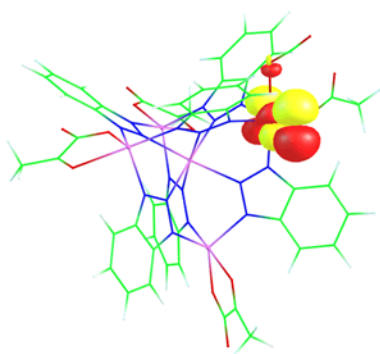
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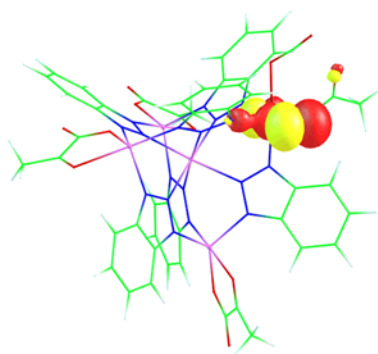
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Figure S3. Singly-occupied natural orbitals (SNOs) of dioxygen activation by the $\text{FeZn}_4(\text{prv})_4(\text{btdd})_3$ MOF. Calculations were done at the UB3LYP-D3(BJ)/B1 level in solvent. Positive values represent alpha-electron occupations. (To be continued)

$^3\text{PC}_{\text{mof}}$

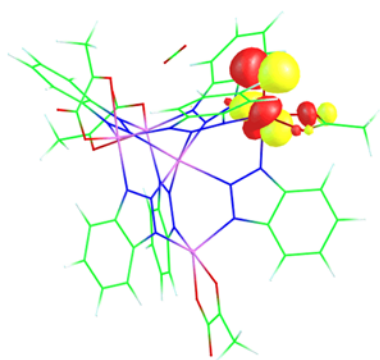


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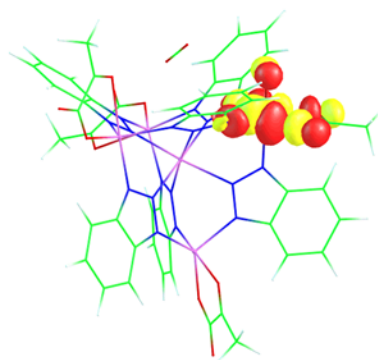


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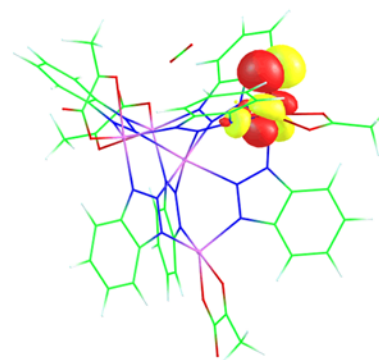
$^5\text{PC}_{\text{mof}}$



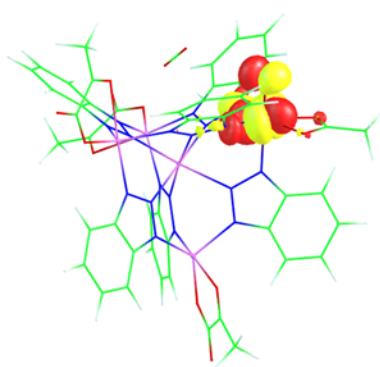
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Figure S3. Singly-occupied natural orbitals (SNOs) of dioxygen activation by the $\text{FeZn}_4(\text{prv})_4(\text{btdd})_3$ MOF. Calculations were done at the UB3LYP-D3(BJ)/B1 level in solvent. Positive values represent alpha-electron occupations.

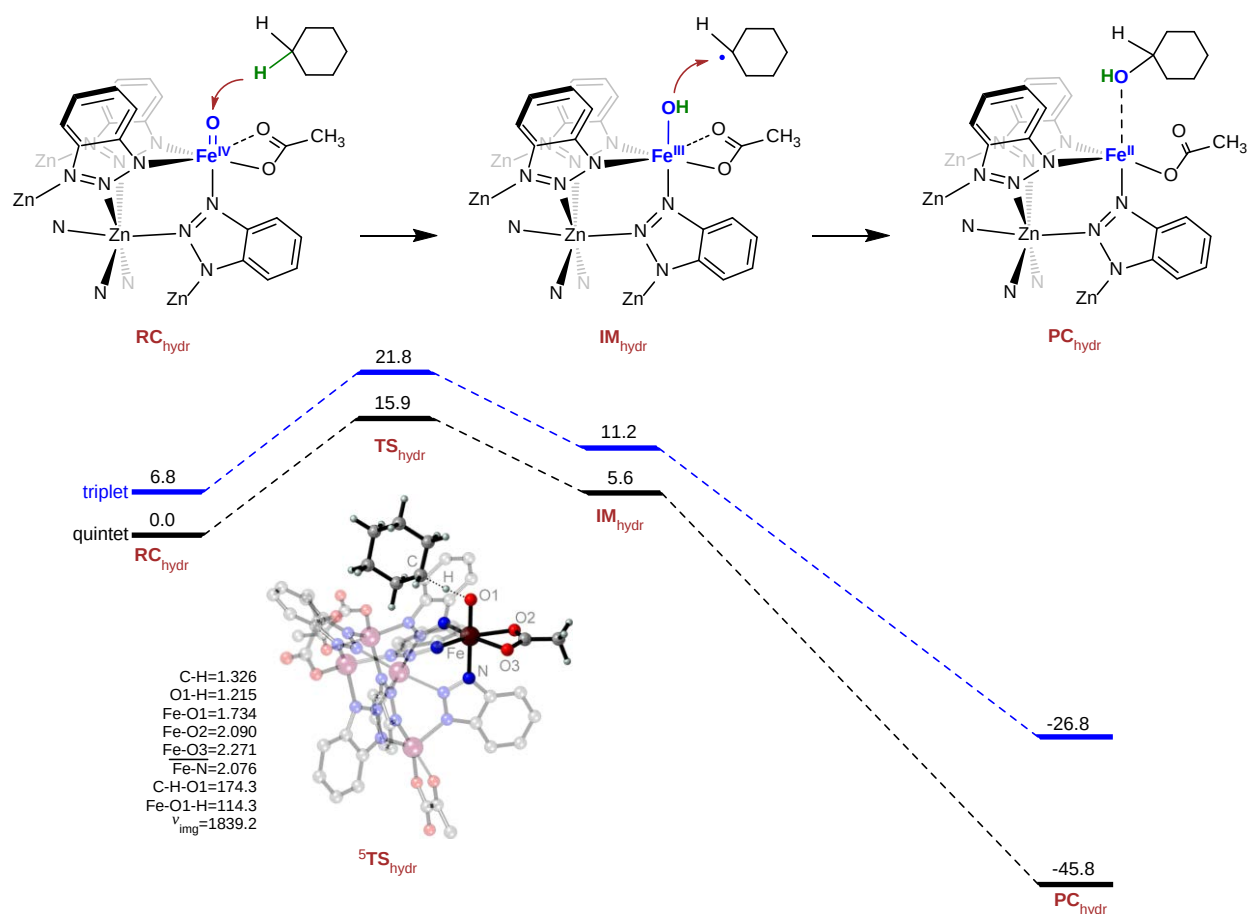
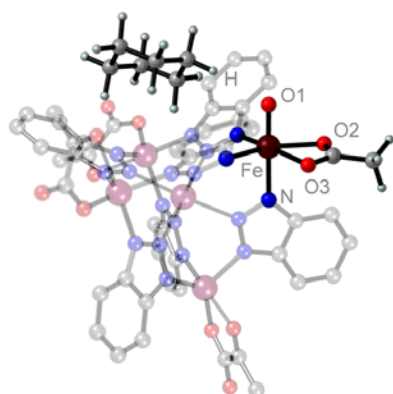


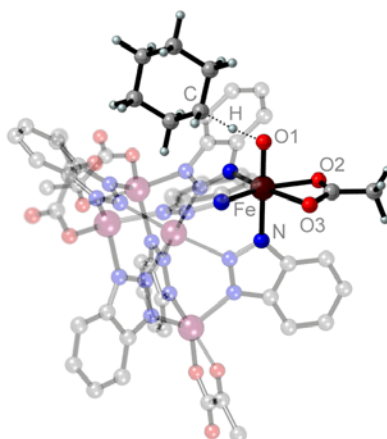
Figure S4. The energy profile (kcal mol⁻¹) for cyclohexane hydroxylation by the iron(IV)-oxo species of the FeZn₄(prv)₄(btdd)₃ MOF. Values are Gibbs free energies calculated at the UB3LYP-D3(BJ)/B2 level. Hydrogen atoms of the supporting ligand are omitted for clarity. Lengths are in Å units, angles are in degree units and imaginary frequencies are in cm⁻¹ units.

Table S3. Various SCF and Gibbs free energies of the intermediates of cyclohexane hydroxylation by the iron(IV)-oxo species of the FeZn₄(prv)₄(btdd)₃ MOF. Calculations were done at the UB3LYP-D3(BJ)/B2//B1 level in vacuum environment.

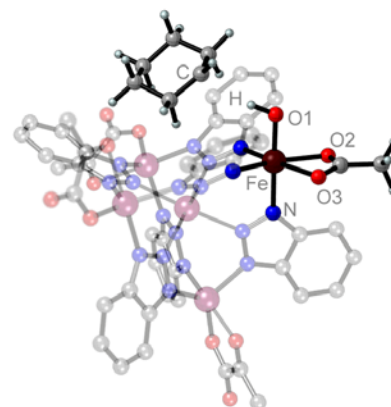
	OPT/B1+ZPE	ΔE	SPE/B2+ZPE	ΔE	G/B2	ΔG
³ RC _{hydr}	-12314.132590	4.9	-12319.647628	5.5	-12319.777453	6.8
⁵ RC _{hydr}	-12314.140457	0.0	-12319.656459	0.0	-12319.788260	0.0
³ TS _{hydr}	-12314.110858	18.6	-12319.624280	20.2	-12319.753545	21.8
⁵ TS _{hydr}	-12314.118119	14.0	-12319.632418	15.1	-12319.762968	15.9
³ IM _{hydr}	-12314.124741	9.9	-12319.640321	10.1	-12319.770395	11.2
⁵ IM _{hydr}	-12314.130882	6.0	-12319.647257	5.8	-12319.779265	5.6
³ PC _{hydr}	-12314.192021	-32.4	-12319.700930	-27.9	-12319.830983	-26.8
⁵ PC _{hydr}	-12314.222327	-51.4	-12319.730795	-46.6	-12319.861296	-45.8

$^{3/5}\text{RC}_{\text{hydr}}$ 

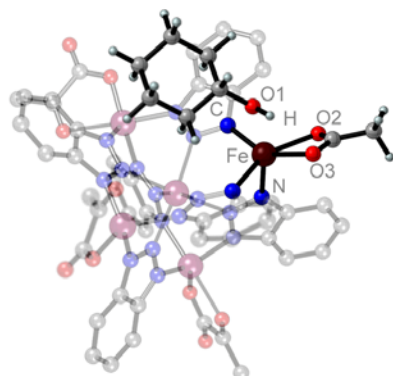
Fe-O1=1.604/1.612
 O1-H=2.677/3.070
 Fe-O2=2.248/2.089
 Fe-O3=2.046/2.233
 Fe-N=2.067/2.096

 $^{3/5}\text{TS}_{\text{hydr}}$ 

C-H=1.328/1.326
 O1-H=1.220/1.215
 Fe-O1=1.731/1.734
 Fe-O2=2.279/2.090
 Fe-O3=2.078/2.271
 Fe-N=2.045/2.076
 C-H-O1=173.2/174.3
 Fe-O1-H=113.7/114.3
 $\nu_{\text{img}}=i$ 1864.3/1839.2

 $^{3/5}\text{IM}_{\text{hydr}}$ 

Fe-O1=1.779/1.780
 C-H=2.165/2.156
 O1-H=0.979/0.979
 Fe-O2=2.311/2.051
 Fe-O3=2.063/2.306
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 $^{3/5}\text{PC}_{\text{hydr}}$ 

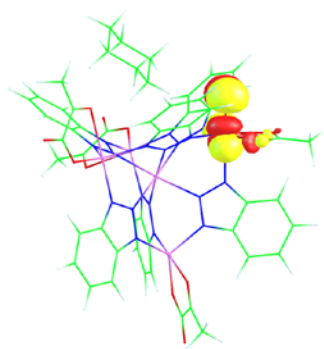
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 O1-C=1.457/1.445
 Fe-O2=2.287/2.195
 Fe-O3=2.008/2.233
 Fe-N=2.083/2.134
 Fe-O1-H=101.2/94.37
 C-O1-H=109.9/111.6

Figure S5. Optimized structures of the intermediates of cyclohexane hydroxylation by the iron(IV)-oxo species of the $\text{FeZn}_4(\text{prv})_4(\text{btdd})_3$ MOF. Calculations were done at the UB3LYP-D3(BJ)/B1 level in vacuum environment. Hydrogen atoms of the L are omitted for clarity. Lengths are in Å units, angles are in degree units and imaginary frequencies are in cm^{-1} units.

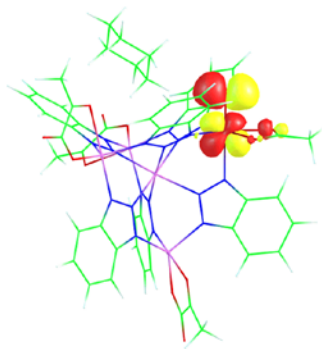
Table S4. Mulliken charges and spin densities of the intermediates of cyclohexane hydroxylation by the FeZn₄(prv)₄(btdd)₃ MOF. Calculations were done at the UB3LYP-D3(BJ)/B1 level in vacuum environment.

	spin						charge					
	Fe	O1	H	L	sub-H	Ac	Fe	O1	H	L	sub-H	Ac
³ RC _{hydr}	1.23	0.83	0.00	-0.05	0.00	-0.01	0.67	-0.31	0.02	-0.04	-0.06	-0.28
⁵ RC _{hydr}	3.09	0.68	0.00	0.09	0.00	0.13	0.80	-0.32	0.02	-0.12	-0.06	-0.31
³ TS _{hydr}	0.93	0.61	-0.04	-0.03	0.55	-0.02	0.66	-0.38	0.19	-0.14	0.00	-0.32
⁵ TS _{hydr}	2.88	0.49	-0.03	0.05	0.53	0.08	0.75	-0.39	0.19	-0.20	0.00	-0.36
³ IM _{hydr}	0.95	0.14	0.01	-0.03	0.96	-0.03	0.66	-0.39	0.19	-0.14	0.00	-0.32
⁵ IM _{hydr}	2.85	0.06	0.01	0.06	0.95	0.07	0.74	-0.39	0.20	-0.19	0.00	-0.35
³ PC _{hydr}	1.99	0.01	0.00	0.00	0.00	0.00	0.70	-0.32	0.21	-0.43	0.25	-0.41
⁵ PC _{hydr}	3.81	0.02	0.00	0.10	0.01	0.06	0.82	-0.33	0.20	-0.44	0.21	-0.46

$^3\text{RC}_{\text{hydr}}$

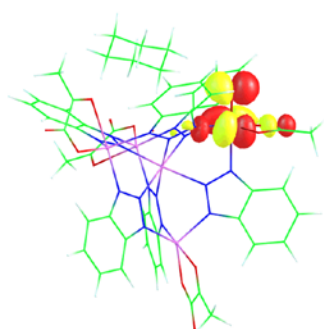


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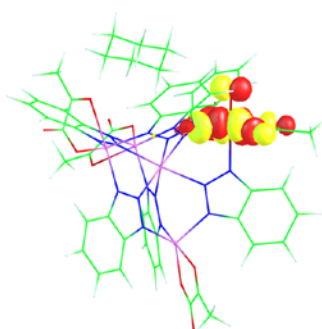


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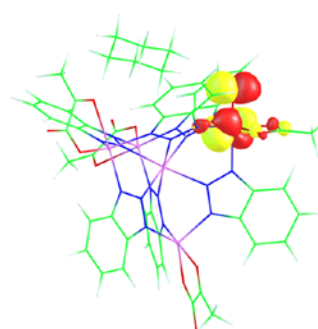
$^5\text{RC}_{\text{hydr}}$



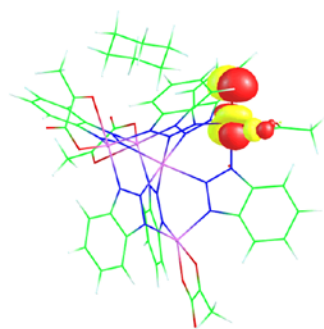
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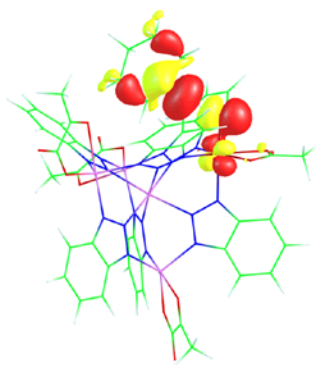
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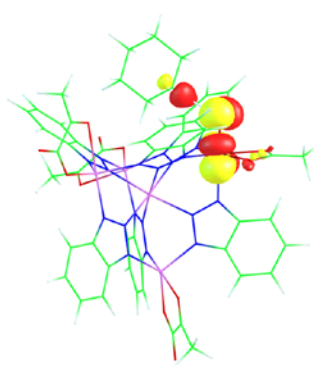
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Figure S6. Singly-occupied natural orbitals (SNOs) of the intermediates of cyclohexane hydroxylation by the $\text{FeZn}_4(\text{prv})_4(\text{btdd})_3$ MOF. Calculations were done at the UB3LYP-D3(BJ)/B1 level in solvent. Positive values represent alpha-electron occupations. (To be continued)

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

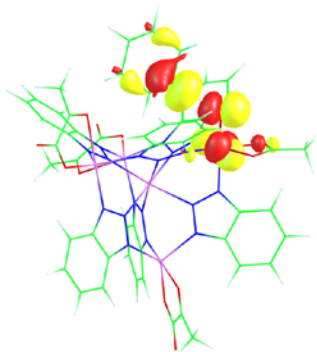


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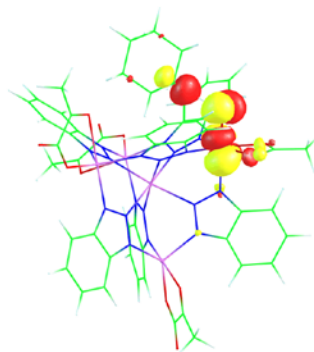


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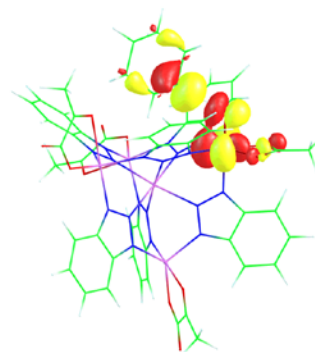
$^5\text{TS}_{\text{hydr}}$



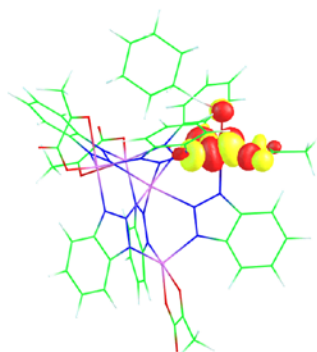
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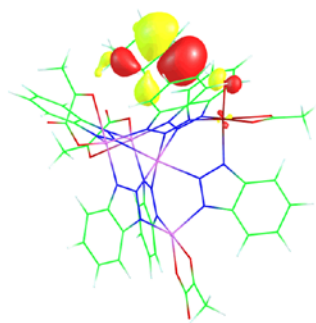
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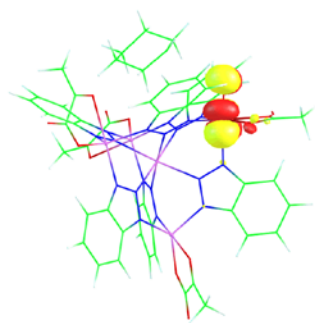
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Figure S6. Singly-occupied natural orbitals (SNOs) of the intermediates of cyclohexane hydroxylation by the $\text{FeZn}_4(\text{prv})_4(\text{btdd})_3$ MOF. Calculations were done at the UB3LYP-D3(BJ)/B1 level in solvent. Positive values represent alpha-electron occupations. (To be continued)

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

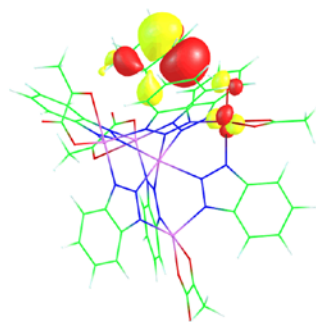


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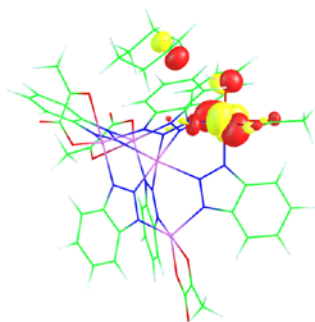


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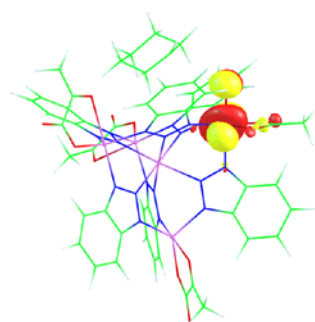
$^5\text{IM}_{\text{hydr}}$



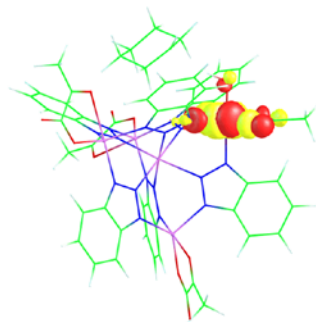
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Figure S6. Singly-occupied natural orbitals (SNOs) of the intermediates of cyclohexane hydroxylation by the $\text{FeZn}_4(\text{prv})_4(\text{btdd})_3$ MOF. Calculations were done at the UB3LYP-D3(BJ)/B1 level in solvent. Positive values represent alpha-electron occupations. (To be continued)

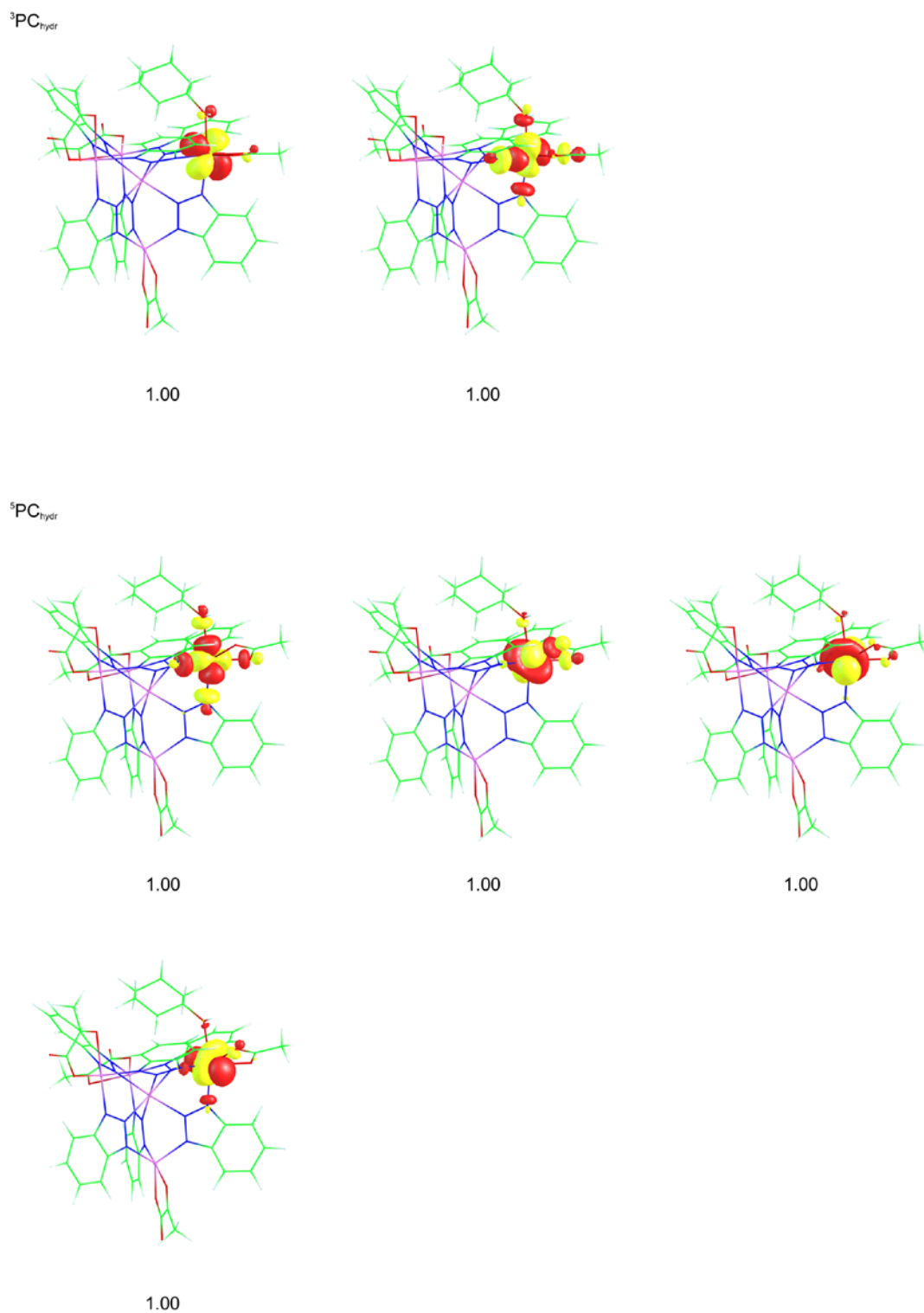


Figure S6. Singly-occupied natural orbitals (SNOs) of the intermediates of cyclohexane hydroxylation by the $\text{FeZn}_4(\text{prv})_4(\text{btdd})_3$ MOF. Calculations were done at the UB3LYP-D3(BJ)/B1 level in solvent. Positive values represent alpha-electron occupations.

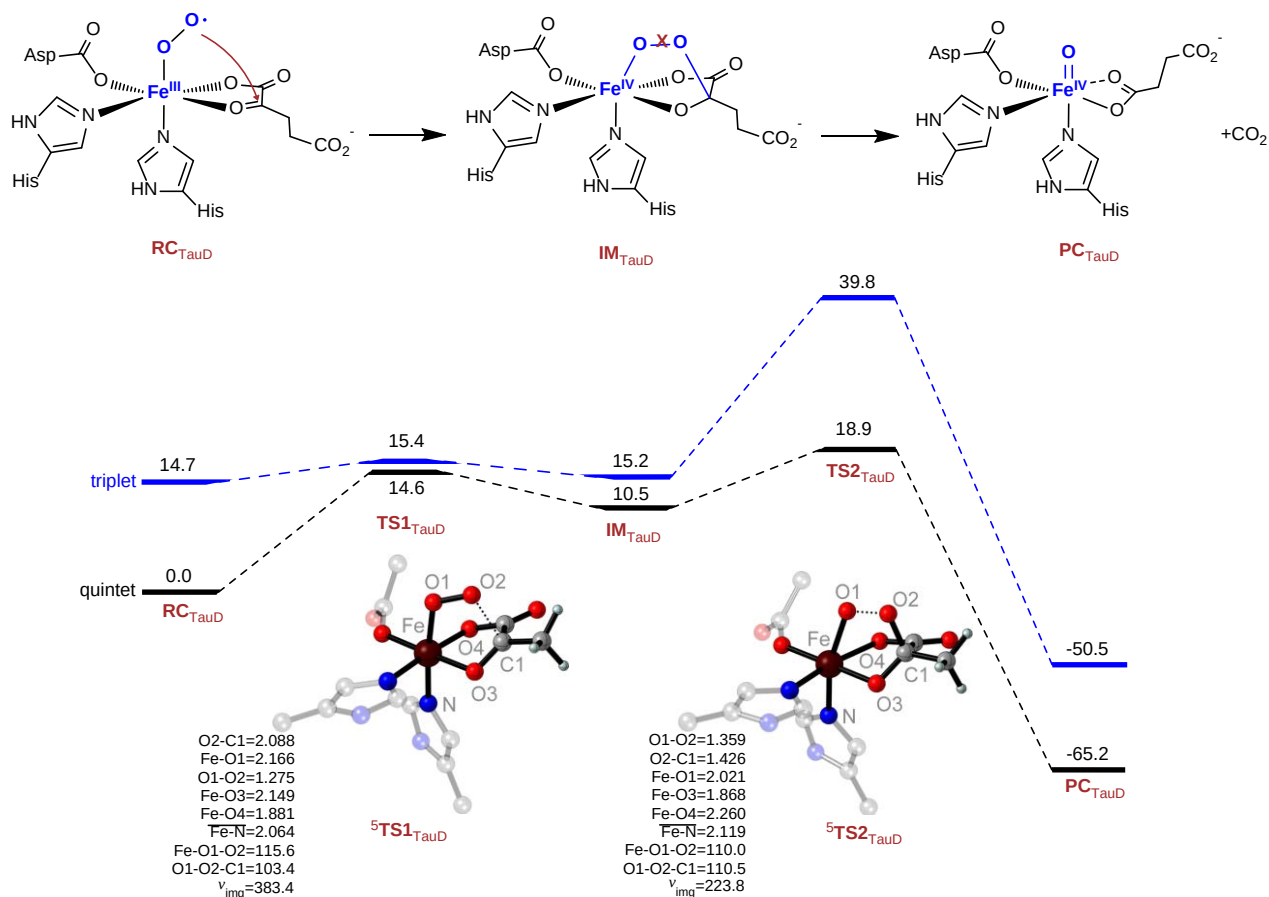
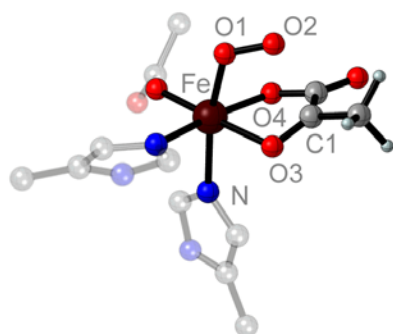


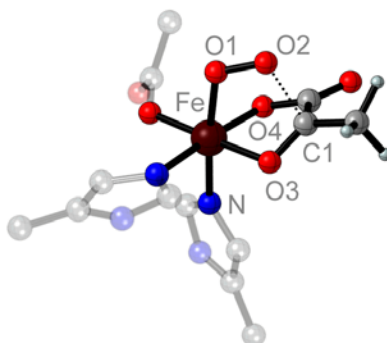
Figure S7. The energy profile (kcal mol⁻¹) for the O₂ activation by the model of the TauD oxygenase. Values are Gibbs free energies calculated at the UB3LYP-D3(BJ)/B2 level. Hydrogen atoms of the supporting ligand are omitted for clarity. Lengths are in Å units, angles are in degree units and imaginary frequencies are in cm⁻¹ units.

Table S5. Various SCF and Gibbs free energies of the intermediates of O₂ activation by the model of the TauD oxygenase. Calculations were done at the UB3LYP-D3(BJ)/B2//B1 level in vacuum environment.

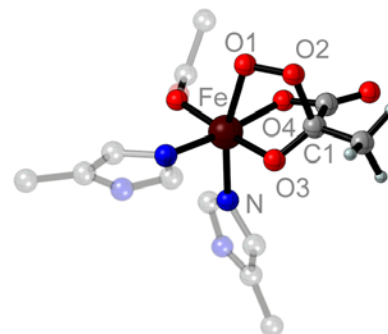
	OPT/B1+ZPE	ΔE	SPE/B2+ZPE	ΔE	G/B2	ΔG
³ RC _{TauD}	-2514.260629	11.4	-2515.860148	12.3	-2515.919325	14.7
⁵ RC _{TauD}	-2514.278811	0.0	-2515.879701	0.0	-2515.942722	0.0
³ TS1 _{TauD}	-2514.260644	11.4	-2515.860150	12.3	-2515.918258	15.4
⁵ TS1 _{TauD}	-2514.258313	12.9	-2515.858252	13.5	-2515.919421	14.6
³ IM _{TauD}	-2514.261488	10.9	-2515.860769	11.9	-2515.918558	15.2
⁵ IM _{TauD}	-2514.266262	7.9	-2515.865383	9.0	-2515.925992	10.5
³ TS2 _{TauD}	-2514.217976	38.2	-2515.821450	36.6	-2515.879334	39.8
⁵ TS2 _{TauD}	-2514.251863	16.9	-2515.852194	17.3	-2515.912650	18.9
³ PC _{TauD}	-2514.355714	-48.3	-2515.960393	-50.6	-2516.023141	-50.5
⁵ PC _{TauD}	-2514.374341	-59.9	-2515.981238	-63.7	-2516.046673	-65.2

^{3/5}RC_{TauD}

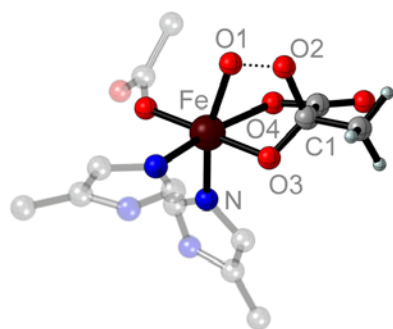
Fe-O1=1.970/2.129
 O1-O2=1.283/1.276
 O2-C1=2.018/2.131
 Fe-O3=1.936/2.144
 Fe-O4=1.917/1.959
 Fe-N=1.980/2.139
 Fe-O1-O2=115.7/116.6

^{3/5}TS1_{TauD}

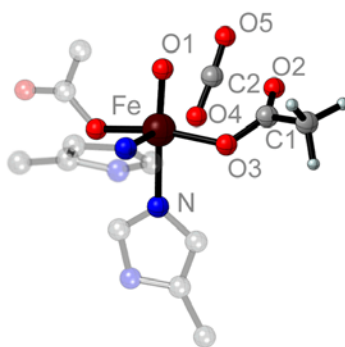
O2-C1=1.873/2.088
 Fe-O1=1.975/2.166
 O1-O2=1.288/1.275
 Fe-O3=1.919/2.149
 Fe-O4=1.917/1.881
 Fe-N=1.977/2.064
 Fe-O1-O2=114.2/115.6
 O1-O2-C1=104.3/103.4
 $\nu_{img=i}$ 158.3/383.4

^{3/5}IM_{TauD}

Fe-O1=1.927/2.442
 O1-O2=1.324/1.294
 O2-C1=1.537/1.599
 Fe-O3=1.873/1.900
 Fe-O4=1.927/1.891
 Fe-N=1.974/2.078
 Fe-O1-O2=110.6/105.0
 O1-O2-C1=108.6/110.1

^{3/5}TS2_{TauD}

O1-O2=2.069/1.359
 O2-C1=1.346/1.426
 Fe-O1=1.662/2.021
 Fe-O3=1.846/1.868
 Fe-O4=1.888/2.260
 Fe-N=2.034/2.119
 Fe-O1-O2=102.7/110.0
 O1-O2-C1=94.5/110.5
 $\nu_{img=i}$ 308.9/223.8

^{3/5}PC_{TauD}

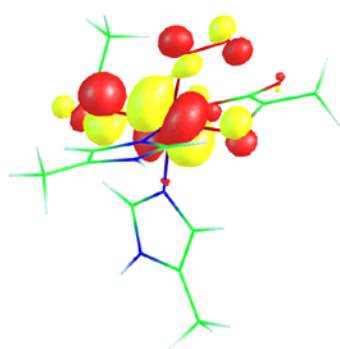
Fe-O1=1.606/1.619
 Fe-O2=3.204/3.278
 O1-O2=3.129/3.066
 O2-C1=1.223/1.218
 Fe-O3=1.949/1.925
 Fe-N=2.024/2.122
 Fe-O1-O2=77.9/82.6
 O1-O2-C1=78.1/76.7
 O4-C2-O5=172.1/174.1

Figure S8. Optimized structures of the intermediates of O₂ activation by the model of the TauD oxygenase. Calculations were done at the UB3LYP-D3(BJ)/B1 level in vacuum environment. Hydrogen atoms of the L are omitted for clarity. Lengths are in Å units, angles are in degree units and imaginary frequencies are in cm⁻¹ units.

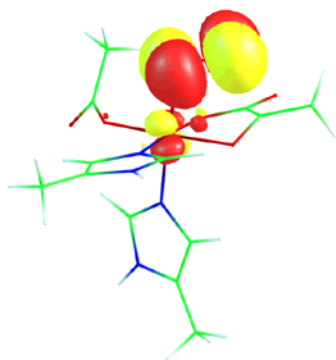
Table S6. Mulliken charges and spin densities of the intermediates of O₂ activation by the model of the TauD oxygenase. Calculations were done at the UB3LYP-D3(BJ)/B1 level in vacuum environment.

	spin					charge				
	Fe	O1	O2	prv	L	Fe	O1	O2	prv	L
³ RC _{TauD}	0.99	0.50	0.54	-0.05	0.03	0.60	-0.14	-0.14	-0.45	0.13
⁵ RC _{TauD}	4.19	-0.34	-0.51	0.31	0.36	0.92	-0.19	-0.14	-0.54	-0.05
³ TS1 _{TauD}	1.01	0.51	0.49	-0.04	0.02	0.60	-0.13	-0.13	-0.47	0.13
⁵ TS1 _{TauD}	2.87	0.49	0.52	-0.03	0.15	0.78	-0.17	-0.15	-0.48	0.01
³ IM _{TauD}	1.07	0.49	0.34	0.08	0.01	0.59	-0.13	-0.12	-0.48	0.14
⁵ IM _{TauD}	2.81	0.66	0.38	0.01	0.13	0.79	-0.14	-0.14	-0.52	0.01
³ TS2 _{TauD}	1.82	0.83	-0.60	-0.12	0.06	0.58	-0.22	-0.19	-0.41	0.24
⁵ TS2 _{TauD}	2.83	0.36	0.28	0.44	0.09	0.80	-0.24	-0.11	-0.47	0.01
³ PC _{TauD}	1.30	0.77	0.01	-0.02	-0.06	0.70	-0.35	-0.30	-0.11	0.06
⁵ PC _{TauD}	3.11	0.66	0.01	0.05	0.17	0.84	-0.37	-0.27	-0.17	-0.03

$^3\text{RC}_{\text{TauD}}$

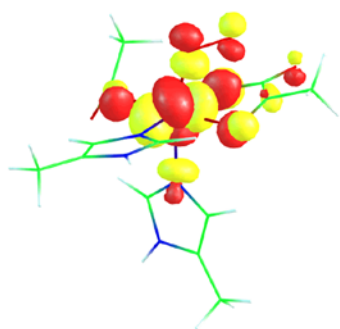


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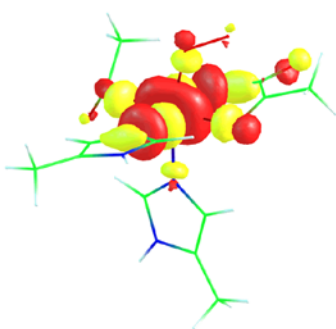


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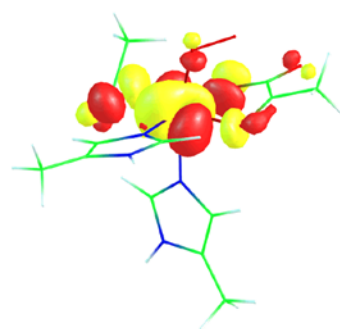
$^5\text{RC}_{\text{TauD}}$



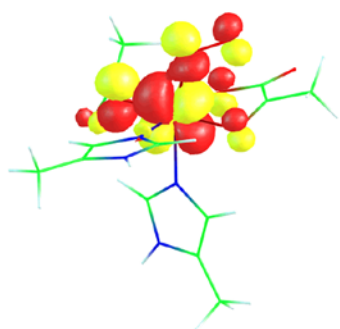
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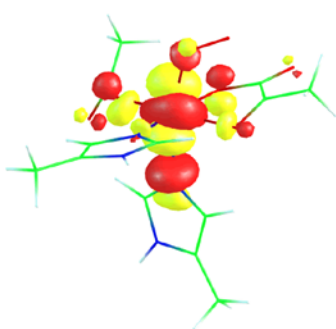
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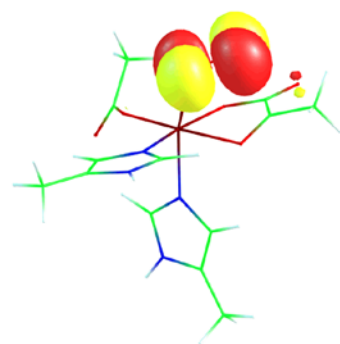
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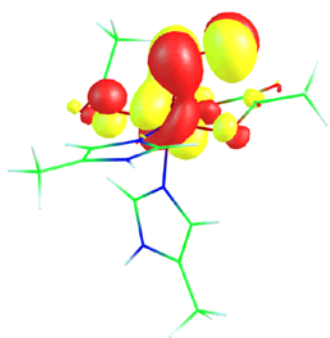
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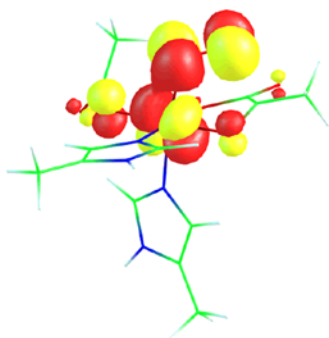
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Figure S9. Singly-occupied natural orbitals (SNOs) of the intermediates of O_2 activation by the model of the TauD oxygenase. Calculations were done at the UB3LYP-D3(BJ)/B1 level in solvent. Positive values represent alpha-electron occupations. (To be continued)

³TS1_{TauD}

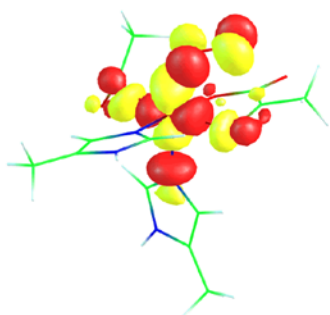


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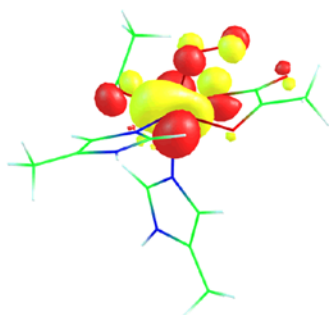


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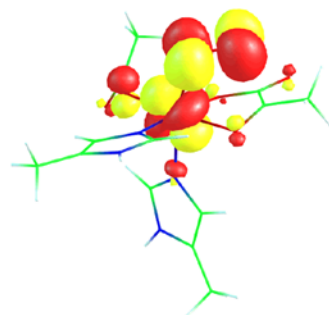
⁵TS1_{TauD}



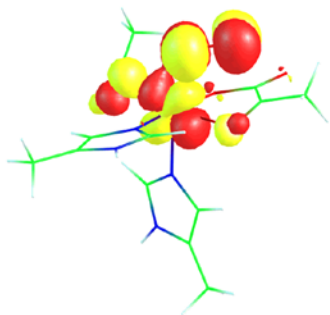
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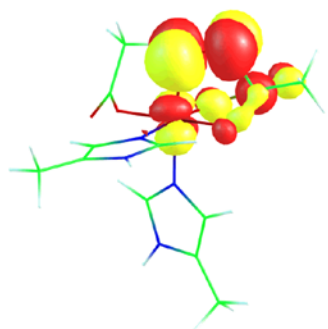
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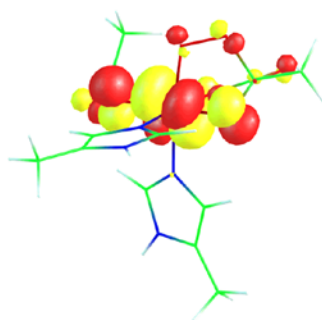
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Figure S9. Singly-occupied natural orbitals (SNOs) of the intermediates of O₂ activation by the model of the TauD oxygenase. Calculations were done at the UB3LYP-D3(BJ)/B1 level in solvent. Positive values represent alpha-electron occupations. (To be continued)

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

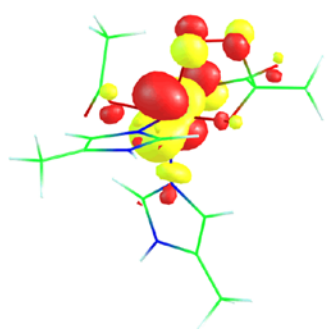


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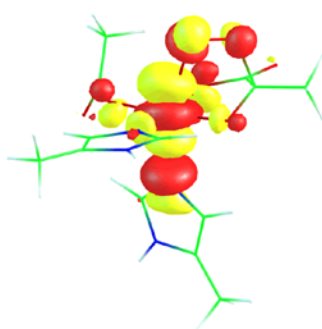


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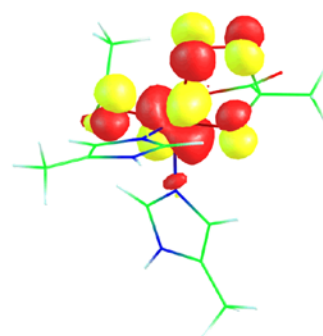
$^5\text{IM}_{\text{TauD}}$



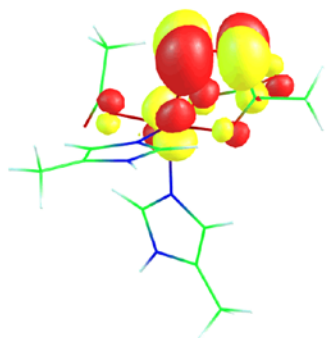
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Figure S9. Singly-occupied natural orbitals (SNOs) of the intermediates of O_2 activation by the model of the TauD oxygenase. Calculations were done at the UB3LYP-D3(BJ)/B1 level in solvent. Positive values represent alpha-electron occupations. (To be continued)

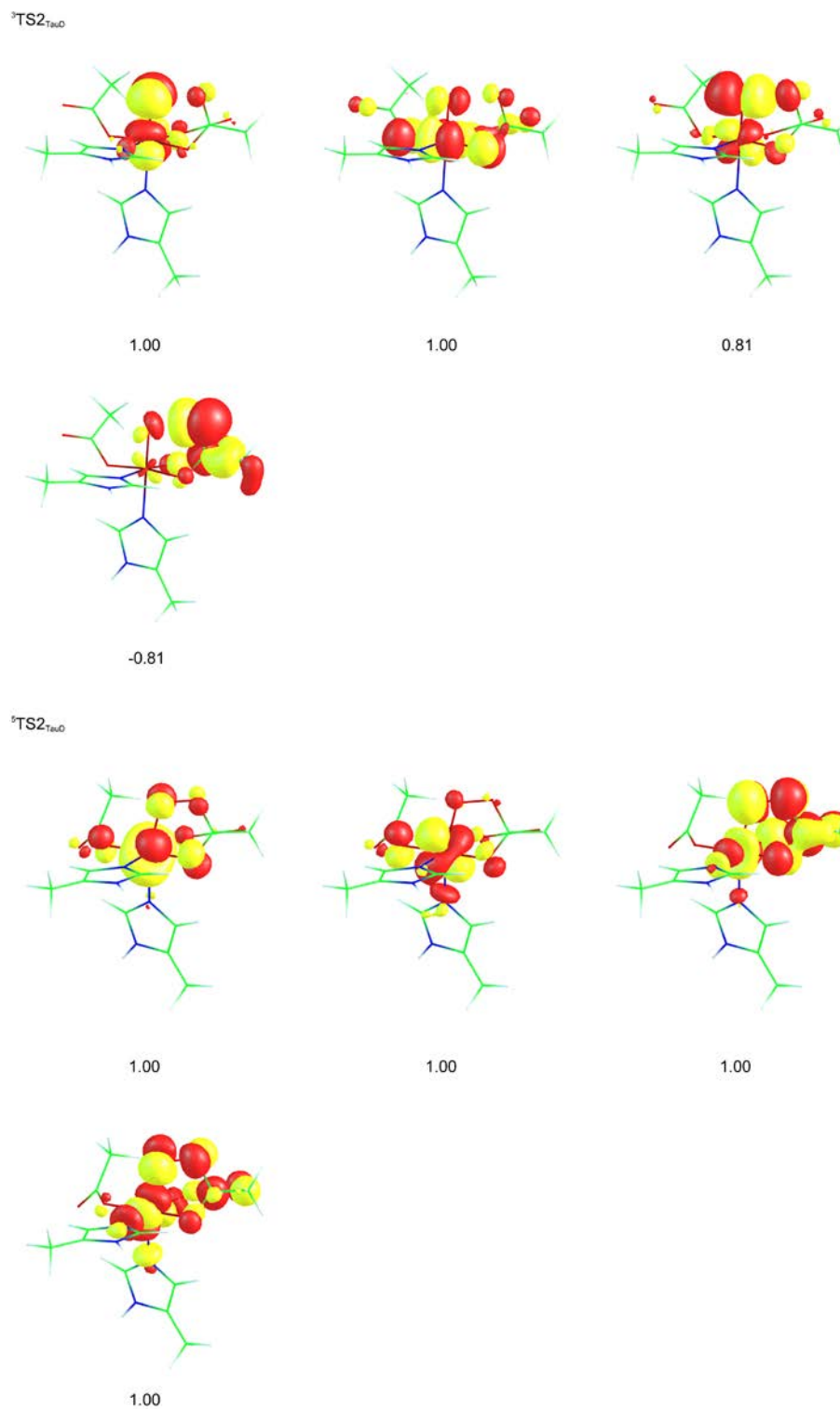
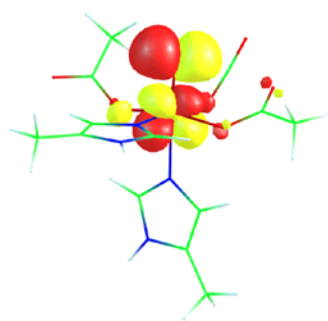
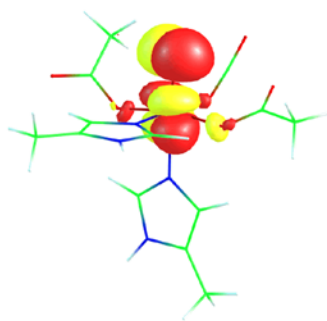


Figure S9. Singly-occupied natural orbitals (SNOs) of the intermediates of O₂ activation by the model of the TauD oxygenase. Calculations were done at the UB3LYP-D3(BJ)/B1 level in solvent. Positive values represent alpha-electron occupations. (To be continued)

$^3\text{PC}_{\text{TauD}}$

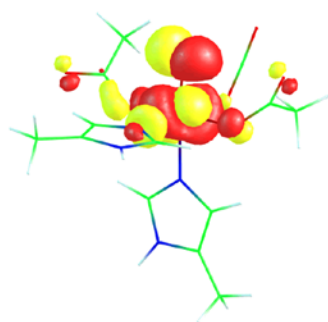


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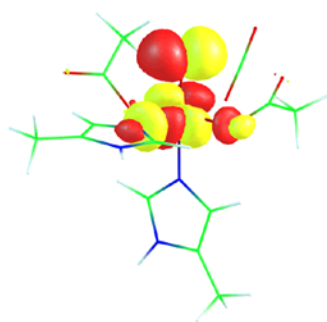


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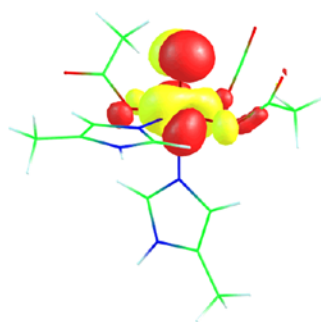
$^5\text{PC}_{\text{TauD}}$



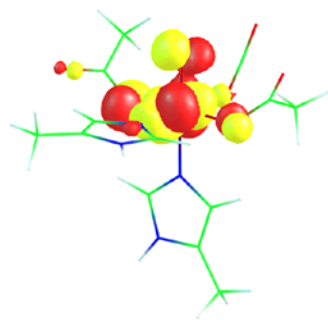
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1.00



1.00

Figure S9. Singly-occupied natural orbitals (SNOs) of the intermediates of O_2 activation by the model of the TauD oxygenase. Calculations were done at the UB3LYP-D3(BJ)/B1 level in solvent. Positive values represent alpha-electron occupations.

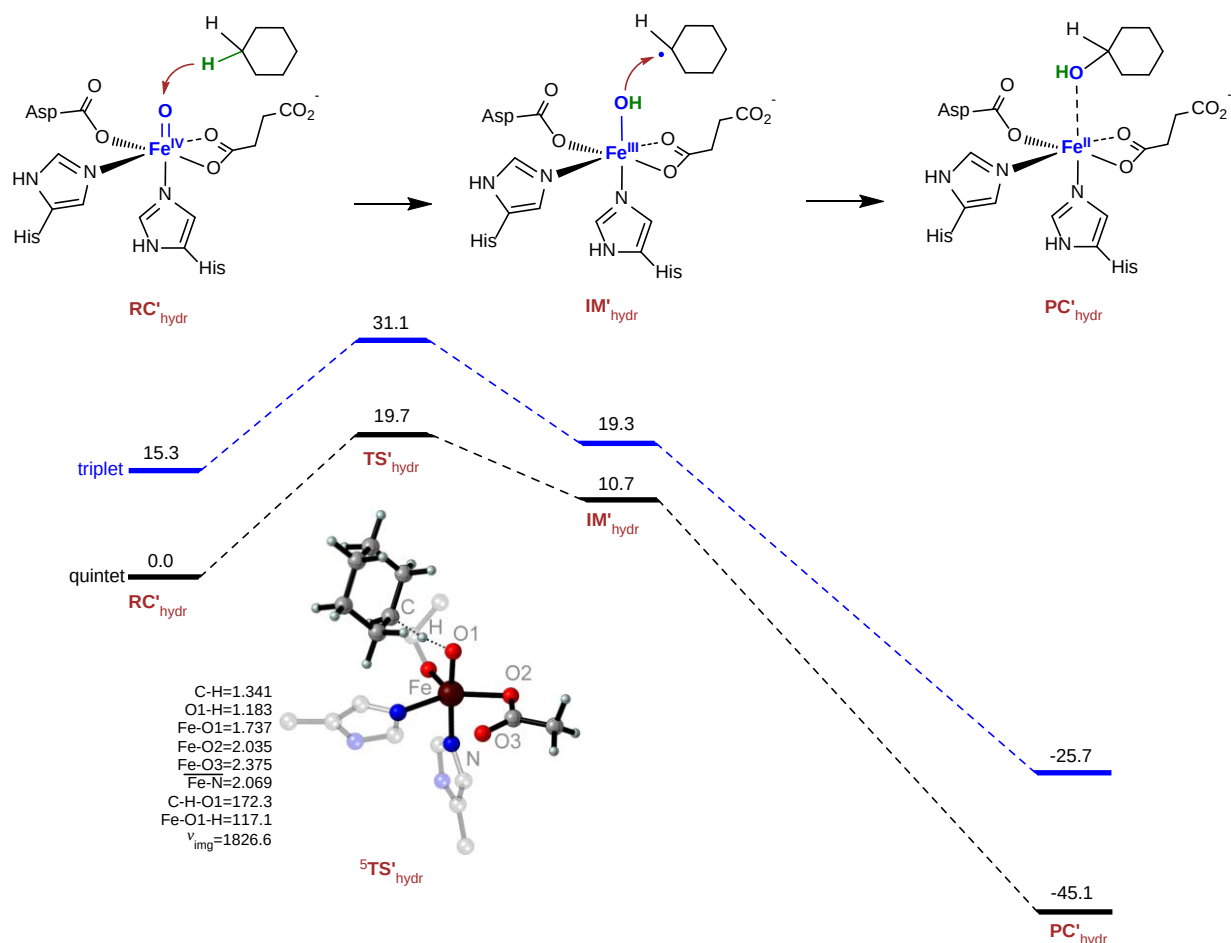
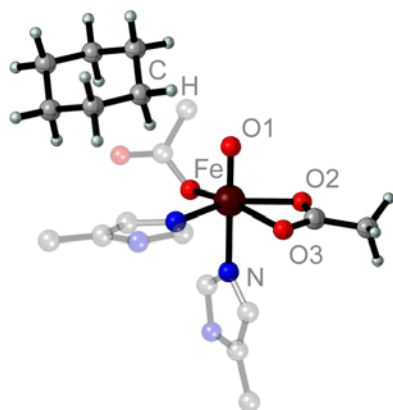


Figure S10. The energy profile (kcal mol⁻¹) for cyclohexane hydroxylation by model of the iron(IV)-oxo species of the TauD oxygenase. Values are Gibbs free energies calculated at the UB3LYP-D3(BJ)/B2 level. Hydrogen atoms of the supporting ligand are omitted for clarity. Lengths are in Å units, angles are in degree units and imaginary frequencies are in cm⁻¹ units.

Table S7. Various SCF and Gibbs free energies of cyclohexane hydroxylation by model of the iron(IV)-oxo species of the TauD oxygenase. Calculations were done at the UB3LYP-D3(BJ)/B2//B1 level in vacuum environment.

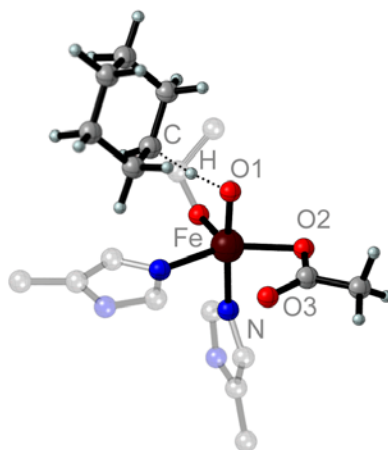
	OPT/B1+ZPE	ΔE	SPE/B2+ZPE	ΔE	G/B2	ΔG
³ RC' _{hydr}	-2561.497545	13.0	-2563.136935	13.6	-2563.205311	15.3
⁵ RC' _{hydr}	-2561.518310	0.0	-2563.158583	0.0	-2563.229660	0.0
³ TS' _{hydr}	-2561.472016	29.0	-2563.111776	29.4	-2563.180048	31.1
⁵ TS' _{hydr}	-2561.490153	17.7	-2563.129384	18.3	-2563.198289	19.7
³ IM' _{hydr}	-2561.487412	19.4	-2563.129671	18.1	-2563.198872	19.3
⁵ IM' _{hydr}	-2561.499185	12.0	-2563.140780	11.2	-2563.212622	10.7
³ PC' _{hydr}	-2561.566727	-30.4	-2563.200938	-26.6	-2563.270605	-25.7
⁵ PC' _{hydr}	-2561.594636	-47.9	-2563.228991	-44.2	-2563.301600	-45.1

^{3/5}RC'_{hydr}



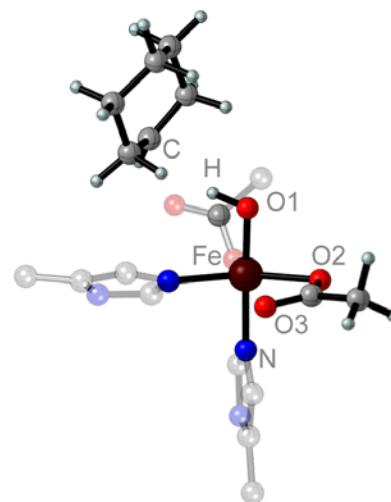
Fe-O1=1.601/1.611
O1-H=3.146/3.185
Fe-O2=2.295/2.075
Fe-O3=2.036/2.286
Fe-N=2.067/2.105

^{3/5}TS'_{hydr}



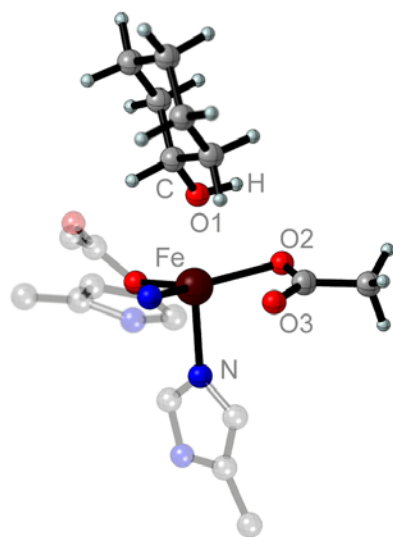
C-H=1.332/1.341
O1-H=1.194/1.183
Fe-O1=1.734/1.737
Fe-O2=2.234/2.035
Fe-O3=2.151/2.375
Fe-N=2.049/2.069
C-H-O1=178.9/172.3
Fe-O1-H=112.8/117.1
 $\nu_{img=i}$ 1820.6/1826.6

^{3/5}IM'_{hydr}



Fe-O1=1.801/1.792
C-H=2.228/2.159
O1-H=0.970/0.973
Fe-O2=2.020/2.021
Fe-O3=2.009/2.386
Fe-N=2.001/2.056
C-H-O1=176.0/162.7
Fe-O1-H=107.2/108.8

^{3/5}PC'_{hydr}



Fe-O1=2.045/2.169
O1-H=0.976/0.970
O1-C=1.437/1.425
Fe-O2=2.002/2.265
Fe-O3=3.443/2.303
Fe-N=2.576/2.170
Fe-O1-H=95.5/106.5
C-O1-H=109.7/113.1

Figure S11. Optimized structures of cyclohexane hydroxylation by model of the iron(IV)-oxo species of the TauD oxygenase. Calculations were done at the UB3LYP-D3(BJ)/B1 level in vacuum environment. Hydrogen atoms of the 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 cyclohexane hydroxylation by model of the iron(IV)-oxo species of the TauD oxygenase. Calculations were done at the UB3LYP-D3(BJ)/B1 level in vacuum environment.

	spin					charge				
	Fe	O1	H50	L	sub-H	Fe	O1	H50	L	sub-H
³ RC' _{hydr}	1.29	0.78	0.00	0.00	-0.07	0.70	-0.36	-0.01	-0.05	-0.28
⁵ RC' _{hydr}	3.11	0.61	0.00	0.00	0.28	0.81	-0.37	-0.02	-0.05	-0.38
³ TS' _{hydr}	0.99	0.58	-0.05	0.55	-0.06	0.64	-0.39	0.18	-0.04	-0.39
⁵ TS' _{hydr}	2.87	0.45	-0.04	0.54	0.17	0.76	-0.40	0.18	-0.04	-0.51
³ IM' _{hydr}	0.97	0.10	0.00	0.98	-0.05	0.56	-0.42	0.20	-0.04	-0.30
⁵ IM' _{hydr}	2.83	0.03	0.00	0.98	0.16	0.75	-0.42	0.21	-0.04	-0.51
³ PC' _{hydr}	1.99	-0.01	0.00	0.00	0.02	0.73	-0.31	0.20	0.23	-0.84
⁵ PC' _{hydr}	3.82	0.02	0.00	0.00	0.16	0.83	-0.33	0.19	0.21	-0.91

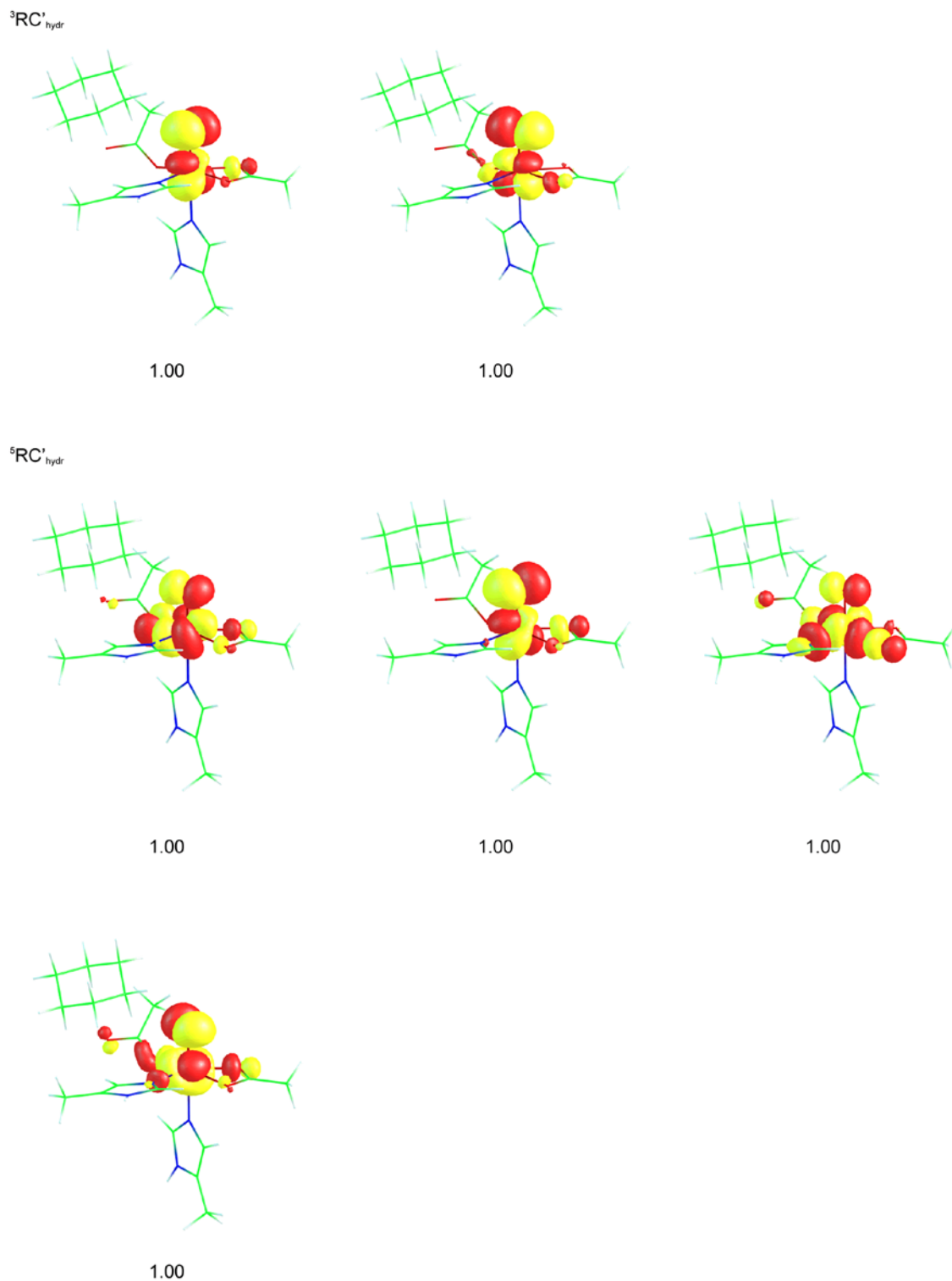


Figure S12. Singly-occupied natural orbitals (SNOs) of cyclohexane hydroxylation by model of the iron(IV)-oxo species of the TauD oxygenase. Calculations were done at the UB3LYP-D3(BJ)/B1 level in solvent. Positive values represent alpha-electron occupations. (To be continued)

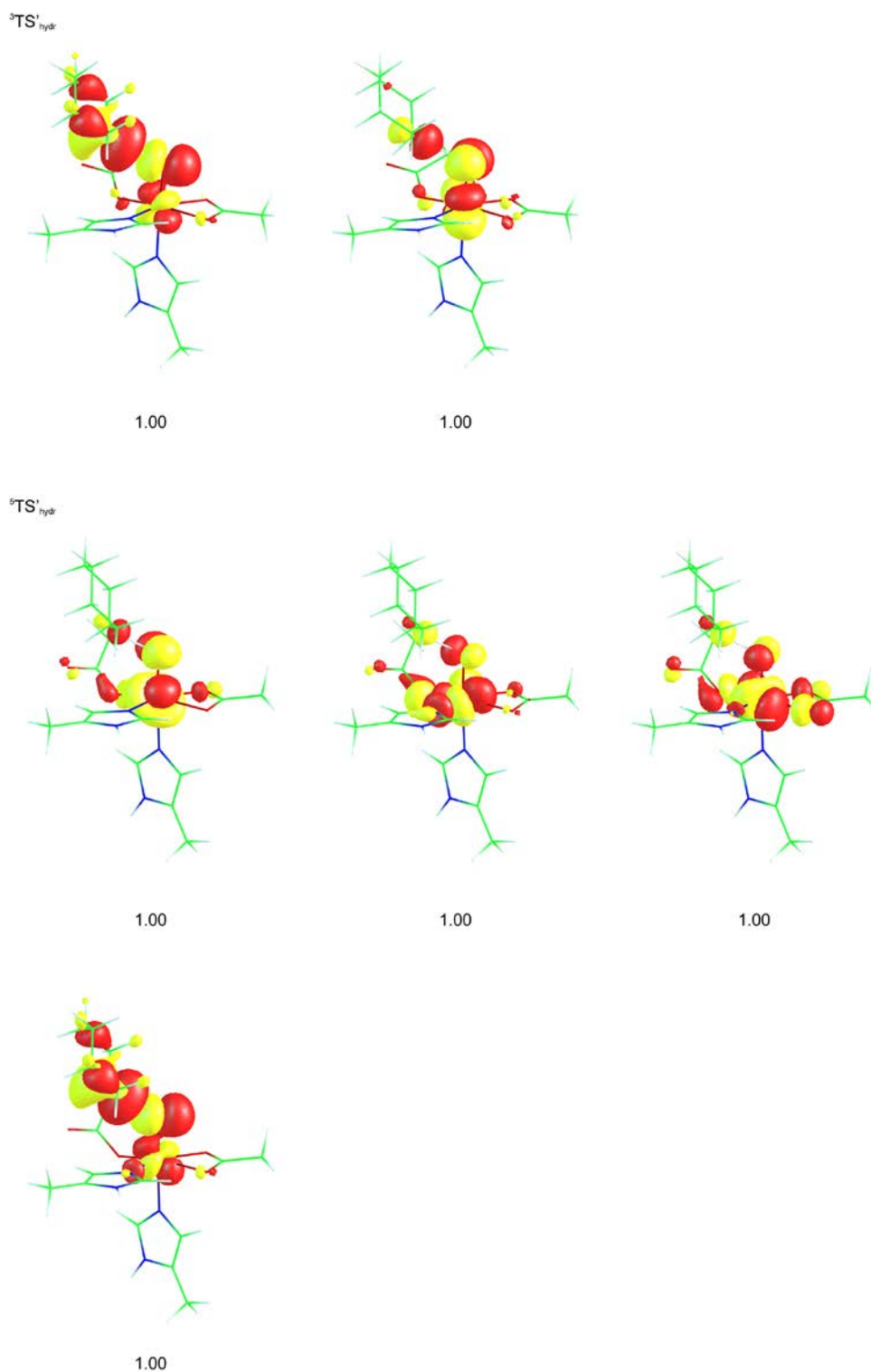


Figure S12. Singly-occupied natural orbitals (SNOs) of cyclohexane hydroxylation by model of the iron(IV)-oxo species of the TauD oxygenase. Calculations were done at the UB3LYP-D3(BJ)/B1 level in solvent. Positive values represent alpha-electron occupations. (To be continued)

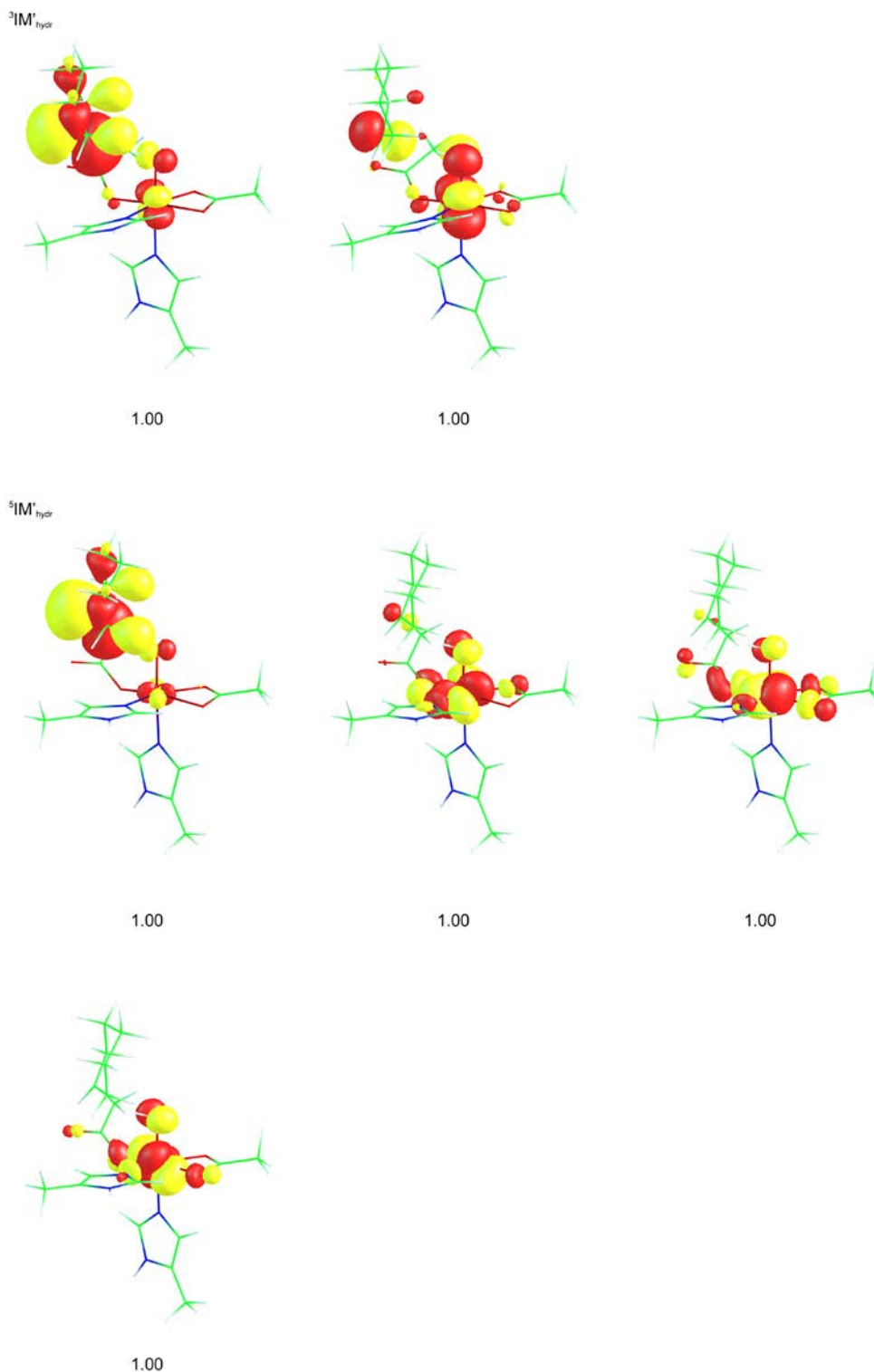


Figure S12. Singly-occupied natural orbitals (SNOs) of cyclohexane hydroxylation by model of the iron(IV)-oxo species of the TauD oxygenase. Calculations were done at the UB3LYP-D3(BJ)/B1 level in solvent. Positive values represent alpha-electron occupations. (To be continued)

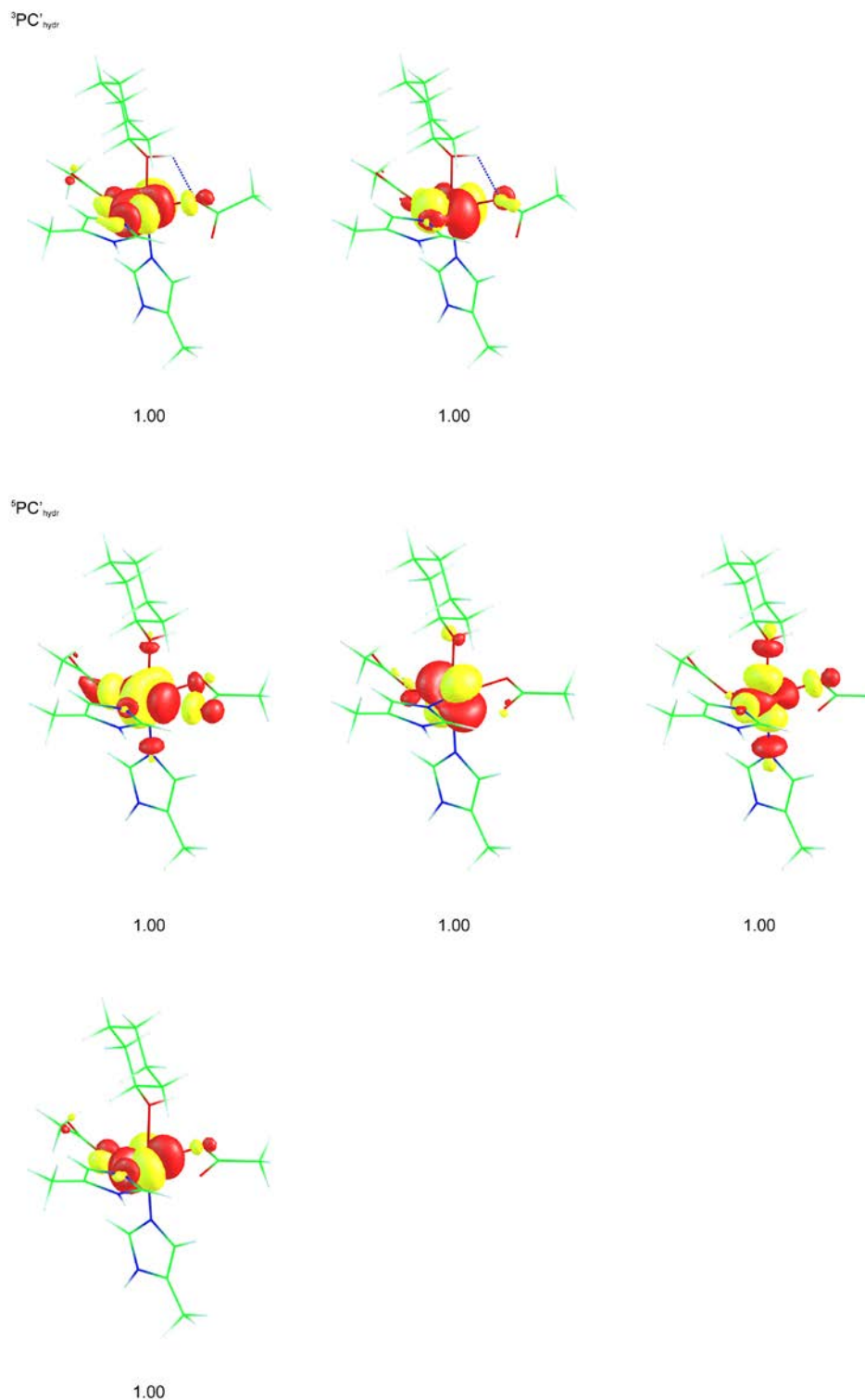


Figure S12. Singly-occupied natural orbitals (SNOs) of cyclohexane hydroxylation by model of the iron(IV)-oxo species of the TauD oxygenase. Calculations were done at the UB3LYP-D3(BJ)/B1 level in solvent. Positive values represent alpha-electron occupations.

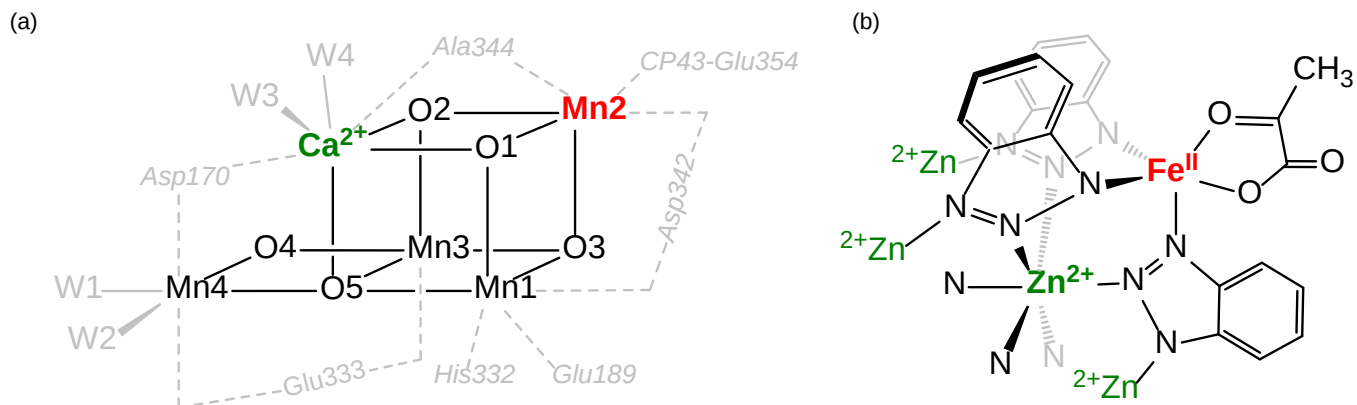


Figure S13. The plot of the structure of (a) the Mn_4CaO_5 active site of the PSII system and (b) the $\text{FeZn}_4(\text{prv})_4(\text{btdd})_3$ site of Long's MOF.

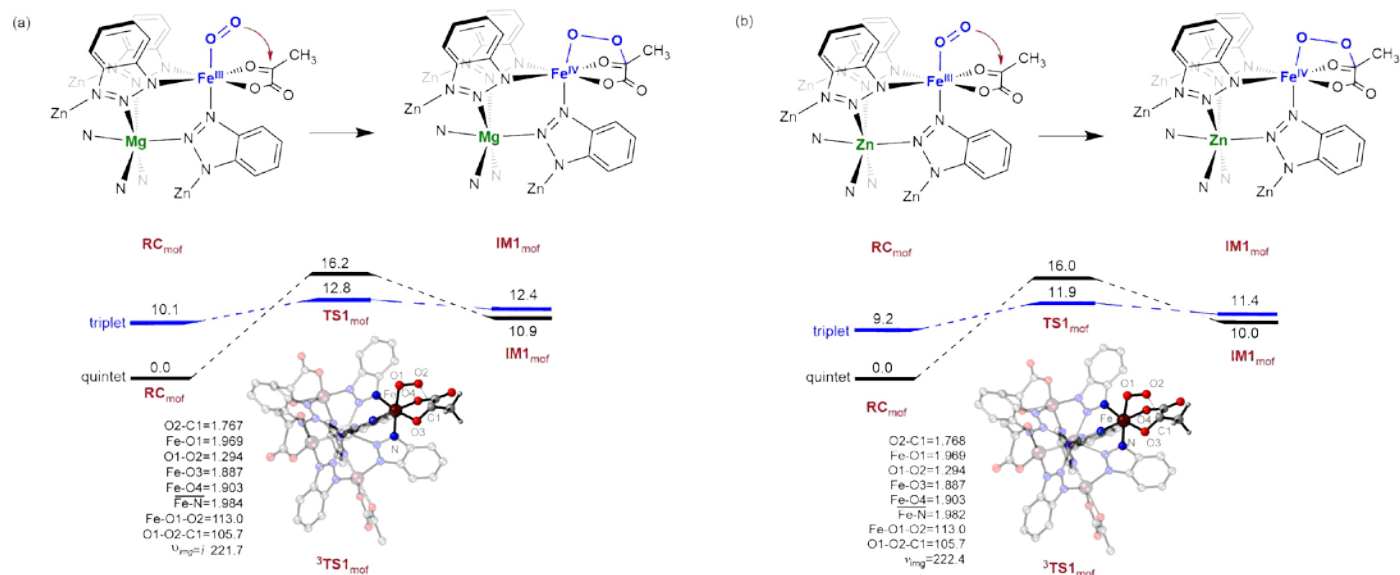


Figure S14. The energy profile (kcal mol⁻¹) for the O₂ activation by the models of (a)FeMgZn₃(prv)₄(btdd)₃ and (b)FeZn₄(prv)₄(btdd)₃ MOF. Values are Gibbs free energies calculated at the UB3LYP-D3(BJ)/B2 level. Hydrogen atoms of the supporting ligand are omitted for clarity. Lengths are in Å units, angles are in degree units and imaginary frequencies are in cm⁻¹ units.

Cartesian coordina

Oxygen activation by MOF

³RC_{mof}

N	-1.035348000	-1.019907000	-2.607589000
C	-0.761130000	-1.153420000	-3.944063000
C	-1.436654000	-1.769370000	-5.020473000
H	-2.387516000	-2.274964000	-4.884269000
N	-0.050448000	-0.338719000	-2.053037000
N	0.865379000	-0.009206000	-2.937595000
C	0.475086000	-0.492154000	-4.149451000
C	1.088803000	-0.413203000	-5.418066000
H	2.039146000	0.109000000	-5.538143000
Fe	-2.645718000	-1.649323000	-1.681224000
Zn	0.125515000	0.103029000	0.044700000
N	-0.146337000	-2.675480000	1.396187000
C	-0.908356000	-3.802058000	1.450503000
C	-0.846776000	-4.919773000	2.305919000
H	-0.106016000	-4.974790000	3.103181000
N	-0.615303000	-1.908071000	0.440674000
N	-1.653835000	-2.459682000	-0.158899000
C	-1.884668000	-3.678136000	0.434081000
C	-2.821050000	-4.711673000	0.214827000
H	-3.558003000	-4.653071000	-0.578986000
N	-2.911476000	0.117460000	-0.754568000
N	3.094880000	-0.262380000	-0.905727000
C	4.274892000	-0.875916000	-0.614744000
C	5.522287000	-0.890558000	-1.271771000
H	5.673882000	-0.349417000	-2.205081000
N	2.222434000	-0.592688000	0.025062000
N	2.760121000	-1.393042000	0.925946000
C	4.059822000	-1.604767000	0.579145000
C	5.094123000	-2.350023000	1.181618000
H	4.933084000	-2.888672000	2.115005000
N	0.853912000	-0.348968000	3.051892000
N	1.539897000	2.512669000	-1.358587000
N	0.280019000	0.475726000	2.199867000
N	-1.972870000	0.688105000	-0.025451000
N	0.723085000	2.160256000	-0.380931000
C	1.580349000	3.872611000	-1.399771000
C	2.256683000	4.778141000	-2.243368000
H	2.893377000	4.428254000	-3.055879000
N	0.223191000	3.212535000	0.233258000

C	0.726881000	4.327591000	-0.364938000
C	0.521802000	5.702248000	-0.118408000
H	-0.143248000	6.025243000	0.684117000
N	-2.400034000	1.799515000	0.533243000
C	-3.689348000	1.993999000	0.154249000
C	-4.584843000	3.041549000	0.448416000
H	-4.274639000	3.882310000	1.068295000
C	-4.035157000	0.903693000	-0.682462000
C	-5.328783000	0.837311000	-1.248566000
H	-5.637976000	0.043867000	-1.918520000
N	-0.119925000	1.584737000	2.796877000
C	0.209024000	1.494141000	4.114595000
C	0.041162000	2.380548000	5.198520000
H	-0.423912000	3.357355000	5.065082000
C	0.838579000	0.236775000	4.281750000
C	1.312841000	-0.197505000	5.538321000
H	1.786809000	-1.174925000	5.641622000
C	-0.827305000	-1.690270000	-6.259525000
H	-1.318475000	-2.152366000	-7.118778000
C	0.415053000	-1.023176000	-6.459146000
H	0.841248000	-0.993709000	-7.464460000
C	6.526546000	-1.634527000	-0.679363000
H	7.510379000	-1.679478000	-1.151291000
C	6.317512000	-2.347932000	0.536095000
H	7.150825000	-2.908800000	0.964776000
C	-1.779424000	-5.916186000	2.089314000
H	-1.779204000	-6.804097000	2.725117000
C	-2.744886000	-5.812927000	1.049596000
H	-3.451104000	-6.633848000	0.907340000
C	-6.207287000	1.861985000	-0.944293000
H	-7.210520000	1.839782000	-1.375154000
C	-5.845156000	2.954952000	-0.109494000
H	-6.577265000	3.742676000	0.080246000
C	2.050088000	6.123624000	-1.997089000
H	2.548198000	6.864838000	-2.626169000
C	1.198406000	6.578477000	-0.948133000
H	1.075508000	7.654169000	-0.803934000
C	0.512119000	1.950540000	6.426152000
H	0.408835000	2.602322000	7.296639000
C	1.134607000	0.679024000	6.593891000
H	1.482900000	0.394784000	7.589337000
C	-4.811766000	-1.709672000	-3.251644000
O	-4.330894000	-2.399482000	-1.035105000
C	-5.077371000	-2.584595000	-2.020343000
O	-3.687934000	-1.053919000	-3.124162000
O	-5.614647000	-1.621950000	-4.153924000
C	-6.316147000	-3.396897000	-1.943395000

H	-6.280568000	-4.090080000	-1.093582000	Zn	0.108664000	0.061412000	-0.024263000
H	-7.173816000	-2.712876000	-1.823523000	N	-1.119544000	-2.174299000	1.771152000
H	-6.464744000	-3.926876000	-2.894021000	C	-2.206447000	-2.965005000	1.970352000
Zn	2.561004000	1.069230000	-2.369515000	C	-2.528975000	-3.865391000	3.005970000
O	3.465245000	1.274902000	-4.077712000	H	-1.858597000	-4.010017000	3.852836000
O	4.532880000	2.277382000	-1.833041000	N	-1.309745000	-1.487864000	0.659836000
C	4.572817000	1.919257000	-4.211508000	N	-2.469108000	-1.782402000	0.101779000
C	5.135462000	2.490919000	-2.873839000	C	-3.079764000	-2.724081000	0.882601000
O	5.206534000	2.118366000	-5.231352000	C	-4.300128000	-3.426281000	0.776133000
C	6.402680000	3.278961000	-2.943569000	H	-4.968477000	-3.296636000	-0.069199000
H	7.185009000	2.667583000	-3.419712000	N	-2.749004000	1.095039000	-0.919785000
H	6.254697000	4.138058000	-3.617307000	N	2.823721000	-1.443632000	-0.638720000
H	6.710348000	3.612411000	-1.944794000	C	3.714845000	-2.348331000	-0.148301000
Zn	1.578224000	-2.182584000	2.390837000	C	4.905962000	-2.887558000	-0.676219000
O	2.182139000	-2.943786000	4.077491000	H	5.264298000	-2.602144000	-1.664605000
O	2.411682000	-4.303293000	1.782053000	N	1.856574000	-1.299421000	0.245938000
C	2.733844000	-4.105445000	4.157498000	N	2.060753000	-2.059728000	1.304692000
C	2.829225000	-4.851804000	2.790867000	C	3.223627000	-2.742524000	1.118424000
O	3.172002000	-4.662003000	5.147097000	C	3.923450000	-3.664098000	1.924271000
C	3.436939000	-6.215759000	2.792958000	H	3.557727000	-3.943540000	2.911844000
H	4.449371000	-6.160181000	3.222922000	N	0.630731000	-0.079555000	3.075580000
H	2.865943000	-6.863351000	3.477200000	N	2.347056000	1.560115000	-1.659650000
H	3.458567000	-6.635329000	1.779661000	N	0.390325000	0.731615000	2.065687000
Zn	-1.198578000	2.943278000	1.736493000	N	-1.628344000	1.402833000	-0.291971000
O	-2.845753000	2.805340000	3.415495000	N	1.437188000	1.690844000	-0.709287000
O	-1.541355000	4.803858000	2.200961000	C	2.878772000	2.788616000	-1.904960000
C	-2.361998000	5.144911000	3.133793000	C	3.853902000	3.236311000	-2.820391000
C	-3.093187000	3.938365000	3.799754000	H	4.333816000	2.549890000	-3.517892000
O	-2.621541000	6.264883000	3.533370000	N	1.342935000	2.941634000	-0.306035000
C	-4.070137000	4.242646000	4.887635000	C	2.229387000	3.686068000	-1.023511000
H	-3.558190000	4.803132000	5.685765000	C	2.535509000	5.064060000	-1.004218000
H	-4.841010000	4.927164000	4.499867000	H	2.021586000	5.733848000	-0.312881000
H	-4.519576000	3.321247000	5.277981000	N	-1.617129000	2.665804000	0.081027000
O	-2.467137000	-3.388383000	-2.565199000	C	-2.782369000	3.238404000	-0.323336000
O	-3.533377000	-3.915749000	-3.039843000	C	-3.262036000	4.559127000	-0.211352000
⁵ RC _{mof}				H	-2.662309000	5.336127000	0.261589000
				C	-3.524538000	2.221116000	-0.968727000
N	-1.225626000	-1.078468000	-2.593271000	C	-4.799602000	2.492779000	-1.511027000
C	-0.952902000	-1.550868000	-3.844360000	H	-5.385664000	1.719366000	-2.000149000
C	-1.769675000	-2.124747000	-4.841972000	N	0.446475000	1.997201000	2.444188000
H	-2.834458000	-2.284841000	-4.676885000	C	0.744234000	2.027566000	3.771694000
N	-0.090644000	-0.664425000	-2.059620000	C	0.945220000	3.090921000	4.676104000
N	0.920848000	-0.826807000	-2.890382000	H	0.880323000	4.129879000	4.352731000
C	0.439929000	-1.383141000	-4.036412000	C	0.860138000	0.678351000	4.183574000
C	1.078754000	-1.762650000	-5.236690000	C	1.163427000	0.330090000	5.517596000
H	2.153035000	-1.617973000	-5.360918000	H	1.239119000	-0.718211000	5.810947000
Fe	-3.112766000	-0.851376000	-1.709300000	C	-1.134933000	-2.494308000	-6.014588000

H	-1.721802000	-2.947292000	-6.816907000	O	1.292531000	-4.494300000	5.990498000
C	0.265219000	-2.312910000	-6.210893000	C	1.019315000	-6.429670000	3.940170000
H	0.705620000	-2.625272000	-7.160532000	H	1.984230000	-6.644582000	4.425507000
C	5.577921000	-3.800806000	0.115888000	H	0.252501000	-6.718283000	4.676614000
H	6.504371000	-4.248713000	-0.249869000	H	0.906425000	-7.000772000	3.010439000
C	5.097675000	-4.177126000	1.403422000	Zn	-0.060201000	3.464823000	1.137517000
H	5.676999000	-4.892888000	1.990651000	O	-1.625786000	4.205784000	2.749511000
C	-3.736126000	-4.529576000	2.897211000	O	0.305954000	5.370307000	1.304396000
H	-4.034982000	-5.236365000	3.674274000	C	-0.321910000	6.131022000	2.133200000
C	-4.603868000	-4.318267000	1.788968000	C	-1.429346000	5.394702000	2.948681000
H	-5.537281000	-4.882802000	1.737394000	O	-0.153388000	7.319208000	2.336920000
C	-5.267244000	3.789158000	-1.387864000	C	-2.199876000	6.200394000	3.942878000
H	-6.248312000	4.041936000	-1.796081000	H	-1.499294000	6.639216000	4.670999000
C	-4.508881000	4.812405000	-0.751711000	H	-2.664314000	7.058399000	3.432061000
H	-4.925242000	5.820541000	-0.696609000	H	-2.953772000	5.582235000	4.445746000
C	4.147080000	4.588052000	-2.798412000	O	-4.673655000	-0.150725000	-4.125268000
H	4.892555000	4.984810000	-3.491344000	O	-3.763536000	0.195268000	-3.372038000
C	3.500668000	5.487285000	-1.900623000				
H	3.776462000	6.543755000	-1.930014000	MECP_{mof}			
C	1.246607000	2.742981000	5.980658000	N	-1.151174000	-1.011525000	-2.591157000
H	1.415154000	3.530400000	6.718799000	C	-0.907169000	-1.181661000	-3.927067000
C	1.349468000	1.382966000	6.395735000	C	-1.645625000	-1.770698000	-4.976028000
H	1.586969000	1.171872000	7.440758000	H	-2.630869000	-2.196620000	-4.806923000
C	-5.334949000	-2.526939000	-2.419652000	N	-0.116160000	-0.386657000	-2.059802000
O	-5.267590000	-0.578624000	-1.035160000	N	0.805640000	-0.131379000	-2.965100000
C	-6.000282000	-1.387229000	-1.592076000	C	0.366928000	-0.609041000	-4.162300000
O	-4.050127000	-2.411496000	-2.460649000	C	0.962877000	-0.602493000	-5.442148000
O	-6.039147000	-3.390122000	-2.902348000	H	1.943824000	-0.148774000	-5.591202000
C	-7.485930000	-1.345692000	-1.514256000	Fe	-2.805043000	-1.574383000	-1.595120000
H	-7.825277000	-0.551898000	-0.837498000	Zn	0.128722000	0.095467000	0.033862000
H	-7.882134000	-1.186725000	-2.531075000	N	-0.230977000	-2.633437000	1.493278000
H	-7.863136000	-2.331762000	-1.203169000	C	-1.052143000	-3.711873000	1.614476000
Zn	2.849370000	-0.293320000	-2.330612000	C	-1.034140000	-4.800356000	2.509574000
O	3.839481000	-0.701703000	-3.954736000	H	-0.274853000	-4.875586000	3.287688000
O	5.093659000	0.264054000	-1.791579000	N	-0.685694000	-1.876280000	0.520367000
C	5.105585000	-0.496940000	-4.073849000	N	-1.770559000	-2.392895000	-0.024685000
C	5.775062000	0.079577000	-2.788241000	C	-2.052172000	-3.568492000	0.624486000
O	5.811015000	-0.701485000	-5.044615000	C	-3.063374000	-4.541574000	0.475162000
C	7.237914000	0.376300000	-2.850476000	H	-3.829363000	-4.451510000	-0.288978000
H	7.780858000	-0.533765000	-3.149661000	N	-2.952947000	0.304702000	-0.654157000
H	7.422710000	1.103894000	-3.656882000	N	3.063370000	-0.463094000	-0.975108000
H	7.599866000	0.757789000	-1.887741000	C	4.211980000	-1.138976000	-0.696194000
Zn	0.652749000	-2.134915000	2.776953000	C	5.437763000	-1.250323000	-1.384066000
O	0.948435000	-2.756446000	4.598781000	H	5.597205000	-0.746795000	-2.336971000
O	0.721284000	-4.489848000	2.569361000	N	2.196980000	-0.713505000	-0.013879000
C	1.073199000	-4.003277000	4.898525000	N	2.710968000	-1.518855000	0.896369000
C	0.916854000	-4.962852000	3.678389000	C	3.985435000	-1.819450000	0.523456000

C	4.986986000	-2.611780000	1.121048000	H	1.519453000	7.554067000	-1.050412000
H	4.816823000	-3.113925000	2.072938000	C	0.794861000	2.093186000	6.352668000
N	0.924418000	-0.310963000	3.037434000	H	0.748874000	2.772610000	7.206768000
N	1.654262000	2.380898000	-1.468194000	C	1.346084000	0.792169000	6.542417000
N	0.377104000	0.521638000	2.175335000	H	1.698958000	0.514169000	7.537989000
N	-1.947289000	0.825283000	0.022379000	C	-5.143125000	-1.581066000	-3.096997000
N	0.842687000	2.105280000	-0.461627000	O	-4.772328000	-2.325005000	-0.850632000
C	1.777148000	3.733947000	-1.548555000	C	-5.523746000	-2.379751000	-1.825553000
C	2.483668000	4.572511000	-2.435517000	O	-3.967371000	-1.022773000	-3.011958000
H	3.073939000	4.161593000	-3.254445000	O	-5.943569000	-1.470202000	-3.999749000
N	0.426339000	3.203059000	0.135456000	C	-6.829669000	-3.089345000	-1.802251000
C	0.981602000	4.268446000	-0.505929000	H	-6.921645000	-3.715403000	-0.906001000
C	0.867524000	5.659493000	-0.294113000	H	-7.637264000	-2.338720000	-1.825236000
H	0.245350000	6.045185000	0.515118000	H	-6.936462000	-3.680006000	-2.723769000
N	-2.273470000	1.983864000	0.555953000	Zn	2.572649000	0.858110000	-2.459299000
C	-3.557911000	2.261831000	0.212374000	O	3.448422000	0.965795000	-4.191390000
C	-4.370054000	3.378355000	0.494913000	O	4.624597000	1.967825000	-2.001913000
H	-3.985840000	4.216601000	1.075409000	C	4.588973000	1.538066000	-4.368335000
C	-4.008966000	1.174037000	-0.575148000	C	5.215599000	2.112681000	-3.061003000
C	-5.317119000	1.178483000	-1.108222000	O	5.209110000	1.669262000	-5.407399000
H	-5.686438000	0.381753000	-1.744567000	C	6.526826000	2.818073000	-3.182884000
N	0.057352000	1.667968000	2.750228000	H	7.257463000	2.146083000	-3.659456000
C	0.412969000	1.594140000	4.061870000	H	6.414754000	3.665384000	-3.878190000
C	0.322057000	2.517500000	5.123869000	H	6.879849000	3.159777000	-2.202089000
H	-0.088733000	3.515827000	4.973161000	Zn	1.539883000	-2.197734000	2.419959000
C	0.972763000	0.307422000	4.250128000	O	2.144968000	-2.947891000	4.110538000
C	1.449774000	-0.120654000	5.507859000	O	2.236018000	-4.380507000	1.848857000
H	1.868652000	-1.121070000	5.628143000	C	2.608388000	-4.145847000	4.213751000
C	-1.051786000	-1.764989000	-6.225001000	C	2.626178000	-4.932397000	2.866488000
H	-1.586446000	-2.210823000	-7.066518000	O	3.018102000	-4.708589000	5.212015000
C	0.232270000	-1.192067000	-6.456563000	C	3.128491000	-6.338285000	2.897585000
H	0.645367000	-1.219359000	-7.467416000	H	4.152546000	-6.347941000	3.302923000
C	6.409443000	-2.039901000	-0.796055000	H	2.526693000	-6.919840000	3.613810000
H	7.375076000	-2.160503000	-1.291741000	H	3.094059000	-6.787108000	1.897247000
C	6.189767000	-2.705298000	0.444525000	Zn	-0.959709000	3.068789000	1.686959000
H	6.997302000	-3.306971000	0.867220000	O	-2.566962000	3.075088000	3.409668000
C	-2.035671000	-5.740934000	2.359332000	O	-1.175632000	4.958329000	2.108564000
H	-2.071423000	-6.602442000	3.029501000	C	-1.955841000	5.373461000	3.046044000
C	-3.030381000	-5.613471000	1.349415000	C	-2.741730000	4.231644000	3.762046000
H	-3.795433000	-6.388512000	1.266430000	O	-2.142081000	6.517809000	3.416402000
C	-6.113225000	2.272013000	-0.815417000	C	-3.677985000	4.624903000	4.856921000
H	-7.127071000	2.311359000	-1.219013000	H	-3.117793000	5.175853000	5.628840000
C	-5.649979000	3.360925000	-0.025174000	H	-4.413650000	5.343379000	4.462431000
H	-6.319876000	4.203060000	0.160167000	H	-4.173820000	3.743620000	5.282137000
C	2.366224000	5.934380000	-2.223232000	O	-2.695948000	-3.411953000	-2.414522000
H	2.890335000	6.626007000	-2.886713000	O	-3.737839000	-3.885373000	-2.960296000
C	1.573126000	6.469273000	-1.166105000				

³TS1_{mof}

N	-1.041707000	-0.922970000	-2.641776000	C	-4.008255000	1.036714000	-0.636297000
C	-0.761242000	-1.040731000	-3.980788000	C	-5.325141000	0.978978000	-1.144860000
C	-1.465987000	-1.575249000	-5.079767000	H	-5.671265000	0.169461000	-1.775699000
H	-2.455683000	-2.007131000	-4.969333000	N	-0.063677000	1.576009000	2.795530000
N	-0.015268000	-0.323150000	-2.061866000	C	0.243829000	1.461556000	4.116619000
N	0.927575000	-0.038259000	-2.927097000	C	0.116623000	2.352601000	5.202357000
C	0.520484000	-0.464952000	-4.156403000	H	-0.287514000	3.355964000	5.067891000
C	1.155157000	-0.397575000	-5.414447000	C	0.795760000	0.168376000	4.286154000
H	2.141670000	0.058630000	-5.509197000	C	1.228435000	-0.297765000	5.546312000
Fe	-2.705655000	-1.459933000	-1.751944000	H	1.641968000	-1.302114000	5.650912000
Zn	0.134677000	0.095166000	0.046667000	C	-0.836700000	-1.509122000	-6.310753000
N	-0.313927000	-2.668771000	1.360622000	H	-1.350781000	-1.909524000	-7.187373000
C	-1.142462000	-3.745832000	1.400748000	C	0.452631000	-0.930530000	-6.479367000
C	-1.159331000	-4.868432000	2.252392000	H	0.892357000	-0.905865000	-7.478864000
H	-0.431983000	-4.971025000	3.057320000	C	6.452549000	-1.976664000	-0.569268000
N	-0.727258000	-1.870283000	0.400988000	H	7.443033000	-2.069279000	-1.019864000
N	-1.786910000	-2.356976000	-0.213715000	C	6.178949000	-2.689072000	0.633850000
C	-2.098644000	-3.558679000	0.373584000	H	6.971634000	-3.297235000	1.074891000
C	-3.099341000	-4.529580000	0.148538000	C	-2.149637000	-5.804399000	2.024225000
H	-3.834442000	-4.414389000	-0.639694000	H	-2.210722000	-6.692049000	2.657491000
N	-2.900209000	0.234457000	-0.747845000	C	-3.099887000	-5.636233000	0.978844000
N	3.103902000	-0.421987000	-0.856143000	H	-3.859624000	-6.407044000	0.832164000
C	4.243283000	-1.100067000	-0.546284000	C	-6.176032000	2.017767000	-0.813856000
C	5.502600000	-1.174962000	-1.175887000	H	-7.198303000	2.003409000	-1.197617000
H	5.704088000	-0.633756000	-2.099684000	C	-5.764020000	3.112688000	-0.004265000
N	2.194793000	-0.713794000	0.052910000	H	-6.477064000	3.911910000	0.208857000
N	2.669620000	-1.549514000	0.956165000	C	2.398560000	6.017081000	-1.938749000
C	3.963511000	-1.827132000	0.635201000	H	2.944861000	6.734998000	-2.554712000
C	4.943068000	-2.631823000	1.252479000	C	1.548536000	6.509804000	-0.905731000
H	4.732869000	-3.169271000	2.176723000	H	1.475082000	7.589763000	-0.759882000
N	0.791203000	-0.413299000	3.054453000	C	0.546739000	1.891098000	6.433502000
N	1.701616000	2.433253000	-1.323730000	H	0.472326000	2.544989000	7.305356000
N	0.277387000	0.447030000	2.199422000	C	1.090266000	0.584125000	6.603354000
N	-1.927162000	0.785021000	-0.050228000	H	1.409085000	0.276238000	7.601638000
N	0.848472000	2.118276000	-0.363943000	C	-4.824848000	-1.377527000	-3.384071000
C	1.808241000	3.789855000	-1.359630000	O	-4.379966000	-2.105757000	-1.168729000
C	2.544933000	4.663827000	-2.185723000	C	-4.998653000	-2.436506000	-2.264158000
H	3.180934000	4.285872000	-2.986126000	O	-3.701126000	-0.742572000	-3.206636000
N	0.387215000	3.191815000	0.242813000	O	-5.652278000	-1.197783000	-4.248362000
C	0.956461000	4.282845000	-0.340971000	C	-6.291708000	-3.179908000	-2.185839000
C	0.813355000	5.665134000	-0.093309000	H	-6.222346000	-4.012238000	-1.472554000
H	0.149069000	6.017445000	0.697434000	H	-7.067858000	-2.480576000	-1.838876000
N	-2.315753000	1.905017000	0.520643000	H	-6.579590000	-3.537589000	-3.182736000
C	-3.614010000	2.121845000	0.184721000	Zn	2.675708000	0.947348000	-2.314951000
C	-4.483065000	3.183889000	0.506500000	O	3.603649000	1.102080000	-4.016514000
H	-4.139628000	4.021702000	1.112416000	O	4.693448000	2.047970000	-1.759551000
				C	4.744224000	1.689178000	-4.137450000

C	5.319209000	2.231125000	-2.792723000	C	-2.767843000	-3.041687000	0.754696000
O	5.398682000	1.855688000	-5.149846000	C	-3.969488000	-3.774082000	0.656232000
C	6.625266000	2.953747000	-2.845842000	H	-4.717383000	-3.544020000	-0.096496000
H	7.381238000	2.303946000	-3.313633000	N	-2.843505000	0.785384000	-0.837256000
H	6.529022000	3.819766000	-3.520142000	N	2.975600000	-1.020928000	-0.813752000
H	6.937452000	3.270450000	-1.843051000	C	3.978966000	-1.863126000	-0.443869000
Zn	1.413395000	-2.283915000	2.389591000	C	5.207363000	-2.197568000	-1.050110000
O	1.949327000	-3.087354000	4.079698000	H	5.500408000	-1.765003000	-2.006073000
O	2.143087000	-4.443345000	1.778375000	N	2.026545000	-1.089279000	0.099050000
C	2.435605000	-4.277748000	4.160287000	N	2.348445000	-1.931408000	1.062571000
C	2.510365000	-5.020785000	2.790555000	C	3.575203000	-2.448927000	0.779156000
O	2.828997000	-4.862656000	5.152401000	C	4.399572000	-3.366103000	1.462976000
C	3.037528000	-6.417946000	2.794245000	H	4.097288000	-3.794444000	2.418080000
H	4.042629000	-6.424597000	3.244346000	N	0.721502000	-0.325489000	3.057223000
H	2.415997000	-7.035299000	3.462267000	N	2.118869000	2.005579000	-1.468668000
H	3.054390000	-6.831824000	1.778508000	N	0.352034000	0.545692000	2.140595000
Zn	-1.066034000	2.990594000	1.727933000	N	-1.780213000	1.162534000	-0.152155000
O	-2.716054000	2.932987000	3.407270000	N	1.215484000	1.914346000	-0.507767000
O	-1.312548000	4.865158000	2.196288000	C	2.475328000	3.313860000	-1.586481000
C	-2.115719000	5.245704000	3.129000000	C	3.366269000	3.981844000	-2.452110000
C	-2.905892000	4.076327000	3.793822000	H	3.925155000	3.442458000	-3.216740000
O	-2.318963000	6.376777000	3.529918000	N	0.958210000	3.092298000	0.022915000
C	-3.865527000	4.427089000	4.882979000	C	1.723614000	4.019885000	-0.616111000
H	-3.326377000	4.962047000	5.680684000	C	1.838275000	5.417781000	-0.456576000
H	-4.602765000	5.148134000	4.495911000	H	1.246914000	5.937178000	0.299217000
H	-4.358832000	3.528393000	5.273241000	N	-1.935817000	2.375787000	0.330884000
O	-2.700860000	-3.170879000	-2.727225000	C	-3.156071000	2.836091000	-0.053090000
O	-3.890404000	-3.602283000	-2.996966000	C	-3.794796000	4.073044000	0.169026000
⁵TS1_{mof}				H	-3.298798000	4.866997000	0.726483000
N	-1.154924000	-0.880529000	-2.650789000	C	-3.760149000	1.803809000	-0.810353000
C	-0.876261000	-1.167509000	-3.957969000	C	-5.051153000	1.969483000	-1.357241000
C	-1.654188000	-1.687450000	-5.014166000	H	-5.526598000	1.184264000	-1.936180000
H	-2.696620000	-1.959186000	-4.869093000	N	0.214178000	1.756086000	2.654119000
N	-0.051830000	-0.416056000	-2.090308000	C	0.511922000	1.686227000	3.980198000
N	0.943498000	-0.372269000	-2.950264000	C	0.550453000	2.662437000	4.997338000
C	0.486500000	-0.829991000	-4.149136000	H	0.322588000	3.707782000	4.788643000
C	1.131038000	-0.985634000	-5.395106000	C	0.837734000	0.333716000	4.243679000
H	2.180375000	-0.710729000	-5.512053000	C	1.198677000	-0.106888000	5.535461000
Fe	-2.992162000	-1.027881000	-1.672907000	H	1.437087000	-1.156609000	5.713828000
Zn	0.142897000	0.066344000	0.009179000	C	-1.014025000	-1.839327000	-6.231120000
N	-0.780312000	-2.478592000	1.576746000	H	-1.574900000	-2.240954000	-7.078041000
C	-1.808014000	-3.352803000	1.747802000	C	0.355101000	-1.493024000	-6.421088000
C	-2.014119000	-4.383695000	2.686851000	H	0.800206000	-1.635709000	-7.408373000
H	-1.279879000	-4.590681000	3.464972000	C	6.002913000	-3.107596000	-0.378050000
N	-1.080770000	-1.683822000	0.568857000	H	6.962866000	-3.401114000	-0.808170000
N	-2.256813000	-1.986316000	0.054408000	C	5.608066000	-3.677633000	0.866746000
				H	6.282766000	-4.381708000	1.358457000

C	-3.195966000	-5.092642000	2.579166000	O	-0.409711000	5.176931000	1.851342000
H	-3.405346000	-5.900447000	3.283628000	C	-1.143209000	5.753082000	2.740398000
C	-4.157434000	-4.792674000	1.572953000	C	-2.137858000	4.787770000	3.456623000
H	-5.073783000	-5.385028000	1.529489000	O	-1.146679000	6.925837000	3.065679000
C	-5.673402000	3.182532000	-1.123738000	C	-3.027351000	5.371473000	4.504620000
H	-6.671530000	3.352901000	-1.532967000	H	-2.406128000	5.840037000	5.284333000
C	-5.055290000	4.224653000	-0.376052000	H	-3.612364000	6.194588000	4.065000000
H	-5.592299000	5.165564000	-0.238359000	H	-3.683499000	4.603323000	4.932080000
C	3.472290000	5.351774000	-2.291865000	O	-5.058274000	-0.594974000	-3.759860000
H	4.145969000	5.915373000	-2.941295000	O	-3.948411000	-0.094821000	-3.399538000
C	2.722528000	6.058203000	-1.306271000				
H	2.850388000	7.140138000	-1.228330000	³ IM _{mof}			
C	0.909238000	2.224614000	6.259530000	N	-1.018391000	-1.119274000	-2.568234000
H	0.957339000	2.942926000	7.081093000	C	-0.718332000	-1.370090000	-3.883107000
C	1.224038000	0.859721000	6.524965000	C	-1.413338000	-2.004409000	-4.935593000
H	1.496954000	0.574773000	7.543458000	H	-2.399648000	-2.432155000	-4.785376000
C	-4.676942000	-2.943341000	-2.705709000	N	0.012044000	-0.494624000	-2.029528000
O	-5.040188000	-1.170457000	-1.189221000	N	0.977518000	-0.309587000	-2.901701000
C	-5.579824000	-1.875305000	-2.073714000	C	0.578504000	-0.839615000	-4.091190000
O	-3.407041000	-2.651286000	-2.528089000	C	1.231510000	-0.905223000	-5.340605000
O	-5.110742000	-3.922039000	-3.267315000	H	2.229527000	-0.481642000	-5.462565000
C	-7.053356000	-1.948515000	-2.265551000	Fe	-2.729713000	-1.527883000	-1.671953000
H	-7.531922000	-1.016349000	-1.938921000	Zn	0.139910000	0.098520000	0.026856000
H	-7.289193000	-2.172808000	-3.313905000	N	-0.430378000	-2.535407000	1.557716000
H	-7.440117000	-2.783808000	-1.656672000	C	-1.279208000	-3.593479000	1.645682000
Zn	2.820498000	0.313949000	-2.358731000	C	-1.350904000	-4.650473000	2.575516000
O	3.796616000	0.211850000	-4.037377000	H	-0.657454000	-4.706198000	3.414290000
O	4.995231000	1.065556000	-1.797862000	N	-0.794388000	-1.804808000	0.523654000
C	5.026468000	0.577390000	-4.153378000	N	-1.838918000	-2.321078000	-0.087953000
C	5.663818000	1.077118000	-2.820200000	C	-2.192913000	-3.470004000	0.571288000
O	5.720564000	0.570890000	-5.153144000	C	-3.195081000	-4.444373000	0.369463000
C	7.080715000	1.547257000	-2.870500000	H	-3.879708000	-4.390447000	-0.469864000
H	7.714577000	0.746495000	-3.282308000	N	-2.898160000	0.241902000	-0.763046000
H	7.158029000	2.378202000	-3.589799000	N	3.103731000	-0.587481000	-0.761874000
H	7.425132000	1.856114000	-1.875834000	C	4.211860000	-1.276738000	-0.373397000
Zn	1.008985000	-2.327039000	2.547128000	C	5.478411000	-1.448194000	-0.968645000
O	1.427853000	-3.063744000	4.300049000	H	5.715684000	-0.993613000	-1.929869000
O	1.332659000	-4.624092000	2.126907000	N	2.169174000	-0.770181000	0.149694000
C	1.682598000	-4.313018000	4.485909000	N	2.596751000	-1.543658000	1.128905000
C	1.600104000	-5.171532000	3.185962000	C	3.885043000	-1.892207000	0.858458000
O	1.970678000	-4.873554000	5.527054000	C	4.823651000	-2.676190000	1.560200000
C	1.858949000	-6.636799000	3.311662000	H	4.577482000	-3.126768000	2.521217000
H	2.852164000	-6.791623000	3.761650000	N	0.721208000	-0.172309000	3.079663000
H	1.144043000	-7.068322000	4.030229000	N	1.812211000	2.262634000	-1.500278000
H	1.783519000	-7.132012000	2.335778000	N	0.254742000	0.629874000	2.145031000
Zn	-0.501894000	3.264196000	1.497220000	N	-1.898088000	0.853169000	-0.156252000
O	-2.154936000	3.607703000	3.140833000	N	0.929135000	2.060141000	-0.537938000

C	1.968040000	3.606695000	-1.649372000	C	-4.962677000	-2.613641000	-2.183138000
C	2.752747000	4.380690000	-2.529214000	O	-3.704183000	-0.831159000	-3.225002000
H	3.391109000	3.913485000	-3.278990000	O	-5.763948000	-1.195408000	-4.135053000
N	0.493841000	3.197264000	-0.036201000	C	-6.349387000	-3.197379000	-2.112919000
C	1.113838000	4.214274000	-0.696926000	H	-6.380581000	-3.977100000	-1.338068000
C	1.016241000	5.616750000	-0.570757000	H	-7.058620000	-2.401597000	-1.852417000
H	0.350078000	6.058540000	0.172059000	H	-6.631170000	-3.621672000	-3.084793000
N	-2.260847000	2.023571000	0.317101000	Zn	2.744122000	0.661438000	-2.344897000
C	-3.571061000	2.217480000	0.008505000	O	3.710929000	0.646419000	-4.032183000
C	-4.422919000	3.312823000	0.252828000	O	4.793220000	1.737966000	-1.837486000
H	-4.053646000	4.205652000	0.756125000	C	4.874741000	1.179649000	-4.175924000
C	-3.999969000	1.058282000	-0.681892000	C	5.444853000	1.810130000	-2.868197000
C	-5.338653000	0.951983000	-1.118219000	O	5.553951000	1.238678000	-5.184208000
H	-5.712674000	0.064885000	-1.614519000	C	6.779240000	2.476333000	-2.952381000
N	-0.045409000	1.820135000	2.634883000	H	7.518271000	1.760692000	-3.345173000
C	0.241546000	1.809725000	3.965500000	H	6.730859000	3.284095000	-3.700050000
C	0.140871000	2.797517000	4.967057000	H	7.083568000	2.865886000	-1.973083000
H	-0.216915000	3.801637000	4.739206000	Zn	1.284560000	-2.115418000	2.588780000
C	0.735828000	0.514710000	4.255819000	O	1.759487000	-2.784400000	4.354791000
C	1.133594000	0.143676000	5.558376000	O	1.964355000	-4.338762000	2.183727000
H	1.502477000	-0.863990000	5.756357000	C	2.201573000	-3.978501000	4.550199000
C	-0.767200000	-2.066227000	-6.157133000	C	2.285062000	-4.838632000	3.251389000
H	-1.270772000	-2.549824000	-6.997285000	O	2.549662000	-4.488242000	5.599233000
C	0.533612000	-1.523817000	-6.360792000	C	2.762978000	-6.246811000	3.388796000
H	0.988360000	-1.603568000	-7.350725000	H	3.755891000	-6.247475000	3.865228000
C	6.387654000	-2.229186000	-0.278371000	H	2.103967000	-6.783641000	4.089627000
H	7.381753000	-2.393888000	-0.699483000	H	2.790295000	-6.746921000	2.412855000
C	6.067221000	-2.828349000	0.973884000	Zn	-0.980091000	3.174013000	1.434798000
H	6.829240000	-3.424985000	1.479952000	O	-2.647669000	3.306331000	3.098874000
C	-2.348231000	-5.585370000	2.375591000	O	-1.171979000	5.086459000	1.747699000
H	-2.450093000	-6.422922000	3.069079000	C	-1.961215000	5.566871000	2.645525000
C	-3.250085000	-5.484877000	1.279150000	C	-2.790190000	4.481736000	3.399888000
H	-4.010848000	-6.258447000	1.153844000	O	-2.126104000	6.732532000	2.954514000
C	-6.173554000	2.025640000	-0.864251000	C	-3.727139000	4.949641000	4.464568000
H	-7.214050000	1.973531000	-1.191814000	H	-3.159575000	5.513965000	5.221428000
C	-5.724224000	3.198184000	-0.196543000	H	-4.434282000	5.674253000	4.031090000
H	-6.425746000	4.020099000	-0.038788000	H	-4.256041000	4.102776000	4.918874000
C	2.650626000	5.754410000	-2.401720000	O	-2.757580000	-3.196588000	-2.473950000
H	3.235383000	6.397612000	-3.063245000	O	-4.077884000	-3.555110000	-2.755133000
C	1.798234000	6.362870000	-1.434452000				
H	1.761551000	7.453252000	-1.382207000	⁵ IM _{mof}			
C	0.536791000	2.428732000	6.240254000	N	-1.273603000	-0.811689000	-2.632718000
H	0.481197000	3.159644000	7.050161000	C	-1.038582000	-1.033684000	-3.965601000
C	1.021382000	1.120160000	6.532067000	C	-1.847640000	-1.486138000	-5.028536000
H	1.315301000	0.888273000	7.558155000	H	-2.888040000	-1.756778000	-4.873531000
C	-4.836258000	-1.358326000	-3.394154000	N	-0.148974000	-0.376287000	-2.084531000
O	-4.471228000	-2.020731000	-1.111914000	N	0.813354000	-0.294666000	-2.971954000

C	0.317780000	-0.689275000	-4.179362000	C	1.001423000	0.298641000	4.227048000
C	0.926569000	-0.775976000	-5.449328000	C	1.431893000	-0.146311000	5.495923000
H	1.973266000	-0.496704000	-5.578562000	H	1.704760000	-1.191373000	5.650466000
Fe	-2.990427000	-1.075048000	-1.664116000	C	-1.244024000	-1.569624000	-6.270928000
Zn	0.132152000	0.059047000	0.027198000	H	-1.833282000	-1.917764000	-7.122180000
N	-0.653287000	-2.525725000	1.584066000	C	0.120419000	-1.221039000	-6.480851000
C	-1.664721000	-3.418269000	1.757729000	H	0.536796000	-1.308878000	-7.486768000
C	-1.846262000	-4.464637000	2.684790000	C	6.030016000	-3.004034000	-0.656320000
H	-1.100099000	-4.675337000	3.450804000	H	6.974885000	-3.277459000	-1.130819000
N	-0.980040000	-1.729792000	0.582638000	C	5.697109000	-3.595950000	0.596311000
N	-2.153412000	-2.045722000	0.077081000	H	6.402148000	-4.296429000	1.049022000
C	-2.640410000	-3.110116000	0.778712000	C	-3.020787000	-5.186949000	2.580811000
C	-3.835248000	-3.854073000	0.685006000	H	-3.210976000	-6.007098000	3.276538000
H	-4.594147000	-3.616753000	-0.055290000	C	-3.999540000	-4.886224000	1.591112000
N	-2.868840000	0.745989000	-0.780140000	H	-4.909456000	-5.488852000	1.553181000
N	2.956364000	-0.958204000	-0.933847000	C	-5.788154000	3.054330000	-0.859302000
C	3.987307000	-1.789661000	-0.619131000	H	-6.804782000	3.206381000	-1.228345000
C	5.193230000	-2.097573000	-1.281672000	C	-5.181617000	4.083694000	-0.086164000
H	5.439025000	-1.648177000	-2.243258000	H	-5.744263000	4.998938000	0.109781000
N	2.048965000	-1.051531000	0.018664000	C	3.262733000	5.455438000	-2.315273000
N	2.424538000	-1.900597000	0.955758000	H	3.901031000	6.044418000	-2.977796000
C	3.645177000	-2.396346000	0.612354000	C	2.528688000	6.129378000	-1.295804000
C	4.511034000	-3.309962000	1.247831000	H	2.632684000	7.212961000	-1.206218000
H	4.255093000	-3.755200000	2.208660000	C	1.115968000	2.168751000	6.260603000
N	0.848535000	-0.350439000	3.039059000	H	1.183119000	2.879095000	7.087748000
N	2.019192000	2.065486000	-1.496417000	C	1.477346000	0.809727000	6.494905000
N	0.415147000	0.520932000	2.151126000	H	1.803375000	0.520787000	7.496517000
N	-1.797242000	1.134669000	-0.110776000	C	-4.582877000	-3.008181000	-2.666341000
N	1.150745000	1.938733000	-0.507504000	O	-4.786835000	-1.210264000	-1.141317000
C	2.339680000	3.383809000	-1.607521000	C	-5.446174000	-1.837598000	-2.117491000
C	3.185128000	4.085508000	-2.491792000	O	-3.305298000	-2.684397000	-2.587472000
H	3.732396000	3.570851000	-3.281481000	O	-5.032263000	-4.041361000	-3.091329000
N	0.882032000	3.102469000	0.047308000	C	-6.897110000	-2.134342000	-1.868928000
C	1.603175000	4.057502000	-0.603086000	H	-7.425746000	-1.220421000	-1.564906000
C	1.688831000	5.455454000	-0.427109000	H	-7.350814000	-2.558501000	-2.774727000
H	1.110457000	5.949272000	0.355418000	H	-6.974329000	-2.877330000	-1.062654000
N	-1.980975000	2.313884000	0.438704000	Zn	2.717967000	0.403679000	-2.435511000
C	-3.229510000	2.746934000	0.115472000	O	3.612191000	0.350264000	-4.161099000
C	-3.899483000	3.950892000	0.411848000	O	4.901014000	1.180065000	-1.964024000
H	-3.411145000	4.736869000	0.986735000	C	4.829678000	0.738692000	-4.327337000
C	-3.820779000	1.726714000	-0.667227000	C	5.522179000	1.219662000	-3.015189000
C	-5.133514000	1.874364000	-1.165199000	O	5.473739000	0.765452000	-5.359486000
H	-5.603640000	1.099093000	-1.759757000	C	6.929779000	1.707697000	-3.120703000
N	0.269546000	1.721453000	2.685106000	H	7.553434000	0.921462000	-3.574150000
C	0.629078000	1.645010000	3.995259000	H	6.965548000	2.551419000	-3.828253000
C	0.688942000	2.610762000	5.021339000	H	7.315208000	2.003419000	-2.137179000
H	0.425762000	3.652190000	4.835899000	Zn	1.158513000	-2.342044000	2.495928000

O	1.674101000	-3.075736000	4.224219000	H	5.709458000	-1.021429000	-1.932907000
O	1.511283000	-4.630915000	2.051620000	N	2.163221000	-0.785813000	0.145598000
C	1.936228000	-4.324970000	4.398784000	N	2.585538000	-1.566080000	1.121718000
C	1.810139000	-5.180912000	3.100898000	C	3.871872000	-1.921208000	0.850464000
O	2.262219000	-4.886844000	5.428041000	C	4.805407000	-2.713784000	1.549325000
C	2.068430000	-6.647251000	3.215971000	H	4.556097000	-3.167031000	2.508280000
H	3.072218000	-6.806453000	3.640009000	N	0.717884000	-0.193009000	3.078786000
H	1.370553000	-7.078418000	3.951413000	N	1.827831000	2.257494000	-1.490368000
H	1.965428000	-7.139751000	2.241223000	N	0.259839000	0.617993000	2.147562000
Zn	-0.532876000	3.219050000	1.574587000	N	-1.891912000	0.867714000	-0.152883000
O	-2.122120000	3.502584000	3.287441000	N	0.943575000	2.056729000	-0.528729000
O	-0.465454000	5.128544000	1.953145000	C	1.992915000	3.601119000	-1.633384000
C	-1.165938000	5.673264000	2.887398000	C	2.782603000	4.373764000	-2.509955000
C	-2.107214000	4.675144000	3.630350000	H	3.417430000	3.905696000	-3.262190000
O	-1.175408000	6.839256000	3.236121000	N	0.516316000	3.194560000	-0.021701000
C	-2.950631000	5.219127000	4.736105000	C	1.143214000	4.210225000	-0.677888000
H	-2.297010000	5.677122000	5.495414000	C	1.055334000	5.612735000	-0.545159000
H	-3.568195000	6.044267000	4.347906000	H	0.392520000	6.055664000	0.199985000
H	-3.573381000	4.430720000	5.176429000	N	-2.245979000	2.038355000	0.326210000
O	-5.468930000	-0.863062000	-3.376996000	C	-3.555540000	2.242162000	0.021273000
O	-4.350767000	-0.214015000	-3.476347000	C	-4.399692000	3.342112000	0.271988000
³TS_{2mof}				H	-4.023295000	4.231082000	0.776901000
N	-1.027343000	-1.097625000	-2.574584000	C	-3.993500000	1.088727000	-0.673069000
C	-0.729701000	-1.342696000	-3.891080000	C	-5.333911000	0.992785000	-1.106499000
C	-1.430069000	-1.965002000	-4.947168000	H	-5.714676000	0.110075000	-1.605504000
H	-2.419727000	-2.385742000	-4.799221000	N	-0.030340000	1.808391000	2.642849000
N	0.008197000	-0.484504000	-2.032434000	C	0.254550000	1.788800000	3.973823000
N	0.974835000	-0.301772000	-2.903784000	C	0.161542000	2.772490000	4.980354000
C	0.571237000	-0.821256000	-4.096393000	H	-0.184933000	3.781669000	4.757349000
C	1.223283000	-0.884367000	-5.346432000	C	0.736762000	0.487965000	4.258397000
H	2.224587000	-0.467968000	-5.466168000	C	1.129018000	0.106732000	5.559707000
Fe	-2.741030000	-1.499849000	-1.679782000	H	1.488968000	-0.905081000	5.752959000
Zn	0.140527000	0.097771000	0.026663000	C	-0.784857000	-2.024425000	-6.169319000
N	-0.448052000	-2.540773000	1.543627000	H	-1.292552000	-2.498810000	-7.012236000
C	-1.303197000	-3.594291000	1.625042000	C	0.520149000	-1.491120000	-6.370136000
C	-1.381498000	-4.656425000	2.548476000	H	0.973928000	-1.568407000	-7.360708000
H	-0.688658000	-4.721354000	3.387084000	C	6.373129000	-2.268180000	-0.286430000
N	-0.807336000	-1.801853000	0.513824000	H	7.366493000	-2.436950000	-0.707665000
N	-1.854679000	-2.308306000	-0.101168000	C	6.048392000	-2.870813000	0.963048000
C	-2.215804000	-3.458954000	0.551149000	H	6.806550000	-3.474136000	1.466981000
C	-3.223669000	-4.426127000	0.343125000	C	-2.384296000	-5.584158000	2.342617000
H	-3.907586000	-4.363137000	-0.496158000	H	-2.491369000	-6.425247000	3.031022000
N	-2.897195000	0.265590000	-0.760272000	C	-3.285155000	-5.471739000	1.246517000
N	3.099374000	-0.604805000	-0.764664000	H	-4.050397000	-6.240063000	1.116293000
C	4.203096000	-1.302421000	-0.378555000	C	-6.161381000	2.070621000	-0.845895000
C	5.468947000	-1.478837000	-0.973837000	H	-7.202985000	2.026486000	-1.171103000
				C	-5.702871000	3.237593000	-0.174652000

H	-6.398519000	4.063637000	-0.012415000	H	-3.421165000	4.402801000	5.444120000
C	2.689981000	5.747556000	-2.376082000	O	-2.780372000	-3.163275000	-2.492256000
H	3.278902000	6.389755000	-3.034882000	O	-4.103106000	-3.511283000	-2.774913000
C	1.842163000	6.357428000	-1.405681000				
H	1.813053000	7.447784000	-1.348376000	⁵ TS _{mof}			
C	0.551806000	2.393504000	6.252417000	N	-1.286775000	-0.820813000	-2.624428000
H	0.502320000	3.121082000	7.065734000	C	-1.058148000	-1.048469000	-3.957493000
C	1.023787000	1.079048000	6.538342000	C	-1.872457000	-1.504533000	-5.014863000
H	1.313980000	0.839233000	7.563666000	H	-2.912384000	-1.773582000	-4.854014000
C	-4.847838000	-1.305387000	-3.399045000	N	-0.159202000	-0.384089000	-2.083282000
O	-4.485337000	-1.984871000	-1.121529000	N	0.798981000	-0.306901000	-2.975538000
C	-4.981400000	-2.567747000	-2.196144000	C	0.297487000	-0.706066000	-4.178952000
O	-3.712021000	-0.787010000	-3.227737000	C	0.900418000	-0.798512000	-5.451299000
O	-5.775260000	-1.131425000	-4.137738000	H	1.946787000	-0.520771000	-5.586458000
C	-6.371717000	-3.143104000	-2.128568000	Fe	-2.999189000	-1.079173000	-1.646706000
H	-6.407430000	-3.927167000	-1.358309000	Zn	0.131863000	0.058872000	0.025600000
H	-7.075837000	-2.344445000	-1.863039000	N	-0.647274000	-2.519799000	1.595408000
H	-6.656672000	-3.559887000	-3.102762000	C	-1.658077000	-3.411544000	1.776719000
Zn	2.748549000	0.653533000	-2.342232000	C	-1.835497000	-4.454793000	2.708086000
O	3.714964000	0.640166000	-4.029718000	H	-1.085768000	-4.663101000	3.471266000
O	4.805055000	1.714504000	-1.830304000	N	-0.978590000	-1.727088000	0.592902000
C	4.881466000	1.167982000	-4.171712000	N	-2.154374000	-2.044397000	0.093899000
C	5.456161000	1.788480000	-2.861218000	C	-2.638280000	-3.106385000	0.801268000
O	5.560068000	1.228668000	-5.180302000	C	-3.833668000	-3.850430000	0.715579000
C	6.794063000	2.447871000	-2.943164000	H	-4.595970000	-3.615598000	-0.022017000
H	7.528782000	1.730497000	-3.340851000	N	-2.871928000	0.745202000	-0.770245000
H	6.749183000	3.260083000	-3.686221000	N	2.949873000	-0.964974000	-0.945111000
H	7.101570000	2.830302000	-1.962054000	C	3.982445000	-1.794942000	-0.631909000
Zn	1.268667000	-2.137156000	2.577960000	C	5.184594000	-2.106542000	-1.299740000
O	1.737836000	-2.817987000	4.341053000	H	5.424529000	-1.663452000	-2.265770000
O	1.935438000	-4.362858000	2.162401000	N	2.047727000	-1.053453000	0.012708000
C	2.173721000	-4.015305000	4.530683000	N	2.428241000	-1.897945000	0.951985000
C	2.253084000	-4.869573000	3.227752000	C	3.647020000	-2.395411000	0.604460000
O	2.518804000	-4.531969000	5.577318000	C	4.516391000	-3.305792000	1.239816000
C	2.723030000	-6.281042000	3.358599000	H	4.265667000	-3.746289000	2.204216000
H	3.715082000	-6.289756000	3.836711000	N	0.861594000	-0.339972000	3.036214000
H	2.059868000	-6.817795000	4.055591000	N	2.011935000	2.058378000	-1.515254000
H	2.749059000	-6.776280000	2.380146000	N	0.424934000	0.528419000	2.146963000
Zn	-0.957256000	3.174785000	1.449673000	N	-1.796969000	1.135492000	-0.107277000
O	-2.613682000	3.311145000	3.108190000	N	1.148863000	1.935973000	-0.521190000
O	-1.135482000	5.086814000	1.773395000	C	2.334550000	3.375756000	-1.631492000
C	-1.915067000	5.569994000	2.677585000	C	3.176413000	4.073681000	-2.522351000
C	-2.750804000	4.482849000	3.427667000	H	3.717202000	3.556675000	-3.314990000
O	-2.064557000	6.736632000	2.991360000	N	0.885463000	3.101676000	0.032095000
C	-3.690102000	4.920212000	4.508995000	C	1.605042000	4.053526000	-0.624681000
H	-3.656845000	6.006359000	4.643801000	C	1.694701000	5.451720000	-0.452532000
H	-4.710045000	4.593779000	4.248432000	H	1.121404000	5.948652000	0.331765000

N	-1.976988000	2.317186000	0.438148000	Zn	2.706690000	0.392130000	-2.450757000
C	-3.226510000	2.750196000	0.118710000	O	3.594265000	0.329724000	-4.179419000
C	-3.893931000	3.956050000	0.413127000	O	4.881189000	1.166263000	-1.995929000
H	-3.402246000	4.743846000	0.982651000	C	4.809690000	0.718837000	-4.355745000
C	-3.822321000	1.727395000	-0.657147000	C	5.506530000	1.207190000	-3.045152000
C	-5.137104000	1.874351000	-1.149872000	O	5.444320000	0.739582000	-5.394052000
H	-5.610695000	1.097101000	-1.739084000	C	6.917713000	1.702441000	-3.125923000
N	0.282040000	1.730884000	2.677308000	H	7.550084000	1.085640000	-2.466721000
C	0.646974000	1.658946000	3.986221000	H	7.288992000	1.667870000	-4.155462000
C	0.711533000	2.628316000	5.008600000	H	6.957160000	2.730403000	-2.730819000
H	0.448034000	3.669193000	4.820558000	Zn	1.168481000	-2.333593000	2.498940000
C	1.019690000	0.313250000	4.221249000	O	1.692271000	-3.061098000	4.227375000
C	1.455302000	-0.127368000	5.489882000	O	1.519075000	-4.623920000	2.061123000
H	1.728452000	-1.171975000	5.646978000	C	1.956038000	-4.309565000	4.404962000
C	-1.274602000	-1.593614000	-6.259653000	C	1.823819000	-5.170082000	3.110713000
H	-1.868056000	-1.944702000	-7.106769000	O	2.287626000	-4.867643000	5.434491000
C	0.089173000	-1.247107000	-6.477278000	C	2.083817000	-6.635821000	3.229480000
H	0.500857000	-1.339466000	-7.484720000	H	3.089990000	-6.792813000	3.648661000
C	6.024865000	-3.009805000	-0.674260000	H	1.390228000	-7.064948000	3.970154000
H	6.966721000	-3.286356000	-1.152953000	H	1.975962000	-7.131779000	2.257013000
C	5.698947000	-3.595070000	0.583335000	Zn	-0.523241000	3.225201000	1.564603000
H	6.406405000	-4.293308000	1.035739000	O	-2.105550000	3.517546000	3.282487000
C	-3.010643000	-5.177184000	2.611998000	O	-0.451065000	5.135907000	1.936290000
H	-3.197763000	-5.994986000	3.311311000	C	-1.146953000	5.685092000	2.871370000
C	-3.993926000	-4.879537000	1.625861000	C	-2.087406000	4.691298000	3.621147000
H	-4.904108000	-5.482122000	1.594122000	O	-1.152755000	6.852231000	3.216301000
C	-5.789160000	3.056255000	-0.845937000	C	-2.926077000	5.240715000	4.727819000
H	-6.807264000	3.207850000	-1.211073000	H	-2.269089000	5.700489000	5.483133000
C	-5.178126000	4.088154000	-0.079744000	H	-3.543708000	6.065377000	4.338700000
H	-5.738958000	5.004784000	0.114922000	H	-3.548542000	4.454944000	5.173227000
C	3.258082000	5.443920000	-2.349348000	O	-5.485600000	-0.871906000	-3.348525000
H	3.893385000	6.029992000	-3.017327000	O	-4.367395000	-0.224190000	-3.455863000
C	2.531346000	6.121813000	-1.327278000				
H	2.638101000	7.205383000	-1.240831000	³ PC _{mof}			
C	1.143540000	2.190532000	6.247640000	N	0.525129000	0.807022000	-2.856020000
H	1.214428000	2.903782000	7.071967000	C	-0.005286000	0.849942000	-4.117523000
C	1.505334000	0.832197000	6.485261000	C	0.392055000	1.480830000	-5.317070000
H	1.835445000	0.546681000	7.486519000	H	1.270061000	2.121720000	-5.354604000
C	-4.597940000	-3.014878000	-2.633677000	N	-0.285425000	0.094710000	-2.097139000
O	-4.793106000	-1.210733000	-1.114808000	N	-1.316719000	-0.355118000	-2.779813000
C	-5.457654000	-1.841405000	-2.085294000	C	-1.193804000	0.081251000	-4.064095000
O	-3.319751000	-2.691766000	-2.562341000	C	-2.016219000	-0.114309000	-5.194573000
O	-5.050218000	-4.049383000	-3.052309000	H	-2.923844000	-0.714784000	-5.116208000
C	-6.907610000	-2.135971000	-1.828607000	Fe	2.281778000	1.598049000	-2.259732000
H	-7.433992000	-1.220447000	-1.525490000	Zn	-0.114880000	-0.110900000	0.050514000
H	-7.366073000	-2.563119000	-2.730598000	N	0.281103000	2.849010000	0.997468000
H	-6.981570000	-2.875861000	-1.019185000	C	0.985678000	3.996004000	0.787630000

C	1.027932000	5.213466000	1.497614000	C	-6.592231000	1.483797000	0.119135000
H	0.442786000	5.355256000	2.405950000	H	-7.638133000	1.462390000	-0.194412000
N	0.607828000	1.984558000	0.060183000	C	-6.216774000	2.344244000	1.190904000
N	1.495144000	2.504242000	-0.761393000	H	-6.988405000	2.947698000	1.673775000
C	1.771708000	3.783263000	-0.367044000	C	1.857611000	6.196002000	0.990519000
C	2.599510000	4.797321000	-0.890116000	H	1.929774000	7.156622000	1.505136000
H	3.168152000	4.634359000	-1.801950000	C	2.622430000	5.992594000	-0.194247000
N	2.724352000	-0.172599000	-1.166436000	H	3.247117000	6.810076000	-0.560752000
N	-3.201525000	0.118866000	-0.474012000	C	6.086372000	-1.711567000	-1.600042000
C	-4.338211000	0.755466000	-0.078699000	H	7.030956000	-1.665753000	-2.146598000
C	-5.672330000	0.679293000	-0.528560000	C	5.910649000	-2.731894000	-0.623245000
H	-5.952417000	0.025071000	-1.353373000	H	6.720127000	-3.444742000	-0.451547000
N	-2.204600000	0.569814000	0.261422000	C	-2.187615000	-6.351653000	-0.921861000
N	-2.617721000	1.472211000	1.130723000	H	-2.756349000	-7.169002000	-1.371073000
C	-3.960608000	1.629061000	0.968756000	C	-1.177482000	-6.665743000	0.033777000
C	-4.908712000	2.435627000	1.631147000	H	-1.007908000	-7.713914000	0.289905000
H	-4.618994000	3.086999000	2.455092000	C	0.518134000	-1.155036000	6.583121000
N	-0.390118000	0.715235000	3.052496000	H	0.768686000	-1.695605000	7.498678000
N	-1.677198000	-2.686018000	-0.818705000	C	-0.101485000	0.124342000	6.692175000
N	0.066597000	-0.204206000	2.226776000	H	-0.300260000	0.525608000	7.688418000
N	1.929058000	-0.702726000	-0.262237000	C	3.637657000	0.864113000	-4.944235000
N	-0.733066000	-2.208249000	-0.026039000	O	3.974894000	2.179226000	-1.570702000
C	-1.689405000	-4.040672000	-0.685654000	C	5.021576000	2.437310000	-2.296401000
C	-2.461961000	-5.048996000	-1.298276000	O	3.143580000	0.336807000	-4.015858000
H	-3.222684000	-4.807704000	-2.040661000	O	4.039005000	1.286619000	-5.939759000
N	-0.120581000	-3.171674000	0.629648000	C	6.155106000	3.047591000	-1.491805000
C	-0.679834000	-4.356413000	0.256260000	H	5.784461000	3.881223000	-0.877733000
C	-0.406362000	-5.687997000	0.636746000	H	6.548550000	2.284322000	-0.801567000
H	0.378555000	-5.903057000	1.363584000	H	6.955704000	3.383267000	-2.162518000
N	2.493440000	-1.722586000	0.352866000	Zn	-2.868271000	-1.385974000	-1.827576000
C	3.735502000	-1.890314000	-0.172673000	O	-4.007874000	-1.788396000	-3.351700000
C	4.739795000	-2.840432000	0.102620000	O	-4.714091000	-2.527878000	-0.875453000
H	4.581326000	-3.625768000	0.841386000	C	-5.111231000	-2.445195000	-3.246177000
C	3.896758000	-0.882157000	-1.154372000	C	-5.458848000	-2.862188000	-1.784132000
C	5.101241000	-0.782724000	-1.885964000	O	-5.885124000	-2.758559000	-4.131748000
H	5.252582000	-0.018009000	-2.642826000	C	-6.705770000	-3.657637000	-1.575004000
N	0.579839000	-1.230197000	2.882711000	H	-7.562311000	-3.106958000	-1.994146000
C	0.453845000	-0.981124000	4.214848000	H	-6.641834000	-4.587200000	-2.162970000
C	0.806140000	-1.728568000	5.357692000	H	-6.855267000	-3.876426000	-0.510509000
H	1.268577000	-2.711748000	5.270523000	Zn	-1.251004000	2.447934000	2.296580000
C	-0.172680000	0.283940000	4.326122000	O	-1.620790000	3.403343000	3.951353000
C	-0.459729000	0.865252000	5.580015000	O	-2.235521000	4.468986000	1.572360000
H	-0.936035000	1.845259000	5.638077000	C	-2.174094000	4.566665000	3.975047000
C	-0.418558000	1.284619000	-6.420991000	C	-2.495413000	5.139577000	2.560022000
H	-0.148356000	1.759479000	-7.366945000	O	-2.463331000	5.240866000	4.946105000
C	-1.601773000	0.494033000	-6.364843000	C	-3.113853000	6.497084000	2.492073000
H	-2.199534000	0.376264000	-7.271392000	H	-4.040246000	6.503878000	3.087458000

H	-2.445974000	7.221199000	2.985425000	N	0.533629000	-3.121603000	0.502701000
H	-3.307273000	6.786509000	1.451826000	N	0.568620000	0.877667000	1.957930000
Zn	1.515959000	-2.714662000	1.848513000	N	1.980625000	0.562735000	-0.942475000
O	3.391297000	-2.379966000	3.231467000	N	1.025978000	-1.911153000	0.709264000
O	1.944200000	-4.505589000	2.485004000	C	1.424430000	-4.024301000	0.997028000
C	2.920428000	-4.738149000	3.292560000	C	1.428652000	-5.434238000	1.029099000
C	3.724539000	-3.462031000	3.690526000	H	0.609388000	-6.012670000	0.602073000
O	3.270951000	-5.806304000	3.759315000	N	2.191103000	-1.962249000	1.319946000
C	4.875643000	-3.638777000	4.625568000	C	2.500886000	-3.272082000	1.527474000
H	4.517257000	-4.110120000	5.554335000	C	3.622559000	-3.892305000	2.119014000
H	5.587160000	-4.357991000	4.190041000	H	4.442147000	-3.288705000	2.511992000
H	5.361972000	-2.677488000	4.832321000	N	3.121129000	0.285212000	-0.348041000
O	2.109906000	2.837594000	-3.269946000	C	4.090031000	0.221507000	-1.297479000
O	5.145734000	2.194139000	-3.494087000	C	5.461015000	-0.088581000	-1.196715000
⁵PC_{mof}				H	5.912744000	-0.316023000	-0.230695000
				C	3.456815000	0.484679000	-2.537345000
				C	4.194594000	0.404147000	-3.740345000
N	-0.363379000	-0.404610000	-3.047434000	H	3.704919000	0.527661000	-4.702335000
C	-0.948091000	-1.212109000	-3.977605000	N	1.736810000	0.787731000	2.569877000
C	-1.166340000	-1.065291000	-5.362654000	C	1.650710000	1.475069000	3.742316000
H	-0.850173000	-0.164644000	-5.887816000	C	2.574378000	1.702064000	4.783264000
N	-0.409487000	-1.016271000	-1.878045000	H	3.580888000	1.284751000	4.749065000
N	-0.987569000	-2.192840000	-1.981276000	C	0.336372000	1.998934000	3.798689000
C	-1.348369000	-2.377820000	-3.282012000	C	-0.108085000	2.786233000	4.881965000
C	-1.988560000	-3.451652000	-3.936449000	H	-1.120976000	3.193121000	4.892187000
H	-2.284619000	-4.340903000	-3.377889000	C	-1.798473000	-2.121580000	-5.995199000
Fe	0.499262000	1.431854000	-3.397466000	H	-1.995461000	-2.059156000	-7.067933000
Zn	0.081351000	-0.056746000	0.023967000	C	-2.202987000	-3.295173000	-5.294394000
N	-1.314663000	2.723468000	0.127500000	H	-2.696196000	-4.094089000	-5.852681000
C	-1.331123000	3.938831000	-0.479929000	C	-5.883592000	-2.431198000	1.765808000
C	-1.893633000	5.173163000	-0.096385000	H	-6.710532000	-3.143393000	1.806746000
H	-2.403432000	5.291112000	0.860142000	C	-6.060378000	-1.143043000	2.348926000
N	-0.647507000	1.886514000	-0.644999000	H	-7.013790000	-0.911434000	2.828695000
N	-0.219682000	2.485854000	-1.736442000	C	-1.742287000	6.220871000	-0.985969000
C	-0.629838000	3.786246000	-1.699534000	H	-2.157185000	7.200136000	-0.736949000
C	-0.482646000	4.860252000	-2.601396000	C	-1.050907000	6.062923000	-2.221953000
H	0.068475000	4.730349000	-3.530299000	H	-0.963437000	6.926560000	-2.884905000
N	2.136315000	0.714780000	-2.247249000	C	5.542111000	0.105172000	-3.633179000
N	-2.412340000	-1.852093000	0.622686000	H	6.140045000	0.024440000	-4.543881000
C	-3.674609000	-1.831572000	1.128083000	C	6.173889000	-0.131052000	-2.380135000
C	-4.699561000	-2.799031000	1.152543000	H	7.238125000	-0.375508000	-2.361177000
H	-4.561827000	-3.777932000	0.693726000	C	2.530469000	-6.035242000	1.610952000
N	-1.865926000	-0.673878000	0.836233000	H	2.582846000	-7.125415000	1.656838000
N	-2.696402000	0.131427000	1.471385000	C	3.609747000	-5.275428000	2.149813000
C	-3.857965000	-0.544869000	1.686212000	H	4.453322000	-5.808185000	2.594361000
C	-5.064074000	-0.183653000	2.320414000	C	2.130298000	2.468816000	5.846130000
H	-5.192618000	0.801372000	2.767990000	H	2.807952000	2.671829000	6.678465000
N	-0.288891000	1.588049000	2.661480000				

Oxidation of cyclohexane to cyclohexanol by MOF

³RC_{hydr}

N	0.529901000	0.455549000	-2.913421000
C	1.070956000	1.378152000	-3.762531000
C	1.431125000	1.325759000	-5.124739000
H	1.272627000	0.422423000	-5.711377000
N	0.395370000	1.008544000	-1.723958000
N	0.815821000	2.256365000	-1.733777000
C	1.258013000	2.547656000	-2.989446000
C	1.826105000	3.718033000	-3.536364000
H	1.971432000	4.602777000	-2.915012000
Fe	0.088801000	-1.399448000	-3.411470000
Zn	-0.379715000	0.003625000	0.053387000
N	1.324268000	-2.577492000	0.285876000
C	1.758098000	-3.663438000	-0.411436000
C	2.462864000	-4.815803000	-0.009357000
H	2.729676000	-4.977928000	1.034520000
N	0.710937000	-1.768570000	-0.551000000
N	0.710991000	-2.260467000	-1.770504000
C	1.369502000	-3.461617000	-1.754643000
C	1.695855000	-4.391861000	-2.762102000
H	1.393396000	-4.223177000	-3.792446000
N	-1.936987000	-0.914215000	-2.500628000
N	1.842702000	1.962864000	1.087920000
C	2.987730000	2.044886000	1.817931000
C	3.912711000	3.091069000	2.006049000
H	3.780531000	4.054562000	1.514837000
N	1.364062000	0.742180000	1.209369000
N	2.128060000	0.003861000	1.994255000
C	3.172002000	0.774039000	2.411158000
C	4.278840000	0.509476000	3.243345000
H	4.412691000	-0.463580000	3.713639000
N	-0.316693000	-1.715320000	2.665850000
N	-1.127628000	3.014875000	0.491449000
N	-1.095085000	-1.035512000	1.848665000
N	-2.021067000	-0.738172000	-1.196688000
N	-1.552743000	1.765920000	0.590757000
C	-2.155352000	3.834620000	0.843428000
C	-2.273702000	5.238906000	0.899067000
H	-1.441749000	5.888525000	0.627319000
N	-2.804193000	1.712803000	0.996039000
C	-3.243928000	2.989767000	1.171432000
C	-4.492768000	3.508350000	1.577156000
H	-5.316668000	2.834709000	1.817672000
N	-3.273541000	-0.606259000	-0.798891000

C	-4.070253000	-0.677756000	-1.895082000	C	1.403605000	5.827395000	1.616064000
C	-5.467606000	-0.554773000	-2.034715000	O	2.310481000	7.123073000	-0.173698000
H	-6.104508000	-0.386012000	-1.165978000	C	1.612951000	6.961158000	2.565827000
C	-3.208628000	-0.862895000	-3.005575000	H	2.676164000	7.248425000	2.557452000
C	-3.736766000	-0.888174000	-4.316737000	H	1.069693000	7.845543000	2.196900000
H	-3.079921000	-0.939673000	-5.180883000	H	1.283958000	6.689583000	3.576460000
N	-2.345842000	-1.022112000	2.274187000	Zn	1.692592000	-1.978135000	2.209275000
C	-2.401957000	-1.728461000	3.436384000	O	2.234659000	-3.156902000	3.659385000
C	-3.462288000	-2.022268000	4.318292000	O	3.979380000	-2.421498000	1.769568000
H	-4.472005000	-1.656647000	4.131204000	C	3.422224000	-3.645325000	3.761734000
C	-1.084940000	-2.182703000	3.689499000	C	4.387040000	-3.198516000	2.620081000
C	-0.771733000	-2.963182000	4.823092000	O	3.857610000	-4.387814000	4.622080000
H	0.248799000	-3.312157000	4.988395000	C	5.774809000	-3.748205000	2.633669000
C	1.984440000	2.478559000	-5.652758000	H	6.251366000	-3.502071000	3.595608000
H	2.282680000	2.492629000	-6.703564000	H	5.724372000	-4.848460000	2.608935000
C	2.181939000	3.654479000	-4.871429000	H	6.359649000	-3.362614000	1.789672000
H	2.629091000	4.530292000	-5.347033000	Zn	-3.771299000	-0.146938000	1.123179000
C	5.000322000	2.817530000	2.815019000	O	-5.039324000	-2.115871000	1.250106000
H	5.751318000	3.591739000	2.985250000	O	-5.536725000	0.479058000	1.671614000
C	5.176727000	1.545321000	3.430941000	C	-6.522621000	-0.326502000	1.867683000
H	6.051803000	1.386886000	4.064764000	C	-6.175567000	-1.821267000	1.588713000
C	2.776775000	-5.725344000	-1.002207000	O	-7.653010000	-0.056402000	2.229906000
H	3.322521000	-6.635440000	-0.743869000	C	-7.269371000	-2.824196000	1.758319000
C	2.402866000	-5.510811000	-2.359615000	H	-7.670559000	-2.751762000	2.781399000
H	2.681134000	-6.260636000	-3.103322000	H	-8.108719000	-2.557590000	1.096574000
C	-5.110104000	-0.773360000	-4.445152000	H	-6.906784000	-3.837435000	1.545545000
H	-5.551471000	-0.777548000	-5.444460000	O	1.505122000	-1.617324000	-4.132725000
C	-5.969331000	-0.617129000	-3.321105000	O	-0.902629000	-1.288317000	-5.426148000
H	-7.044483000	-0.518999000	-3.486411000	C	3.638907000	-0.362589000	-1.440001000
C	-3.500063000	5.739788000	1.297408000	C	4.266650000	1.033868000	-1.505107000
H	-3.643319000	6.821325000	1.353068000	C	5.546824000	1.110592000	-0.666191000
C	-4.591974000	4.887061000	1.633827000	C	6.548872000	0.023417000	-1.071306000
H	-5.536220000	5.342937000	1.939830000	C	5.917769000	-1.371906000	-0.992469000
C	-3.147237000	-2.782796000	5.430160000	C	4.637757000	-1.456588000	-1.830693000
H	-3.933250000	-3.035697000	6.145331000	H	2.761302000	-0.418650000	-2.095583000
C	-1.822874000	-3.249466000	5.676116000	H	3.288540000	-0.552330000	-0.412354000
H	-1.637846000	-3.850541000	6.569153000	H	4.502225000	1.276945000	-2.557335000
O	-0.728413000	-3.094860000	-4.212759000	H	3.543576000	1.794243000	-1.170690000
C	-1.091614000	-2.531186000	-5.300397000	H	6.003852000	2.110665000	-0.751662000
C	-1.778218000	-3.336128000	-6.364400000	H	5.288850000	0.977331000	0.398786000
H	-1.362109000	-4.351754000	-6.404970000	H	6.889229000	0.211478000	-2.106538000
H	-2.845483000	-3.417290000	-6.100823000	H	7.447694000	0.075357000	-0.433352000
H	-1.691271000	-2.836564000	-7.337750000	H	6.641622000	-2.139346000	-1.316580000
Zn	0.817907000	3.377274000	0.023748000	H	5.660435000	-1.595500000	0.056933000
O	1.616667000	5.028410000	-0.627041000	H	4.886917000	-1.348248000	-2.902086000
O	0.922494000	4.754093000	1.945566000	H	4.172271000	-2.449637000	-1.720886000
C	1.828741000	6.047815000	0.131661000				

⁵RC_{hydr}

N	0.130547000	0.370356000	-3.062640000	C	-3.412924000	-1.169078000	-2.682429000
C	0.562249000	1.252915000	-4.006017000	C	-4.083942000	-1.309858000	-3.919502000
C	0.722796000	1.144750000	-5.402003000	H	-3.526709000	-1.461031000	-4.839636000
H	0.480314000	0.220511000	-5.925932000	N	-2.069707000	-0.900605000	2.496851000
N	0.189107000	0.957826000	-1.882168000	C	-2.019864000	-1.535189000	3.699821000
N	0.634210000	2.192712000	-1.991636000	C	-2.999634000	-1.785722000	4.682567000
C	0.884086000	2.441082000	-3.308646000	H	-4.027621000	-1.445065000	4.557989000
C	1.379085000	3.582006000	-3.975479000	C	-0.679148000	-1.956395000	3.870748000
H	1.620828000	4.487006000	-3.416330000	C	-0.260197000	-2.656295000	5.022826000
Fe	-0.300983000	-1.620450000	-3.353878000	H	0.778316000	-2.973943000	5.128189000
Zn	-0.299582000	-0.002618000	0.042945000	C	1.210876000	2.267491000	-6.047169000
N	1.550820000	-2.481991000	0.337735000	H	1.359105000	2.238736000	-7.129060000
C	1.980207000	-3.591044000	-0.323398000	C	1.532863000	3.466110000	-5.345765000
C	2.826067000	-4.649973000	0.065159000	H	1.915362000	4.317349000	-5.913387000
H	3.245192000	-4.698704000	1.069539000	C	5.022305000	3.213766000	2.485412000
N	0.761934000	-1.803722000	-0.475900000	H	5.743062000	4.025822000	2.602374000
N	0.642987000	-2.403078000	-1.639589000	C	5.221217000	2.010894000	3.223011000
C	1.402827000	-3.537000000	-1.613675000	H	6.081521000	1.942663000	3.892240000
C	1.671137000	-4.528152000	-2.580471000	C	3.082549000	-5.617014000	-0.888636000
H	1.218175000	-4.476196000	-3.567422000	H	3.733694000	-6.457620000	-0.638898000
N	-2.092707000	-1.183204000	-2.305971000	C	2.517359000	-5.551664000	-2.194817000
N	1.935948000	2.099158000	0.773223000	H	2.758410000	-6.342334000	-2.908660000
C	3.058925000	2.289115000	1.518261000	C	-5.463203000	-1.192460000	-3.905417000
C	3.947176000	3.377540000	1.631048000	H	-6.010760000	-1.286007000	-4.846088000
H	3.796811000	4.290155000	1.055256000	C	-6.194782000	-0.925534000	-2.714645000
N	1.503635000	0.871905000	0.988091000	H	-7.281369000	-0.830500000	-2.769621000
N	2.277531000	0.236821000	1.848643000	C	-3.477850000	5.747543000	1.111978000
C	3.273155000	1.084430000	2.226801000	H	-3.646982000	6.826583000	1.092146000
C	4.362097000	0.933305000	3.109061000	C	-4.517005000	4.901205000	1.598249000
H	4.509572000	0.011749000	3.671107000	H	-5.447815000	5.359543000	1.939673000
N	-0.005352000	-1.545565000	2.759868000	C	-2.581640000	-2.469630000	5.810161000
N	-1.097036000	3.018791000	0.342284000	H	-3.302232000	-2.686167000	6.602080000
N	-0.857443000	-0.924671000	1.970436000	C	-1.233125000	-2.901023000	5.975710000
N	-2.039339000	-0.888878000	-1.017607000	H	-0.964520000	-3.438900000	6.887618000
N	-1.479595000	1.772563000	0.568213000	O	-1.077938000	-3.680689000	-3.723608000
C	-2.117545000	3.841782000	0.707692000	C	-1.576328000	-3.237483000	-4.786837000
C	-2.271338000	5.243133000	0.661026000	C	-2.367884000	-4.120155000	-5.712460000
H	-1.482291000	5.887150000	0.273221000	H	-2.044445000	-5.164327000	-5.614919000
N	-2.695479000	1.726203000	1.071940000	H	-3.429496000	-4.058629000	-5.421703000
C	-3.155151000	3.003063000	1.182761000	H	-2.274549000	-3.774280000	-6.750300000
C	-4.383884000	3.524915000	1.642093000	Zn	0.797697000	3.404225000	-0.307917000
H	-5.168415000	2.855012000	1.997395000	O	1.461186000	5.038530000	-1.129870000
N	-3.242383000	-0.718213000	-0.511758000	O	0.986683000	4.917161000	1.503842000
C	-4.149922000	-0.880232000	-1.507877000	C	1.680110000	6.117864000	-0.461611000
C	-5.553756000	-0.754976000	-1.502524000	C	1.380490000	5.986277000	1.063394000
H	-6.087879000	-0.500561000	-0.586942000	O	2.082985000	7.188800000	-0.876771000
				C	1.597089000	7.195721000	1.912718000

H	2.638439000	7.535825000	1.799141000	C	-2.142247000	0.359233000	4.918091000
H	0.977815000	8.021626000	1.528232000	H	-2.084791000	-0.657005000	5.303771000
H	1.361794000	6.982578000	2.962743000	N	-0.609518000	0.728447000	1.719086000
Zn	1.984472000	-1.754661000	2.191973000	N	-1.012905000	1.964122000	1.935179000
O	2.667934000	-2.760296000	3.712959000	C	-1.635413000	1.999888000	3.146697000
O	4.278030000	-2.078100000	1.691899000	C	-2.268149000	3.050587000	3.845635000
C	3.893260000	-3.145427000	3.809529000	H	-2.306945000	4.053314000	3.417494000
C	4.780490000	-2.726554000	2.597290000	Fe	-0.503561000	-1.983414000	2.923328000
O	4.414322000	-3.774371000	4.711899000	Zn	0.385831000	0.056050000	-0.084103000
C	6.212811000	-3.146186000	2.610235000	N	-1.239542000	-2.402855000	-1.072033000
H	6.690157000	-2.776692000	3.531309000	C	-1.729244000	-3.605645000	-0.666898000
H	6.264066000	-4.244684000	2.677002000	C	-2.343212000	-4.657064000	-1.378061000
H	6.735685000	-2.782044000	1.717417000	H	-2.470091000	-4.607995000	-2.459579000
Zn	-3.596557000	-0.131319000	1.414679000	N	-0.760656000	-1.777934000	-0.015170000
O	-4.794559000	-2.118365000	1.757883000	N	-0.907071000	-2.499080000	1.073493000
O	-5.336754000	0.485036000	2.048695000	C	-1.520237000	-3.675414000	0.729011000
C	-6.272665000	-0.331260000	2.392816000	C	-1.943625000	-4.790557000	1.481619000
C	-5.903657000	-1.832018000	2.182428000	H	-1.777523000	-4.824093000	2.555481000
O	-7.372819000	-0.066229000	2.841079000	N	1.561505000	-1.433259000	2.423922000
C	-6.942928000	-2.849750000	2.521055000	N	-1.695862000	2.248197000	-0.958852000
H	-7.248262000	-2.718529000	3.571060000	C	-2.766663000	2.488186000	-1.763050000
H	-7.849114000	-2.651564000	1.926907000	C	-3.676888000	3.562499000	-1.825583000
H	-6.568359000	-3.865023000	2.341440000	H	-3.594986000	4.410353000	-1.145566000
O	1.044103000	-1.841066000	-4.214107000	N	-1.203452000	1.068040000	-1.272544000
O	-1.446333000	-1.995652000	-5.059813000	N	-1.885890000	0.509627000	-2.255820000
C	3.438503000	-0.049859000	-2.312939000	C	-2.887004000	1.362347000	-2.611414000
C	4.403608000	0.983532000	-1.725950000	C	-3.905946000	1.282893000	-3.582174000
C	5.266633000	0.367604000	-0.619722000	H	-3.985055000	0.425036000	-4.248539000
C	6.010644000	-0.878391000	-1.113757000	N	0.641134000	-1.076566000	-2.983391000
C	5.039514000	-1.912154000	-1.696775000	N	1.215040000	3.064556000	0.157303000
C	4.170116000	-1.303482000	-2.801324000	N	1.315631000	-0.621723000	-1.946838000
H	2.862149000	0.387634000	-3.139874000	N	1.827259000	-0.977789000	1.214051000
H	2.709041000	-0.337255000	-1.537303000	N	1.636301000	1.840033000	-0.113514000
H	5.058321000	1.366955000	-2.530159000	C	2.291260000	3.896162000	0.104876000
H	3.843526000	1.852398000	-1.342180000	C	2.431749000	5.281808000	0.326311000
H	5.975097000	1.113045000	-0.220797000	H	1.577048000	5.900890000	0.598945000
H	4.620440000	0.070266000	0.220337000	N	2.931068000	1.814814000	-0.348668000
H	6.742910000	-0.585056000	-1.889078000	C	3.405479000	3.085476000	-0.223787000
H	6.590498000	-1.323184000	-0.287484000	C	4.704304000	3.622968000	-0.354162000
H	5.590859000	-2.787280000	-2.080501000	H	5.546128000	2.974461000	-0.601701000
H	4.392338000	-2.282129000	-0.885049000	N	3.124386000	-0.829499000	1.021463000
H	4.811341000	-1.030784000	-3.660198000	C	3.761958000	-1.185942000	2.166659000
H	3.440900000	-2.036623000	-3.179285000	C	5.128756000	-1.178393000	2.511185000
				H	5.885914000	-0.857141000	1.795389000
				C	2.751949000	-1.565897000	3.085373000
				C	3.087961000	-1.918456000	4.411346000
				H	2.312832000	-2.125171000	5.144694000
³ TS _{hydr}							
N	-0.926034000	-0.060827000	2.724927000				
C	-1.577498000	0.685457000	3.667056000				

N	2.614072000	-0.594778000	-2.188785000	Zn	-1.409643000	-1.385814000	-2.832255000
C	2.814140000	-1.055170000	-3.454535000	O	-1.843402000	-2.211341000	-4.533251000
C	3.978687000	-1.228424000	-4.230526000	O	-3.744452000	-1.884908000	-2.657838000
H	4.962711000	-0.967329000	-3.841007000	C	-3.013932000	-2.671175000	-4.814478000
C	1.533334000	-1.372512000	-3.968855000	C	-4.066890000	-2.473347000	-3.678539000
C	1.359491000	-1.892732000	-5.269017000	O	-3.376125000	-3.222866000	-5.836999000
H	0.362770000	-2.144071000	-5.635946000	C	-5.435207000	-3.025089000	-3.911693000
C	-2.759456000	1.395833000	5.595726000	H	-5.838185000	-2.615915000	-4.851002000
H	-3.214401000	1.198458000	6.569134000	H	-5.359178000	-4.111895000	-4.076587000
C	-2.823962000	2.718988000	5.068180000	H	-6.095685000	-2.804622000	-3.063996000
H	-3.328892000	3.491814000	5.652269000	Zn	3.878556000	-0.028236000	-0.696883000
C	-4.682655000	3.466938000	-2.770600000	O	5.116926000	-1.984001000	-1.049088000
H	-5.418242000	4.269697000	-2.855000000	O	5.711338000	0.619209000	-0.877034000
C	-4.789956000	2.345417000	-3.642848000	C	6.701310000	-0.174984000	-1.096112000
H	-5.598426000	2.328179000	-4.376871000	C	6.294196000	-1.679082000	-1.166988000
C	-2.751260000	-5.748845000	-0.634359000	O	7.875326000	0.110309000	-1.245683000
H	-3.230610000	-6.591947000	-1.136884000	C	7.384266000	-2.677164000	-1.382351000
C	-2.558551000	-5.809367000	0.776169000	H	7.930405000	-2.423119000	-2.304272000
H	-2.904092000	-6.695570000	1.313038000	H	8.123253000	-2.583594000	-0.570696000
C	4.432497000	-1.915227000	4.739575000	H	6.978361000	-3.695235000	-1.428866000
H	4.730955000	-2.172340000	5.758480000	O	-2.126656000	-2.326090000	3.418189000
C	5.443312000	-1.558329000	3.802706000	O	0.065290000	-2.292090000	5.108072000
H	6.487184000	-1.562982000	4.124068000	C	-4.000888000	-1.588527000	1.866381000
C	3.707241000	5.801471000	0.196630000	C	-3.696832000	-0.397869000	0.983374000
H	3.868924000	6.869144000	0.361768000	C	-4.961685000	0.012727000	0.201547000
C	4.825786000	4.984562000	-0.141008000	C	-6.133473000	0.276533000	1.151799000
H	5.808505000	5.453520000	-0.227029000	C	-6.405332000	-0.923411000	2.066036000
C	3.800780000	-1.732714000	-5.506640000	C	-5.135049000	-1.341553000	2.836209000
H	4.672006000	-1.883395000	-6.148103000	H	-2.975538000	-1.927821000	2.638289000
C	2.511313000	-2.064122000	-6.016378000	H	-4.117563000	-2.523910000	1.294868000
H	2.436802000	-2.464377000	-7.029912000	H	-3.382669000	0.455701000	1.605730000
O	0.112767000	-3.856631000	3.577148000	H	-2.881006000	-0.610754000	0.283466000
C	0.239451000	-3.503519000	4.797702000	H	-4.746155000	0.907156000	-0.405029000
C	0.651200000	-4.523019000	5.823342000	H	-5.216549000	-0.790640000	-0.510900000
H	0.154066000	-5.483281000	5.628762000	H	-5.898514000	1.158827000	1.775102000
H	1.738061000	-4.685189000	5.736141000	H	-7.040634000	0.531872000	0.578610000
H	0.423968000	-4.163642000	6.834999000	H	-7.216934000	-0.694974000	2.777156000
Zn	-0.767974000	3.405922000	0.454311000	H	-6.751010000	-1.776312000	1.454348000
O	-1.608867000	4.936365000	1.316332000	H	-4.849974000	-0.530151000	3.529559000
O	-0.643277000	5.110054000	-1.176347000	H	-5.329482000	-2.235432000	3.449630000
C	-1.729012000	6.081076000	0.738239000				
C	-1.145125000	6.120396000	-0.707767000	⁵ TS _{hydr}			
O	-2.235233000	7.096194000	1.180023000	N	-0.683964000	0.010709000	2.867325000
C	-1.236115000	7.413481000	-1.450142000	C	-1.312052000	0.741007000	3.830091000
H	-2.290362000	7.727955000	-1.501151000	C	-1.797721000	0.399836000	5.109366000
H	-0.725963000	8.198777000	-0.870084000	H	-1.689495000	-0.614824000	5.491108000
H	-0.801724000	7.319291000	-2.453052000	N	-0.462217000	0.795493000	1.832665000

N	-0.901858000	2.018624000	2.056358000	H	4.663349000	-0.905400000	-4.122021000
C	-1.448939000	2.048118000	3.303820000	C	1.228796000	-1.282806000	-4.047111000
C	-2.074514000	3.080997000	4.034904000	C	0.972109000	-1.777042000	-5.343877000
H	-2.169474000	4.080957000	3.608875000	H	-0.047255000	-2.013067000	-5.654014000
Fe	-0.203434000	-2.010242000	2.958838000	C	-2.413009000	1.417997000	5.816355000
Zn	0.328628000	0.071514000	-0.065134000	H	-2.811383000	1.210897000	6.812301000
N	-1.344168000	-2.395220000	-1.029300000	C	-2.548272000	2.736278000	5.288519000
C	-1.719542000	-3.648308000	-0.655122000	H	-3.044532000	3.494893000	5.898136000
C	-2.385438000	-4.680553000	-1.347459000	C	-4.855318000	3.549167000	-2.432353000
H	-2.668721000	-4.569890000	-2.394075000	H	-5.581908000	4.363248000	-2.476787000
N	-0.743048000	-1.825107000	-0.001488000	C	-5.026106000	2.430980000	-3.299068000
N	-0.700302000	-2.631146000	1.036125000	H	-5.872418000	2.427761000	-3.989317000
C	-1.309357000	-3.802741000	0.690045000	C	-2.638734000	-5.837839000	-0.633565000
C	-1.572103000	-4.985523000	1.411617000	H	-3.151296000	-6.668525000	-1.123968000
H	-1.238980000	-5.084503000	2.442808000	C	-2.242384000	-5.983982000	0.727438000
N	1.697796000	-1.464212000	2.355582000	H	-2.469837000	-6.921565000	1.239551000
N	-1.795055000	2.282199000	-0.784361000	C	4.744855000	-1.885016000	4.453718000
C	-2.903922000	2.539291000	-1.528797000	H	5.124457000	-2.144077000	5.444737000
C	-3.799949000	3.627521000	-1.541670000	C	5.673600000	-1.489851000	3.450213000
H	-3.669950000	4.472384000	-0.865583000	H	6.737903000	-1.465811000	3.694109000
N	-1.337795000	1.094737000	-1.125296000	C	3.686351000	5.818114000	0.025802000
N	-2.081205000	0.549458000	-2.071486000	H	3.860377000	6.884527000	0.186449000
C	-3.086718000	1.417339000	-2.370843000	C	4.780500000	5.000573000	-0.382759000
C	-4.157040000	1.354824000	-3.286231000	H	5.757425000	5.467815000	-0.525445000
H	-4.284421000	0.499257000	-3.947948000	C	3.395888000	-1.631374000	-5.727218000
N	0.400986000	-0.998364000	-3.003144000	H	4.225146000	-1.776719000	-6.423234000
N	1.189399000	3.086621000	0.122993000	C	2.074898000	-1.943183000	-6.162988000
N	1.141767000	-0.566984000	-2.002517000	H	1.935113000	-2.323657000	-7.177246000
N	1.865067000	-0.988331000	1.131938000	O	0.511063000	-4.098960000	3.491946000
N	1.589899000	1.862244000	-0.178623000	C	0.643444000	-3.663219000	4.661913000
C	2.262474000	3.916407000	0.009813000	C	1.096642000	-4.567802000	5.779635000
C	2.419666000	5.300550000	0.229547000	H	0.673598000	-5.572929000	5.649078000
H	1.584701000	5.920078000	0.556861000	H	2.194326000	-4.657625000	5.729919000
N	2.868228000	1.836761000	-0.491557000	H	0.820508000	-4.151904000	6.756916000
C	3.352793000	3.105403000	-0.389366000	Zn	-0.767062000	3.444340000	0.553204000
C	4.642826000	3.640326000	-0.594956000	O	-1.550680000	4.980622000	1.458889000
H	5.466720000	2.991186000	-0.895604000	O	-0.733298000	5.140913000	-1.087059000
N	3.138244000	-0.806740000	0.854324000	C	-1.700247000	6.123651000	0.884619000
C	3.865403000	-1.154960000	1.948228000	C	-1.200525000	6.155772000	-0.592939000
C	5.253042000	-1.109107000	2.189643000	O	-2.177451000	7.142122000	1.350445000
H	5.943285000	-0.757458000	1.422416000	C	-1.326402000	7.447309000	-1.332739000
C	2.936090000	-1.570037000	2.933239000	H	-2.379989000	7.767941000	-1.323812000
C	3.380117000	-1.925428000	4.226227000	H	-0.779127000	8.231096000	-0.785392000
H	2.667611000	-2.167269000	5.009748000	H	-0.951101000	7.347807000	-2.358719000
N	2.423197000	-0.545739000	-2.323813000	Zn	-1.641535000	-1.324865000	-2.730950000
C	2.541441000	-0.984624000	-3.607167000	O	-2.153438000	-2.082371000	-4.444136000
C	3.655243000	-1.152114000	-4.455451000	O	-3.954596000	-1.866010000	-2.463510000

C	-3.326793000	-2.557852000	-4.682136000	H	-2.552525000	4.251737000	2.938440000
C	-4.322092000	-2.422111000	-3.487364000	Fe	0.061760000	-1.487067000	3.334031000
O	-3.730994000	-3.080941000	-5.704029000	Zn	0.324232000	-0.007775000	-0.094677000
C	-5.691980000	-2.988498000	-3.669445000	N	-1.033701000	-2.777611000	-0.403206000
H	-6.152410000	-2.546006000	-4.566400000	C	-1.407738000	-3.884310000	0.295283000
H	-5.608020000	-4.065351000	-3.887031000	C	-1.987627000	-5.101633000	-0.115735000
H	-6.308513000	-2.816779000	-2.778451000	H	-2.192809000	-5.301117000	-1.167410000
Zn	3.781606000	-0.001924000	-0.913162000	N	-0.533643000	-1.906064000	0.449108000
O	4.971757000	-1.966220000	-1.349299000	N	-0.554194000	-2.370703000	1.679137000
O	5.609605000	0.626919000	-1.189021000	C	-1.105618000	-3.625803000	1.651724000
C	6.572461000	-0.176348000	-1.484558000	C	-1.392392000	-4.567435000	2.662234000
C	6.142679000	-1.674790000	-1.541577000	H	-1.158986000	-4.344909000	3.700579000
O	7.736781000	0.096999000	-1.711281000	N	1.942139000	-0.820961000	2.497907000
C	7.203184000	-2.684019000	-1.836574000	N	-2.102230000	1.665037000	-1.230708000
H	7.691962000	-2.427246000	-2.789405000	C	-3.146523000	1.627659000	-2.103424000
H	7.994114000	-2.608211000	-1.073435000	C	-4.180289000	2.543744000	-2.382712000
H	6.781758000	-3.696375000	-1.866328000	H	-4.244631000	3.497569000	-1.860573000
O	-1.803508000	-2.385439000	3.510276000	N	-1.457959000	0.517441000	-1.315077000
O	0.444472000	-2.425677000	4.901588000	N	-2.015673000	-0.281854000	-2.203576000
C	-3.731410000	-1.741003000	1.990819000	C	-3.083971000	0.367397000	-2.743281000
C	-3.552585000	-0.397084000	1.321509000	C	-4.029016000	-0.010998000	-3.718154000
C	-4.823639000	-0.037208000	0.524070000	H	-3.961886000	-0.972378000	-4.226761000
C	-6.065351000	-0.084651000	1.419998000	N	0.606315000	-1.708181000	-2.705867000
C	-6.207848000	-1.439094000	2.123643000	N	0.650714000	3.088443000	-0.470224000
C	-4.929574000	-1.801171000	2.910019000	N	1.246376000	-0.917541000	-1.868772000
H	-2.688254000	-2.036178000	2.753674000	N	2.017437000	-0.535916000	1.210683000
H	-3.695483000	-2.581536000	1.279709000	N	1.250071000	1.913033000	-0.570157000
H	-3.386655000	0.378806000	2.087429000	C	1.567189000	4.049819000	-0.767582000
H	-2.681016000	-0.394937000	0.657501000	C	1.492105000	5.458041000	-0.795454000
H	-4.707359000	0.963918000	0.077898000	H	0.569006000	5.981007000	-0.546442000
H	-4.930569000	-0.744454000	-0.315659000	N	2.511351000	2.042559000	-0.925473000
H	-5.990621000	0.711904000	2.182890000	C	2.774802000	3.371400000	-1.064307000
H	-6.970621000	0.133596000	0.828753000	C	3.953818000	4.066039000	-1.411521000
H	-7.077183000	-1.436038000	2.802469000	H	4.871676000	3.518002000	-1.629952000
H	-6.397618000	-2.223621000	1.369036000	N	3.249967000	-0.235915000	0.850357000
H	-4.794966000	-1.077119000	3.733407000	C	4.039712000	-0.302352000	1.953002000
H	-5.025115000	-2.798104000	3.368143000	C	5.413030000	-0.036280000	2.126631000
³IM_{hydr}				H	6.034747000	0.271800000	1.285868000
				C	3.195609000	-0.669154000	3.030017000
N	-0.627900000	0.302795000	2.846229000	C	3.710202000	-0.746348000	4.343737000
C	-1.184797000	1.181494000	3.731193000	H	3.052946000	-0.942416000	5.186705000
C	-1.414556000	1.107991000	5.121092000	N	2.492239000	-0.711690000	-2.257972000
H	-1.103037000	0.232724000	5.689420000	C	2.689480000	-1.399004000	-3.416465000
N	-0.653767000	0.849563000	1.647282000	C	3.805476000	-1.525358000	-4.269151000
N	-1.214152000	2.042757000	1.678986000	H	4.742496000	-1.011023000	-4.055538000
C	-1.576609000	2.305738000	2.966163000	C	1.465003000	-2.048206000	-3.706389000
C	-2.241712000	3.404813000	3.551566000	C	1.303162000	-2.860524000	-4.848976000

H	0.349934000	-3.354162000	-5.046270000	C	-5.317014000	-4.224115000	-2.960962000
C	-2.058531000	2.194334000	5.685382000	H	-5.758211000	-3.978160000	-3.939503000
H	-2.265977000	2.192242000	6.757886000	H	-5.213124000	-5.320856000	-2.955956000
C	-2.470791000	3.320560000	4.913433000	H	-5.959959000	-3.886185000	-2.138884000
H	-2.984256000	4.141527000	5.419100000	Zn	3.734572000	0.343688000	-1.045031000
C	-5.113053000	2.156772000	-3.328117000	O	5.265594000	-1.434096000	-1.162872000
H	-5.937184000	2.829397000	-3.575098000	O	5.412895000	1.212954000	-1.528058000
C	-5.032710000	0.900003000	-3.994542000	C	6.504036000	0.553114000	-1.711407000
H	-5.790402000	0.653252000	-4.741328000	C	6.358216000	-0.980577000	-1.467516000
C	-2.262419000	-6.021099000	0.879768000	O	7.595129000	0.982135000	-2.039016000
H	-2.710434000	-6.981374000	0.614659000	C	7.582535000	-1.821315000	-1.625935000
C	-1.973504000	-5.752933000	2.248821000	H	7.996187000	-1.671576000	-2.635523000
H	-2.215911000	-6.514858000	2.992932000	H	8.360298000	-1.458303000	-0.935366000
C	5.060994000	-0.491448000	4.504613000	H	7.356350000	-2.878938000	-1.442530000
H	5.491937000	-0.531942000	5.507613000	O	-1.457220000	-1.880638000	4.172250000
C	5.906867000	-0.147600000	3.412706000	O	0.940256000	-1.393047000	5.469326000
H	6.962836000	0.055070000	3.604550000	C	-4.078914000	-1.301465000	2.543255000
C	2.651120000	6.132087000	-1.135678000	C	-3.746530000	-1.172654000	1.091524000
H	2.644779000	7.224014000	-1.167338000	C	-4.837599000	-0.371602000	0.348117000
C	3.862723000	5.446079000	-1.442060000	C	-5.087916000	0.972653000	1.035877000
H	4.745276000	6.034538000	-1.702563000	C	-5.512024000	0.772995000	2.495276000
C	3.639545000	-2.320437000	-5.389219000	C	-4.466740000	-0.056643000	3.278119000
H	4.473978000	-2.448023000	-6.082523000	H	-2.246454000	-1.727047000	3.613807000
C	2.408224000	-2.980730000	-5.672910000	H	-4.331883000	-2.283391000	2.956174000
H	2.340596000	-3.597058000	-6.572119000	H	-2.797036000	-0.617565000	0.974693000
O	0.940266000	-3.156050000	4.169585000	H	-3.605191000	-2.151980000	0.615156000
C	1.176520000	-2.621054000	5.306347000	H	-4.548472000	-0.236146000	-0.702913000
C	1.789625000	-3.452754000	6.398708000	H	-5.773201000	-0.958413000	0.340188000
H	1.405781000	-4.481165000	6.360831000	H	-4.165347000	1.580668000	0.999757000
H	2.879185000	-3.492926000	6.234608000	H	-5.856980000	1.544712000	0.490607000
H	1.596953000	-2.998376000	7.379030000	H	-5.658171000	1.744535000	2.995136000
Zn	-1.348506000	3.168973000	-0.065365000	H	-6.484137000	0.249102000	2.518376000
O	-2.382840000	4.671396000	0.617391000	H	-3.578340000	0.585352000	3.409018000
O	-1.571000000	4.602807000	-1.933752000	H	-4.829176000	-0.285070000	4.291881000
C	-2.705326000	5.684547000	-0.109294000				
C	-2.200241000	5.589114000	-1.581771000	⁵ IM _{hydr}			
O	-3.339066000	6.671467000	0.216539000	N	-0.434862000	0.341433000	2.929703000
C	-2.519469000	6.728622000	-2.493127000	C	-1.005874000	1.177923000	3.838596000
H	-3.609976000	6.881155000	-2.513976000	C	-1.169528000	1.077783000	5.235925000
H	-2.104513000	7.656387000	-2.068111000	H	-0.791543000	0.212009000	5.779480000
H	-2.124634000	6.545934000	-3.500154000	N	-0.559345000	0.883409000	1.735501000
Zn	-1.370541000	-2.217186000	-2.336998000	N	-1.191723000	2.041636000	1.798050000
O	-1.773652000	-3.411412000	-3.815737000	C	-1.502349000	2.280866000	3.102901000
O	-3.635225000	-2.841301000	-1.967743000	C	-2.197414000	3.336805000	3.731387000
C	-2.925781000	-3.966325000	-3.973991000	H	-2.579887000	4.173381000	3.144936000
C	-3.961551000	-3.605289000	-2.863337000	Fe	0.339354000	-1.580859000	3.300667000
O	-3.282447000	-4.713762000	-4.865769000	Zn	0.274666000	0.005684000	-0.079742000

N	-1.023344000	-2.798359000	-0.463754000	C	-2.356033000	3.228127000	5.101872000
C	-1.311480000	-3.953280000	0.196541000	H	-2.888620000	4.015379000	5.640338000
C	-1.901813000	-5.159929000	-0.230775000	C	-5.327520000	2.186221000	-3.004427000
H	-2.196269000	-5.307830000	-1.269578000	H	-6.167411000	2.856553000	-3.198990000
N	-0.462777000	-1.967703000	0.393166000	C	-5.265367000	0.946520000	-3.704291000
N	-0.361307000	-2.505536000	1.589584000	H	-6.052424000	0.710771000	-4.423757000
C	-0.892136000	-3.764511000	1.533945000	C	-2.068716000	-6.139060000	0.731584000
C	-1.066429000	-4.768065000	2.509796000	H	-2.520226000	-7.093775000	0.452613000
H	-0.731558000	-4.605823000	3.531599000	C	-1.661662000	-5.941610000	2.082642000
N	2.057542000	-0.889176000	2.415829000	H	-1.819026000	-6.750776000	2.799204000
N	-2.223161000	1.674541000	-1.054963000	C	5.266645000	-0.442905000	4.261208000
C	-3.305268000	1.646242000	-1.879768000	H	5.755043000	-0.486035000	5.237413000
C	-4.357963000	2.559208000	-2.091124000	C	6.030816000	-0.028374000	3.134777000
H	-4.407152000	3.499269000	-1.542857000	H	7.083779000	0.226430000	3.273070000
N	-1.572544000	0.535613000	-1.193665000	C	2.483432000	6.206484000	-1.086583000
N	-2.162594000	-0.247997000	-2.075880000	H	2.460036000	7.298612000	-1.093037000
C	-3.259989000	0.402138000	-2.551451000	C	3.692281000	5.546177000	-1.454299000
C	-4.243384000	0.038387000	-3.493679000	H	4.555469000	6.153812000	-1.734901000
H	-4.189999000	-0.909354000	-4.028566000	C	3.389045000	-2.070974000	-5.607170000
N	0.463342000	-1.581060000	-2.782024000	H	4.195574000	-2.166691000	-6.337640000
N	0.554639000	3.118367000	-0.414534000	C	2.150466000	-2.727496000	-5.866457000
N	1.132693000	-0.819237000	-1.941167000	H	2.049539000	-3.309443000	-6.785241000
N	2.050027000	-0.567112000	1.131419000	O	1.375476000	-3.535867000	3.951060000
N	1.166276000	1.954455000	-0.562787000	C	1.583868000	-2.928144000	5.025501000
C	1.444885000	4.100083000	-0.724861000	C	2.263281000	-3.599324000	6.191412000
C	1.348271000	5.507257000	-0.717791000	H	2.067702000	-4.679362000	6.176142000
H	0.428135000	6.010213000	-0.421052000	H	3.351117000	-3.447851000	6.093647000
N	2.411028000	2.112206000	-0.962801000	H	1.936806000	-3.154506000	7.140588000
C	2.649941000	3.447356000	-1.082138000	Zn	-1.426536000	3.177732000	0.079104000
C	3.804609000	4.167321000	-1.458117000	O	-2.445606000	4.667552000	0.811137000
H	4.721486000	3.638544000	-1.723273000	O	-1.734718000	4.619867000	-1.770985000
N	3.243822000	-0.198019000	0.721683000	C	-2.803037000	5.682772000	0.104119000
C	4.093812000	-0.250175000	1.779865000	C	-2.354908000	5.600174000	-1.387705000
C	5.458781000	0.085126000	1.881951000	O	-3.431267000	6.662822000	0.460199000
H	6.011591000	0.446642000	1.014771000	C	-2.715685000	6.743977000	-2.277927000
C	3.329712000	-0.684653000	2.889853000	H	-3.806920000	6.890692000	-2.254787000
C	3.923848000	-0.766174000	4.169650000	H	-2.288993000	7.671108000	-1.863255000
H	3.328155000	-1.025492000	5.039837000	H	-2.359824000	6.570113000	-3.300914000
N	2.360717000	-0.591244000	-2.372828000	Zn	-1.483277000	-2.154553000	-2.341064000
C	2.514445000	-1.231963000	-3.564084000	O	-1.928347000	-3.275968000	-3.864716000
C	3.595970000	-1.318393000	-4.464744000	O	-3.709369000	-2.868384000	-1.899502000
H	4.538563000	-0.806895000	-4.269273000	C	-3.067306000	-3.864110000	-3.994401000
C	1.282394000	-1.877010000	-3.829134000	C	-4.056139000	-3.596988000	-2.816682000
C	1.078824000	-2.645919000	-4.994937000	O	-3.443724000	-4.578390000	-4.905082000
H	0.120984000	-3.137892000	-5.172745000	C	-5.393433000	-4.258469000	-2.879333000
C	-1.848339000	2.119172000	5.842346000	H	-5.892125000	-3.979544000	-3.820719000
H	-2.010651000	2.094396000	6.922335000	H	-5.252659000	-5.349588000	-2.936976000

H	-6.004503000	-3.986112000	-2.009961000	H	-1.867846000	-5.409643000	-1.348528000
Zn	3.641458000	0.435188000	-1.182108000	N	-0.527505000	-1.916944000	0.358499000
O	5.173971000	-1.327306000	-1.402232000	N	-0.372950000	-2.436369000	1.552052000
O	5.299347000	1.329488000	-1.692717000	C	-0.743842000	-3.750363000	1.473334000
C	6.381794000	0.678904000	-1.948816000	C	-0.784191000	-4.792373000	2.427296000
C	6.251216000	-0.861518000	-1.741262000	H	-0.435919000	-4.617298000	3.444186000
O	7.454552000	1.121221000	-2.316407000	N	1.809034000	-0.721650000	2.584107000
C	7.469445000	-1.692859000	-1.976251000	N	-2.221953000	1.682092000	-1.193727000
H	7.838324000	-1.513318000	-2.998253000	C	-3.394495000	1.584580000	-1.876877000
H	8.275626000	-1.346601000	-1.310074000	C	-4.468261000	2.482978000	-2.037956000
H	7.254064000	-2.756020000	-1.813065000	H	-4.456697000	3.464434000	-1.563179000
O	-1.151394000	-2.030165000	4.163675000	N	-1.570858000	0.544621000	-1.328636000
O	1.263978000	-1.691918000	5.127863000	N	-2.245949000	-0.305633000	-2.079556000
C	-3.850221000	-1.614190000	2.676721000	C	-3.409049000	0.295540000	-2.459136000
C	-3.638285000	-1.341781000	1.222790000	C	-4.490923000	-0.134968000	-3.254125000
C	-4.777142000	-0.464197000	0.658495000	H	-4.492890000	-1.119640000	-3.719034000
C	-4.944649000	0.808702000	1.491625000	N	0.489621000	-1.581733000	-2.778200000
C	-5.238306000	0.472697000	2.958242000	N	0.662804000	3.092552000	-0.753418000
C	-4.145808000	-0.443046000	3.559733000	N	1.161205000	-0.879051000	-1.887798000
H	-1.930616000	-2.019662000	3.570637000	N	1.916342000	-0.440394000	1.299054000
H	-4.088203000	-2.629541000	3.010206000	N	1.242316000	1.905716000	-0.679269000
H	-2.695759000	-0.779192000	1.085395000	C	1.609563000	3.997263000	-1.124120000
H	-3.548138000	-2.267319000	0.639241000	C	1.561963000	5.391692000	-1.329792000
H	-4.577427000	-0.227604000	-0.395780000	H	0.639095000	5.953942000	-1.188127000
H	-5.718738000	-1.041114000	0.675486000	N	2.520252000	1.973214000	-0.988098000
H	-4.020103000	1.410783000	1.427966000	C	2.815369000	3.270566000	-1.279161000
H	-5.751464000	1.435533000	1.076561000	C	4.020671000	3.900102000	-1.658053000
H	-5.316516000	1.392912000	3.560035000	H	4.935864000	3.316208000	-1.768416000
H	-6.215782000	-0.037842000	3.020899000	N	3.177784000	-0.248162000	0.947342000
H	-3.233710000	0.167928000	3.669599000	C	3.948553000	-0.387977000	2.057968000
H	-4.420103000	-0.764050000	4.575964000	C	5.337192000	-0.255221000	2.263199000
³PC_{hydr}				H	6.006074000	0.000109000	1.441069000
N	-0.572197000	0.621706000	2.795161000	C	3.062006000	-0.686383000	3.122045000
C	-0.881401000	1.656498000	3.634727000	C	3.536345000	-0.837543000	4.442991000
C	-0.902498000	1.768092000	5.042372000	H	2.843005000	-0.990512000	5.267984000
H	-0.588865000	0.937459000	5.673372000	N	2.433960000	-0.765769000	-2.220406000
N	-0.706417000	1.050755000	1.556406000	C	2.620553000	-1.425465000	-3.396755000
N	-1.118687000	2.307358000	1.521287000	C	3.756342000	-1.615064000	-4.210451000
C	-1.254520000	2.739685000	2.802403000	H	4.721344000	-1.183578000	-3.944510000
C	-1.686767000	3.974612000	3.333714000	C	1.359597000	-1.961151000	-3.755659000
H	-1.986528000	4.786226000	2.668902000	C	1.182454000	-2.727884000	-4.927035000
Fe	-0.083627000	-1.186107000	3.344933000	H	0.205243000	-3.148085000	-5.171065000
Zn	0.245806000	0.031481000	-0.103432000	C	-1.319852000	2.984497000	5.552465000
N	-0.988825000	-2.795434000	-0.516251000	H	-1.349542000	3.124733000	6.635530000
C	-1.144893000	-3.978012000	0.133077000	C	-1.711658000	4.068771000	4.713163000
C	-1.591853000	-5.240201000	-0.307456000	H	-2.037769000	5.001402000	5.179359000
				C	-5.531119000	2.045075000	-2.807680000

H	-6.390922000	2.701131000	-2.959599000	O	5.413761000	1.007856000	-1.457466000
C	-5.537850000	0.755761000	-3.413740000	C	6.473458000	0.292259000	-1.606289000
H	-6.398920000	0.466449000	-4.020104000	C	6.250923000	-1.226013000	-1.324544000
C	-1.638612000	-6.247578000	0.639522000	O	7.588997000	0.657805000	-1.930226000
H	-1.975229000	-7.244835000	0.347297000	C	7.435661000	-2.127964000	-1.446623000
C	-1.242183000	-6.023408000	1.988409000	H	7.865528000	-2.025882000	-2.455360000
H	-1.284526000	-6.858554000	2.691482000	H	8.223114000	-1.783164000	-0.757784000
C	4.901521000	-0.713610000	4.632710000	H	7.157507000	-3.168284000	-1.237316000
H	5.312358000	-0.814265000	5.639874000	O	-2.109868000	-1.722833000	3.809024000
C	5.792167000	-0.431352000	3.557516000	O	0.484413000	-0.987655000	5.551795000
H	6.859099000	-0.332525000	3.769752000	C	-3.398354000	-1.388871000	3.216418000
C	2.747056000	6.002197000	-1.699936000	C	-3.350109000	-1.404232000	1.689194000
H	2.762669000	7.081527000	-1.867820000	C	-4.671038000	-0.940072000	1.068306000
C	3.957041000	5.266732000	-1.864769000	C	-5.067705000	0.440893000	1.594212000
H	4.860627000	5.805700000	-2.158292000	C	-5.163583000	0.424087000	3.123875000
C	3.573797000	-2.360587000	-5.361770000	C	-3.847293000	-0.038181000	3.759712000
H	4.422865000	-2.533846000	-6.026862000	H	-2.031917000	-2.681986000	3.910672000
C	2.307299000	-2.913335000	-5.711522000	H	-4.109215000	-2.161466000	3.561270000
H	2.228242000	-3.499853000	-6.629588000	H	-2.548233000	-0.728165000	1.364017000
O	0.326250000	-2.842985000	4.402442000	H	-3.097873000	-2.411103000	1.327593000
C	0.543455000	-2.239631000	5.509888000	H	-4.572668000	-0.941627000	-0.028033000
C	0.923999000	-3.053070000	6.719635000	H	-5.470491000	-1.665707000	1.306624000
H	0.348958000	-3.988949000	6.755801000	H	-4.307366000	1.180021000	1.282421000
H	1.989635000	-3.322900000	6.633870000	H	-6.022634000	0.765583000	1.150326000
H	0.779557000	-2.470975000	7.638500000	H	-5.423172000	1.422421000	3.510385000
Zn	-1.312881000	3.279207000	-0.297036000	H	-5.983645000	-0.252412000	3.427491000
O	-2.199801000	4.922434000	0.263277000	H	-3.068290000	0.701447000	3.537507000
O	-1.652015000	4.445484000	-2.315678000	H	-3.926039000	-0.091438000	4.856844000
C	-2.533857000	5.846185000	-0.569073000				
C	-2.197711000	5.506738000	-2.054365000	⁵ PC _{hydr}			
O	-3.065329000	6.915847000	-0.332545000	N	-0.751186000	0.419987000	2.871017000
C	-2.566293000	6.517977000	-3.090377000	C	-1.174072000	1.360450000	3.759310000
H	-3.646872000	6.721916000	-3.028674000	C	-1.375003000	1.315604000	5.154738000
H	-2.075381000	7.474413000	-2.850684000	H	-1.137217000	0.414919000	5.721599000
H	-2.285646000	6.170606000	-4.092378000	N	-0.740440000	0.966747000	1.671033000
Zn	-1.473545000	-2.163163000	-2.381914000	N	-1.153617000	2.221246000	1.710749000
O	-1.869431000	-3.338691000	-3.875963000	C	-1.448102000	2.526235000	3.004106000
O	-3.658046000	-3.021566000	-1.890585000	C	-1.954225000	3.698844000	3.605853000
C	-2.938088000	-4.054104000	-3.944892000	H	-2.175294000	4.580050000	3.001601000
C	-3.923875000	-3.845142000	-2.752425000	Fe	-0.349507000	-1.609738000	3.187579000
O	-3.254863000	-4.847798000	-4.812028000	Zn	0.296253000	0.026161000	-0.021932000
C	-5.163233000	-4.679945000	-2.736615000	N	-0.962746000	-2.725627000	-0.807008000
H	-5.710259000	-4.538305000	-3.681505000	C	-1.219574000	-3.972695000	-0.333006000
H	-4.878388000	-5.744187000	-2.721688000	C	-1.643168000	-5.153518000	-0.976302000
H	-5.789714000	-4.430877000	-1.871110000	H	-1.801349000	-5.183650000	-2.054503000
Zn	3.691503000	0.231553000	-0.961879000	N	-0.564186000	-1.978241000	0.207336000
O	5.135107000	-1.619876000	-1.021352000	N	-0.556641000	-2.654780000	1.337287000

C	-0.964887000	-3.929470000	1.058874000	C	-1.818631000	-6.266166000	-0.173680000
C	-1.148650000	-5.071903000	1.869483000	H	-2.141590000	-7.207621000	-0.623821000
H	-0.957374000	-5.025461000	2.940842000	C	-1.580168000	-6.221417000	1.229752000
N	1.678843000	-1.131989000	2.568103000	H	-1.735079000	-7.130649000	1.815211000
N	-2.042054000	1.846239000	-1.132705000	C	4.613684000	-1.523603000	4.794904000
C	-3.143408000	1.858938000	-1.931132000	H	4.952448000	-1.802801000	5.795216000
C	-4.166423000	2.811787000	-2.109331000	C	5.581407000	-1.083536000	3.845772000
H	-4.169719000	3.745738000	-1.547113000	H	6.631153000	-1.044259000	4.145371000
N	-1.420713000	0.696635000	-1.306106000	C	2.999166000	6.083970000	-0.859464000
N	-2.048205000	-0.054954000	-2.191981000	H	3.042870000	7.174226000	-0.912464000
C	-3.145978000	0.626651000	-2.624772000	C	4.204971000	5.342054000	-1.026096000
C	-4.160326000	0.311725000	-3.552188000	H	5.133826000	5.887669000	-1.206746000
H	-4.151411000	-0.628649000	-4.101062000	C	3.914914000	-1.842679000	-5.310307000
N	0.688194000	-1.321485000	-2.839060000	H	4.800821000	-1.949709000	-5.940378000
N	0.812977000	3.140101000	-0.351149000	C	2.669701000	-2.343844000	-5.790297000
N	1.307403000	-0.725008000	-1.839724000	H	2.643010000	-2.826714000	-6.769698000
N	1.879229000	-0.659080000	1.353135000	O	-0.684500000	-3.469209000	4.377815000
N	1.365814000	1.938228000	-0.363944000	C	-0.257692000	-2.864972000	5.410498000
C	1.795613000	4.056571000	-0.566420000	C	-0.184090000	-3.599757000	6.726298000
C	1.783410000	5.465510000	-0.628183000	H	-1.038254000	-4.282475000	6.833775000
H	0.862673000	6.030797000	-0.484670000	H	0.732472000	-4.212651000	6.731158000
N	2.662048000	2.009626000	-0.584443000	H	-0.137728000	-2.895734000	7.566806000
C	2.996510000	3.322707000	-0.721257000	Zn	-1.184146000	3.340269000	-0.029986000
C	4.233359000	3.960341000	-0.958935000	O	-2.098142000	4.945008000	0.594162000
H	5.144034000	3.370493000	-1.074762000	O	-1.324263000	4.689617000	-1.958131000
N	3.162658000	-0.429071000	1.124411000	C	-2.339720000	5.948062000	-0.176210000
C	3.852962000	-0.756444000	2.248623000	C	-1.871740000	5.737187000	-1.649658000
C	5.224545000	-0.688527000	2.568930000	O	-2.875667000	7.003528000	0.108809000
H	5.955235000	-0.320566000	1.848218000	C	-2.122313000	6.848731000	-2.615647000
C	2.890917000	-1.203004000	3.187430000	H	-3.199528000	7.077447000	-2.632649000
C	3.264671000	-1.586747000	4.493427000	H	-1.636011000	7.764727000	-2.244493000
H	2.506659000	-1.874029000	5.221578000	H	-1.757258000	6.586190000	-3.616251000
N	2.597737000	-0.588250000	-2.085796000	Zn	-1.298619000	-1.894847000	-2.629233000
C	2.850508000	-1.118388000	-3.313798000	O	-1.594961000	-2.907729000	-4.261422000
C	4.031601000	-1.227797000	-4.076337000	O	-3.532429000	-2.729799000	-2.410147000
H	4.980024000	-0.834875000	-3.709971000	C	-2.675292000	-3.567816000	-4.497493000
C	1.611737000	-1.601268000	-3.800541000	C	-3.751274000	-3.448148000	-3.373483000
C	1.501443000	-2.235185000	-5.056608000	O	-2.941116000	-4.249324000	-5.470586000
H	0.539208000	-2.618137000	-5.400512000	C	-5.012390000	-4.230085000	-3.545847000
C	-1.865419000	2.471039000	5.736427000	H	-5.470160000	-3.975641000	-4.514186000
H	-2.037283000	2.495342000	6.815069000	H	-4.762131000	-5.301025000	-3.614126000
C	-2.155121000	3.641507000	4.973671000	H	-5.703711000	-4.043575000	-2.714687000
H	-2.546480000	4.519601000	5.492548000	Zn	3.803621000	0.257827000	-0.677661000
C	-5.164519000	2.486732000	-3.009962000	O	5.219840000	-1.614576000	-0.837607000
H	-5.983960000	3.188303000	-3.180291000	O	5.563600000	1.036823000	-1.000414000
C	-5.156389000	1.255855000	-3.727620000	C	6.620970000	0.316813000	-1.146475000
H	-5.964779000	1.056080000	-4.434273000	C	6.358402000	-1.216570000	-1.030348000

O	7.760976000	0.689236000	-1.357323000	C	2.890950000	-0.050860000	-0.487765000
C	7.535436000	-2.126716000	-1.165700000	O	2.092202000	0.205865000	0.501943000
H	8.031063000	-1.936274000	-2.130508000	O	4.085194000	0.157090000	-0.562587000
H	8.281584000	-1.866841000	-0.398123000	C	2.120103000	-0.668956000	-1.672456000
H	7.229244000	-3.176430000	-1.077489000	O	0.869467000	-0.419993000	-1.706734000
O	-2.620913000	-1.779852000	3.479802000	C	2.864272000	-1.048111000	-2.905232000
O	0.144131000	-1.669918000	5.325985000	H	3.116947000	-0.125701000	-3.454683000
C	-3.805290000	-1.423263000	2.731811000	H	3.808667000	-1.535664000	-2.632342000
C	-3.566001000	-1.483536000	1.223365000	H	2.252102000	-1.695406000	-3.547330000
C	-4.780695000	-0.995068000	0.428692000	C	1.555161000	-1.367541000	3.219758000
C	-5.189491000	0.414328000	0.862880000	H	2.404175000	-1.165566000	2.547908000
C	-5.467462000	0.455937000	2.369224000	H	1.902138000	-1.333924000	4.260505000
C	-4.254040000	-0.031956000	3.167740000	H	1.157892000	-2.359544000	2.963797000
H	-2.598660000	-2.727975000	3.680962000	C	-5.123553000	-1.714034000	0.052291000
H	-4.596781000	-2.147947000	2.998266000	H	-5.814931000	-1.130083000	-0.578666000
H	-2.704178000	-0.841194000	0.990429000	H	-5.397763000	-2.778153000	-0.044565000
H	-3.300027000	-2.507737000	0.923028000	H	-5.292428000	-1.419480000	1.096744000
H	-4.551006000	-1.036549000	-0.646020000	C	-0.981346000	4.809300000	-1.491139000
H	-5.629163000	-1.685982000	0.588769000	H	-1.972584000	5.238660000	-1.266691000
H	-4.371305000	1.117600000	0.626124000	H	-0.226148000	5.588381000	-1.292201000
H	-6.069741000	0.755585000	0.294362000	H	-0.950092000	4.581068000	-2.565174000
H	-5.731074000	1.476611000	2.689626000	H	-3.697269000	-2.135143000	-2.352325000
H	-6.343641000	-0.179417000	2.595155000	H	-2.574573000	-0.654246000	1.441131000
H	-3.419945000	0.664194000	3.006076000	H	-1.193015000	-1.536290000	-2.429146000
H	-4.455114000	-0.033857000	4.250444000	H	-0.825935000	4.341236000	1.295789000
				H	-0.372733000	1.854213000	-2.078649000
				H	-0.315194000	1.967809000	2.145769000

Oxygen activation by TauD

³ RC _{TauD}				⁵ RC _{TauD}			
Fe	0.301848000	-0.379403000	0.143547000	Fe	0.305937000	-0.368348000	0.393742000
O	1.001820000	-2.220496000	0.104229000	O	0.761275000	-2.447190000	0.434255000
O	1.995257000	-2.422450000	-0.682499000	O	1.810193000	-2.813768000	-0.192189000
C	-3.699002000	-1.473790000	-0.313287000	C	-3.836534000	-1.435141000	-0.268042000
N	-3.181483000	-1.749231000	-1.570787000	N	-3.231953000	-1.942792000	-1.410254000
C	-2.635838000	-0.982337000	0.407586000	C	-2.810587000	-0.858812000	0.444377000
C	-1.862734000	-1.431459000	-1.579624000	C	-1.904540000	-1.672090000	-1.358770000
N	-1.516290000	-0.966339000	-0.394375000	N	-1.630488000	-1.016674000	-0.248276000
C	0.524641000	-0.289886000	2.977027000	C	0.251827000	0.637918000	3.166726000
O	-0.251947000	-0.435991000	1.913652000	O	-0.264367000	-0.052926000	2.166721000
O	0.393878000	0.674760000	3.713900000	O	-0.141830000	1.755946000	3.459203000
C	-0.719235000	3.572383000	-0.702499000	C	-0.316182000	3.476423000	-1.516597000
N	-0.687894000	3.546331000	0.683325000	N	-0.635445000	3.734059000	-0.190861000
C	-0.460378000	2.276503000	-1.082043000	C	-0.016684000	2.135237000	-1.548706000
C	-0.418514000	2.286621000	1.103627000	C	-0.524684000	2.588264000	0.523844000
N	-0.281684000	1.504246000	0.045439000	N	-0.151032000	1.606927000	-0.282242000
				C	2.994316000	-0.520552000	-0.369878000
				O	2.228902000	-0.035192000	0.565854000

O	4.205877000	-0.493705000	-0.427483000
C	2.162531000	-1.166892000	-1.497871000
O	0.965469000	-0.799381000	-1.600666000
C	2.879714000	-1.871454000	-2.601003000
H	3.324685000	-1.114458000	-3.269273000
H	3.703485000	-2.471153000	-2.193974000
H	2.182879000	-2.495458000	-3.176424000
C	1.384870000	-0.057691000	3.884715000
H	2.228705000	-0.130446000	3.178685000
H	1.685520000	0.507454000	4.775722000
H	1.095066000	-1.084633000	4.152699000
C	-5.294881000	-1.566053000	0.008749000
H	-5.907061000	-1.082966000	-0.771577000
H	-5.606383000	-2.622237000	0.074267000
H	-5.534711000	-1.087162000	0.967605000
C	-0.327543000	4.523584000	-2.576830000
H	-1.326733000	4.975128000	-2.699420000
H	0.382858000	5.337889000	-2.355037000
H	-0.038278000	4.081857000	-3.540029000
H	-3.701842000	-2.443518000	-2.155202000
H	-2.828961000	-0.355286000	1.407732000
H	-1.172409000	-1.945000000	-2.115512000
H	-0.888217000	4.636326000	0.194566000
H	0.293405000	1.515942000	-2.385718000
H	-0.677816000	2.497402000	1.605192000

³TS1_{TauD}

Fe	0.307898000	-0.368383000	0.150207000
O	1.038115000	-2.202900000	0.139727000
O	2.003930000	-2.381047000	-0.693884000
C	-3.683882000	-1.503979000	-0.305519000
N	-3.165405000	-1.760430000	-1.566651000
C	-2.624056000	-1.012303000	0.420155000
C	-1.849419000	-1.431623000	-1.573369000
N	-1.505645000	-0.978109000	-0.382833000
C	0.501869000	-0.230536000	2.991588000
O	-0.258143000	-0.404467000	1.921299000
O	0.334948000	0.733751000	3.721645000
C	-0.721008000	3.555478000	-0.763559000
N	-0.742892000	3.544360000	0.622697000
C	-0.435118000	2.258612000	-1.119350000
C	-0.478043000	2.291907000	1.066868000
N	-0.293730000	1.500412000	0.022710000
C	2.894332000	-0.056041000	-0.474976000
O	2.091534000	0.240366000	0.501787000
O	4.085036000	0.162948000	-0.559235000
C	2.121228000	-0.756156000	-1.617887000

O	0.870893000	-0.443148000	-1.682528000
C	2.865233000	-1.139052000	-2.853544000
H	3.084132000	-0.221600000	-3.423169000
H	3.824232000	-1.598943000	-2.583358000
H	2.263822000	-1.816163000	-3.475278000
C	1.562900000	-1.274780000	3.250771000
H	2.411887000	-1.050760000	2.585836000
H	1.898709000	-1.224587000	4.294495000
H	1.198601000	-2.280297000	2.998098000
C	-5.106132000	-1.759695000	0.058565000
H	-5.802696000	-1.174525000	-0.565518000
H	-5.371949000	-2.824864000	-0.049605000
H	-5.276489000	-1.477774000	1.106261000
C	-0.963617000	4.781536000	-1.575037000
H	-1.967154000	5.203094000	-1.394772000
H	-0.224475000	5.570141000	-1.354544000
H	-0.887227000	4.542510000	-2.644435000
H	-3.679050000	-2.140496000	-2.352454000
H	-2.564629000	-0.693110000	1.456568000
H	-1.178188000	-1.518619000	-2.423719000
H	-0.910234000	4.344585000	1.220716000
H	-0.301382000	1.825238000	-2.105909000
H	-0.405777000	1.986270000	2.115210000

⁵TS1_{TauD}

Fe	0.243821000	-0.451840000	0.258061000
O	0.927471000	-2.502730000	0.127040000
O	2.003464000	-2.683033000	-0.532365000
C	-3.764377000	-1.398156000	-0.442693000
N	-3.139672000	-1.855568000	-1.596607000
C	-2.752664000	-0.870716000	0.323606000
C	-1.812029000	-1.610803000	-1.505100000
N	-1.561237000	-1.014330000	-0.352927000
C	0.183713000	0.115103000	3.135647000
O	-0.374441000	-0.411151000	2.065132000
O	-0.151098000	1.204429000	3.580368000
C	-0.392099000	3.624490000	-1.092708000
N	-0.652595000	3.695935000	0.267340000
C	-0.132860000	2.294139000	-1.328081000
C	-0.546922000	2.455402000	0.806993000
N	-0.236220000	1.593806000	-0.146242000
C	2.908986000	-0.284289000	-0.290112000
O	2.019085000	0.057838000	0.615477000
O	4.107596000	-0.141298000	-0.189895000
C	2.256175000	-0.876975000	-1.549952000
O	1.039342000	-0.606055000	-1.732516000
C	3.138486000	-1.362627000	-2.651293000

H	3.528632000	-0.488329000	-3.199906000
H	3.998039000	-1.905660000	-2.238616000
H	2.568254000	-1.995486000	-3.344304000
C	1.282444000	-0.716806000	3.758100000
H	2.153537000	-0.661649000	3.084740000
H	1.554316000	-0.326062000	4.746890000
H	0.981448000	-1.772715000	3.821083000
C	-5.229924000	-1.525509000	-0.206304000
H	-5.817430000	-0.996712000	-0.975671000
H	-5.553131000	-2.580059000	-0.200914000
H	-5.486592000	-1.091993000	0.769477000
C	-0.412602000	4.812785000	-1.992015000
H	-1.402360000	5.300218000	-2.009723000
H	0.327827000	5.570968000	-1.685307000
H	-0.170845000	4.507508000	-3.019204000
H	-3.598548000	-2.309849000	-2.377376000
H	-2.773600000	-0.423247000	1.313388000
H	-1.064571000	-1.846364000	-2.259306000
H	-0.861465000	4.539120000	0.788512000
H	0.133743000	1.797780000	-2.257206000
H	-0.657840000	2.211242000	1.870449000

³IM_{TauD}

Fe	0.301492000	-0.382720000	0.159331000
O	0.996331000	-2.179933000	0.197786000
O	1.927096000	-2.338566000	-0.729976000
C	-3.712797000	-1.415368000	-0.351755000
N	-3.189534000	-1.629294000	-1.618923000
C	-2.647644000	-0.983418000	0.403696000
C	-1.865972000	-1.333963000	-1.601590000
N	-1.522296000	-0.943457000	-0.389087000
C	0.403764000	-0.187806000	3.022982000
O	-0.312296000	-0.368886000	1.926387000
O	0.187574000	0.764982000	3.755451000
C	-0.540183000	3.556708000	-0.829594000
N	-0.713857000	3.547835000	0.546270000
C	-0.246717000	2.253704000	-1.154889000
C	-0.529013000	2.289784000	1.014509000
N	-0.251058000	1.494124000	-0.005559000
C	2.903332000	-0.159368000	-0.424154000
O	2.099068000	0.208164000	0.524071000
O	4.084513000	0.074802000	-0.550346000
C	2.101091000	-1.009096000	-1.481857000
O	0.870437000	-0.487158000	-1.621633000
C	2.844904000	-1.348180000	-2.743954000
H	3.047049000	-0.413996000	-3.285576000
H	3.807949000	-1.814958000	-2.499119000

H	2.242933000	-2.016153000	-3.376266000
C	1.483383000	-1.207126000	3.309080000
H	2.339741000	-0.974266000	2.656824000
H	1.799130000	-1.141936000	4.358150000
H	1.143120000	-2.222445000	3.060904000
C	-5.144503000	-1.649213000	-0.010680000
H	-5.819795000	-1.020334000	-0.615327000
H	-5.436681000	-2.701580000	-0.166048000
H	-5.317526000	-1.407133000	1.046500000
C	-0.662580000	4.787635000	-1.660456000
H	-1.669968000	5.232520000	-1.592657000
H	0.065485000	5.558901000	-1.357263000
H	-0.472476000	4.545933000	-2.714945000
H	-3.705899000	-1.959283000	-2.425299000
H	-2.589830000	-0.705597000	1.451941000
H	-1.185461000	-1.396862000	-2.446744000
H	-0.921095000	4.353385000	1.124246000
H	-0.009453000	1.810680000	-2.117272000
H	-0.562955000	1.986357000	2.064475000

⁵IM_{TauD}

Fe	0.063351000	-0.405440000	0.243521000
O	-0.048178000	-2.837776000	0.054256000
O	0.876674000	-3.150344000	-0.795390000
C	-4.063427000	-0.059800000	-0.469542000
N	-3.584170000	-0.555283000	-1.676743000
C	-2.951983000	0.058282000	0.330132000
C	-2.244619000	-0.719120000	-1.583479000
N	-1.844467000	-0.353098000	-0.378895000
C	0.141274000	0.069112000	3.077748000
O	-0.567695000	-0.076101000	1.969339000
O	0.370774000	1.169062000	3.554715000
C	1.228993000	3.561658000	-1.077630000
N	0.982069000	3.750996000	0.275029000
C	0.903128000	2.245891000	-1.309714000
C	0.530462000	2.589753000	0.810613000
N	0.472608000	1.668351000	-0.135674000
C	2.510182000	-1.458238000	-0.162906000
O	1.823125000	-0.846331000	0.775646000
O	3.688953000	-1.721609000	-0.132642000
C	1.581212000	-1.827328000	-1.352453000
O	0.617432000	-0.920059000	-1.499572000
C	2.270429000	-2.297041000	-2.602656000
H	2.844910000	-1.460515000	-3.025276000
H	2.970889000	-3.107126000	-2.359515000
H	1.529793000	-2.639936000	-3.339148000
C	0.627006000	-1.214663000	3.709486000

H	1.462794000	-1.582961000	3.093358000
H	0.974870000	-1.034311000	4.734546000
H	-0.162427000	-1.980097000	3.690500000
C	-5.503967000	0.232243000	-0.225043000
H	-5.893056000	0.994259000	-0.921376000
H	-6.128749000	-0.670672000	-0.330901000
H	-5.636342000	0.612532000	0.796694000
C	1.745537000	4.637323000	-1.970515000
H	1.057949000	5.498940000	-2.019563000
H	2.727403000	5.011891000	-1.634662000
H	1.868524000	4.248194000	-2.990406000
H	-4.145525000	-0.770717000	-2.492192000
H	-2.852431000	0.397031000	1.357311000
H	-1.584553000	-1.092652000	-2.362854000
H	1.137683000	4.608236000	0.792027000
H	0.962869000	1.670022000	-2.229614000
H	0.301948000	2.419391000	1.868446000

³TS₂TauD

Fe	0.191307000	-0.502584000	0.146835000
O	0.002850000	-2.120175000	-0.184461000
O	1.455383000	-2.464567000	-1.617481000
C	-3.675692000	0.256584000	-1.276616000
N	-2.894194000	0.427510000	-2.411666000
C	-2.786778000	-0.027644000	-0.266330000
C	-1.594084000	0.242614000	-2.082785000
N	-1.512755000	-0.025220000	-0.794032000
C	-1.228110000	-1.585451000	2.415631000
O	-0.740619000	-0.534400000	1.759973000
O	-2.414999000	-1.655130000	2.670245000
C	1.192268000	3.614078000	0.483316000
N	0.371225000	3.426643000	1.586563000
C	1.212296000	2.393779000	-0.150413000
C	-0.065821000	2.143492000	1.594098000
N	0.429601000	1.505940000	0.551672000
C	2.750956000	-1.230291000	-0.015663000
O	1.906085000	-0.789061000	0.882830000
O	3.890534000	-1.568904000	0.178375000
C	2.050419000	-1.268662000	-1.452613000
O	1.137092000	-0.209179000	-1.411035000
C	3.090475000	-1.080148000	-2.563996000
H	3.513448000	-0.070314000	-2.471444000
H	3.887444000	-1.822324000	-2.433640000
H	2.612527000	-1.197061000	-3.546323000
C	-0.214898000	-2.625136000	2.834516000
H	0.689762000	-2.141318000	3.229632000
H	-0.658169000	-3.306828000	3.571194000

H	0.094549000	-3.191558000	1.942624000
C	-5.161342000	0.369530000	-1.283873000
H	-5.497270000	1.374640000	-1.590607000
H	-5.623007000	-0.363153000	-1.967024000
H	-5.549922000	0.176961000	-0.274979000
C	1.858264000	4.910665000	0.173596000
H	1.128068000	5.723090000	0.018412000
H	2.541315000	5.223315000	0.981468000
H	2.451962000	4.812881000	-0.745276000
H	-3.237395000	0.638103000	-3.341199000
H	-2.966130000	-0.268721000	0.780578000
H	-0.742719000	0.286787000	-2.757126000
H	0.147705000	4.125472000	2.285026000
H	1.732014000	2.079202000	-1.049940000
H	-0.713614000	1.694782000	2.342374000

⁵TS₂TauD

Fe	0.019014000	-0.418291000	0.303575000
O	0.163131000	-2.388847000	0.726316000
O	0.970219000	-3.001827000	-0.179660000
C	-4.215933000	-0.076375000	-0.573067000
N	-3.724075000	-0.666706000	-1.729603000
C	-3.114147000	0.083543000	0.235688000
C	-2.385490000	-0.841417000	-1.592616000
N	-1.999726000	-0.394551000	-0.414695000
C	0.047310000	0.352976000	3.059688000
O	-0.630056000	0.205252000	1.923694000
O	0.088317000	1.437493000	3.613007000
C	1.393901000	3.314234000	-1.276330000
N	0.976315000	3.668173000	-0.000454000
C	1.080591000	1.980783000	-1.389551000
C	0.440908000	2.583693000	0.609172000
N	0.492750000	1.553542000	-0.219392000
C	2.744033000	-1.339661000	-0.209349000
O	2.235724000	-0.625369000	0.691045000
O	3.873527000	-1.593513000	-0.563107000
C	1.499493000	-2.051485000	-1.101914000
O	0.596261000	-1.078177000	-1.346353000
C	2.011797000	-2.788994000	-2.313993000
H	2.534442000	-2.075650000	-2.963438000
H	2.728106000	-3.559942000	-2.003261000
H	1.173175000	-3.246245000	-2.859412000
C	0.746242000	-0.877006000	3.587717000
H	1.637162000	-1.053581000	2.963775000
H	1.051514000	-0.719031000	4.629713000
H	0.105109000	-1.764445000	3.490971000
C	-5.655572000	0.255553000	-0.377276000

H	-6.021070000	0.968305000	-1.135963000
H	-6.294343000	-0.642648000	-0.425307000
H	-5.798793000	0.714565000	0.610206000
C	2.039644000	4.272129000	-2.217481000
H	1.378321000	5.121243000	-2.460256000
H	2.975458000	4.683280000	-1.802744000
H	2.288166000	3.760280000	-3.156976000
H	-4.273920000	-0.931948000	-2.538074000
H	-3.033286000	0.503548000	1.234933000
H	-1.725682000	-1.282239000	-2.336790000
H	1.074901000	4.583008000	0.423614000
H	1.246590000	1.293854000	-2.214707000
H	0.069298000	2.552070000	1.636116000

³PC_{TauD}

Fe	-0.208098000	-0.545697000	0.118403000
O	-0.223056000	-1.988043000	0.823587000
O	-3.000756000	-0.819347000	1.663934000
C	3.669505000	0.360832000	1.145802000
N	2.941954000	0.904237000	2.197233000
C	2.734630000	-0.183535000	0.298613000
C	1.625457000	0.685096000	1.982874000
N	1.481884000	0.031917000	0.842117000
C	1.241314000	-2.216115000	-1.813976000
O	0.669141000	-1.072931000	-1.509837000
O	2.429939000	-2.287606000	-2.093740000
C	-0.946624000	3.413940000	-1.458358000
N	-0.241272000	2.801864000	-2.485066000
C	-1.035017000	2.454767000	-0.476559000
C	0.064792000	1.535088000	-2.110388000
N	-0.406814000	1.304096000	-0.899952000
C	-2.798068000	-1.948599000	-0.520827000
O	-2.173848000	-1.057111000	-0.966089000
O	-3.417869000	-2.879449000	-0.232435000
C	-2.229664000	0.018595000	2.109078000
O	-1.090644000	0.380560000	1.588508000
C	-2.545081000	0.757392000	3.404803000
H	-2.362018000	1.837294000	3.295724000
H	-3.586055000	0.575253000	3.700259000
H	-1.876077000	0.388052000	4.199328000
C	0.335975000	-3.433098000	-1.836159000
H	-0.553476000	-3.225435000	-2.451026000
H	0.873656000	-4.306240000	-2.226697000
H	-0.011459000	-3.631180000	-0.810813000
C	5.156424000	0.413457000	1.069002000
H	5.532120000	1.450547000	1.042649000
H	5.628452000	-0.094122000	1.927182000

H	5.494073000	-0.091588000	0.154218000
C	-1.449735000	4.814704000	-1.535652000
H	-0.630722000	5.540678000	-1.676255000
H	-2.162616000	4.950115000	-2.366808000
H	-1.971202000	5.074200000	-0.604308000
H	3.328812000	1.381758000	3.002202000
H	2.870682000	-0.723173000	-0.639503000
H	0.801888000	0.986699000	2.622870000
H	0.001590000	3.225024000	-3.372745000
H	-1.500926000	2.505880000	0.502343000
H	0.616856000	0.805836000	-2.698371000

⁵PC_{TauD}

Fe	-0.346953000	-0.438440000	0.053963000
O	-0.666109000	-1.897361000	0.677993000
O	-2.973749000	-0.383836000	2.014432000
C	3.892947000	-0.540957000	0.915118000
N	3.398096000	0.182631000	1.991924000
C	2.793109000	-0.820778000	0.136011000
C	2.054949000	0.313995000	1.844558000
N	1.673807000	-0.281704000	0.733349000
C	0.422505000	-2.314087000	-2.003222000
O	0.158680000	-1.063386000	-1.655480000
O	1.559099000	-2.703519000	-2.200297000
C	-0.232127000	3.663232000	-1.257852000
N	0.309992000	2.983056000	-2.340047000
C	-0.524394000	2.682379000	-0.339652000
C	0.328259000	1.657756000	-2.058549000
N	-0.172011000	1.454015000	-0.854470000
C	-3.358144000	-1.293496000	-0.380391000
O	-2.718960000	-0.431351000	-0.849672000
O	-4.020034000	-2.175196000	-0.028201000
C	-1.990953000	0.252099000	2.350471000
O	-0.980456000	0.561765000	1.572426000
C	-1.830346000	0.783623000	3.767406000
H	-1.527802000	1.841912000	3.754186000
H	-2.765393000	0.661408000	4.328435000
H	-1.029145000	0.217276000	4.270150000
C	-0.792122000	-3.204207000	-2.154837000
H	-1.569147000	-2.692417000	-2.742220000
H	-0.516853000	-4.157408000	-2.623397000
H	-1.201777000	-3.388915000	-1.148988000
C	5.334233000	-0.886044000	0.758220000
H	5.970923000	0.012988000	0.693600000
H	5.703584000	-1.498844000	1.598106000
H	5.474777000	-1.465089000	-0.164387000
C	-0.411547000	5.142442000	-1.231247000

H	0.547406000	5.676554000	-1.343424000
H	-1.083811000	5.489244000	-2.034382000
H	-0.853846000	5.445476000	-0.272574000
H	3.944777000	0.542567000	2.764789000
H	2.716636000	-1.387295000	-0.793519000
H	1.390604000	0.828540000	2.534736000
H	0.632348000	3.403059000	-3.203662000
H	-0.960901000	2.761876000	0.650926000
H	0.693214000	0.869864000	-2.712509000

Oxidation of cyclohexane to cyclohexanol by MOF

³RC_{hydr}

Fe	0.886572000	-0.921965000	-0.163761000
O	-0.223216000	-1.909622000	-0.760083000
O	2.513451000	-2.539999000	-0.210553000
C	-1.126473000	2.623922000	-0.829163000
N	-0.592766000	2.315730000	-2.074400000
C	-0.720756000	1.607326000	0.002002000
C	0.097242000	1.155088000	-1.983387000
N	0.032640000	0.718112000	-0.737864000
C	-1.025788000	-1.007508000	2.048624000
O	0.181954000	-0.722097000	1.616982000
O	-1.782684000	-0.137518000	2.464841000
C	4.346656000	1.588682000	0.902609000
N	3.663447000	1.475980000	2.104373000
C	3.595104000	0.863383000	0.006351000
C	2.557617000	0.712650000	1.907684000
N	2.499314000	0.330755000	0.648273000
C	2.780073000	-2.073531000	-1.337579000
O	2.111300000	-1.065942000	-1.783279000
C	3.904808000	-2.620185000	-2.178197000
H	4.828466000	-2.071395000	-1.930497000
H	4.065738000	-3.682049000	-1.950320000
H	3.694613000	-2.477762000	-3.246780000
C	-1.412811000	-2.471826000	2.026145000
H	-0.620106000	-3.071999000	2.497912000
H	-2.372033000	-2.632784000	2.533618000
H	-1.474367000	-2.798536000	0.977281000
C	-1.981931000	3.817685000	-0.583910000
H	-1.460969000	4.757652000	-0.832372000
H	-2.912289000	3.775497000	-1.173990000
H	-2.265450000	3.854361000	0.475838000
C	5.613476000	2.359510000	0.753063000
H	5.481208000	3.424749000	1.008693000

H	6.416491000	1.959438000	1.395338000
H	5.961327000	2.306063000	-0.287604000
H	-0.718596000	2.855728000	-2.921905000
H	-0.950499000	1.416713000	1.050069000
H	0.631913000	0.658348000	-2.789519000
H	3.942815000	1.887864000	2.986553000
H	3.763619000	0.688317000	-1.052628000
H	1.815720000	0.453918000	2.659647000
C	-4.326975000	-1.673016000	-0.285394000
C	-3.369277000	-0.772072000	-1.073148000
C	-4.007878000	0.584712000	-1.387798000
C	-4.510428000	1.273702000	-0.113430000
C	-5.482953000	0.373646000	0.657913000
C	-4.838885000	-0.979198000	0.983253000
H	-3.824111000	-2.619006000	-0.026833000
H	-5.187264000	-1.940474000	-0.928334000
H	-2.453459000	-0.616510000	-0.483426000
H	-3.043793000	-1.273065000	-1.999408000
H	-3.286867000	1.230284000	-1.917792000
H	-4.859913000	0.439245000	-2.078642000
H	-3.647687000	1.495820000	0.537807000
H	-4.988863000	2.238568000	-0.357386000
H	-5.810160000	0.874054000	1.584852000
H	-6.392438000	0.215374000	0.047621000
H	-3.993852000	-0.809374000	1.671321000
H	-5.559858000	-1.628396000	1.508896000

⁵RC_{hydr}

Fe	0.909071000	-0.942890000	-0.100660000
O	-0.304481000	-1.786753000	-0.740297000
O	2.329336000	-2.373712000	-0.592342000
C	-1.181972000	2.763519000	-0.559317000
N	-0.635329000	2.579880000	-1.822501000
C	-0.733788000	1.695353000	0.182547000
C	0.101378000	1.440067000	-1.819073000
N	0.056645000	0.898536000	-0.618577000
C	-0.923784000	-1.263160000	2.104088000
O	0.312763000	-1.008188000	1.721576000
O	-1.704273000	-0.376033000	2.416305000
C	4.335969000	1.483660000	0.928896000
N	3.755185000	1.223419000	2.161568000
C	3.537233000	0.828918000	0.020803000
C	2.659684000	0.446683000	1.973212000
N	2.511003000	0.192842000	0.687541000
C	2.628119000	-1.844059000	-1.704973000
O	2.079004000	-0.765367000	-2.056844000
C	3.680625000	-2.495456000	-2.568799000

H	3.620993000	-2.122135000	-3.599072000	C	-0.042215000	1.857007000	-1.642269000
H	4.674087000	-2.253250000	-2.157184000	N	-0.010822000	1.232988000	-0.479582000
H	3.568306000	-3.588107000	-2.544165000	C	-0.607943000	-1.505757000	2.176508000
C	-1.301326000	-2.727767000	2.113362000	O	0.019135000	-0.547903000	1.517516000
H	-0.516070000	-3.321454000	2.604547000	O	-1.342959000	-1.243184000	3.113689000
H	-2.270791000	-2.882523000	2.603165000	C	4.552910000	1.032705000	0.737612000
H	-1.350205000	-3.059840000	1.064026000	N	3.931555000	0.916453000	1.972155000
C	-2.083397000	3.899078000	-0.218447000	C	3.621043000	0.577749000	-0.167096000
H	-1.601284000	4.876659000	-0.388774000	C	2.684635000	0.411940000	1.787784000
H	-3.013550000	3.870156000	-0.810044000	N	2.478534000	0.198882000	0.503041000
H	-2.365526000	3.839058000	0.840831000	C	2.156684000	-1.961245000	-1.821274000
C	5.562959000	2.313135000	0.763531000	O	1.767273000	-0.782913000	-2.127307000
H	5.419010000	3.340807000	1.138391000	C	3.052394000	-2.716592000	-2.772203000
H	6.426529000	1.880520000	1.296769000	H	4.100501000	-2.572194000	-2.461933000
H	5.826540000	2.378840000	-0.300811000	H	2.832822000	-3.791823000	-2.723756000
H	-0.780884000	3.182824000	-2.623014000	H	2.934784000	-2.341708000	-3.797437000
H	-0.966981000	1.405252000	1.206961000	C	-0.360711000	-2.928783000	1.709993000
H	0.649714000	1.030904000	-2.664525000	H	0.717471000	-3.129647000	1.621968000
H	4.089997000	1.556092000	3.057752000	H	-0.831546000	-3.634381000	2.406165000
H	3.620192000	0.771182000	-1.060444000	H	-0.771328000	-3.051779000	0.696859000
H	1.988129000	0.089481000	2.749980000	C	-1.689423000	4.423973000	0.376632000
C	-4.169453000	-1.638611000	-0.566245000	H	-1.100177000	5.343629000	0.221598000
C	-3.308429000	-0.570676000	-1.249577000	H	-2.671381000	4.567348000	-0.105108000
C	-4.053496000	0.762486000	-1.370641000	H	-1.861139000	4.311524000	1.455523000
C	-4.565677000	1.240216000	-0.006744000	C	5.939810000	1.551358000	0.567894000
C	-5.444991000	0.175307000	0.659589000	H	6.042785000	2.584565000	0.941256000
C	-4.693736000	-1.154915000	0.791707000	H	6.679310000	0.928713000	1.099689000
H	-3.583447000	-2.564106000	-0.442282000	H	6.208731000	1.551955000	-0.497171000
H	-5.026263000	-1.892715000	-1.219376000	H	-0.791017000	3.745099000	-2.216730000
H	-2.389613000	-0.427469000	-0.661966000	H	-0.687337000	1.713292000	1.491678000
H	-2.977784000	-0.922171000	-2.240925000	H	0.338399000	1.451835000	-2.577628000
H	-3.396525000	1.523951000	-1.824696000	H	4.340855000	1.155570000	2.867225000
H	-4.913409000	0.644714000	-2.057146000	H	3.685324000	0.491522000	-1.248222000
H	-3.701264000	1.442901000	0.648842000	H	1.953669000	0.213699000	2.568550000
H	-5.120807000	2.189015000	-0.111391000	C	-3.727507000	-1.606111000	0.319246000
H	-5.780758000	0.524736000	1.650573000	C	-2.893337000	-0.405752000	-0.068026000
H	-6.358152000	0.027551000	0.052095000	C	-3.515635000	0.459990000	-1.140608000
H	-3.843715000	-1.011019000	1.479365000	C	-4.929188000	0.907711000	-0.718691000
H	-5.349144000	-1.919699000	1.242767000	C	-5.801718000	-0.296560000	-0.345477000
				C	-5.142242000	-1.157727000	0.737848000
				H	-3.247868000	-2.155786000	1.142204000
				H	-3.808098000	-2.296860000	-0.540135000
				H	-2.539541000	0.158293000	0.806271000
				H	-1.752034000	-0.878212000	-0.565261000
				H	-2.884301000	1.337687000	-1.353171000
				H	-3.589775000	-0.115900000	-2.081205000
				H	-4.845964000	1.579850000	0.155077000
³TS_{hydr}							
Fe	0.673264000	-0.603687000	-0.284089000				
O	-0.732862000	-1.321279000	-1.001719000				
O	1.830616000	-2.465579000	-0.715592000				
C	-0.990546000	3.216944000	-0.147324000				
N	-0.626987000	3.069807000	-1.480039000				
C	-0.589111000	2.052355000	0.464019000				

H	-5.402038000	1.493872000	-1.525990000	C	-3.878746000	-1.462100000	0.328556000
H	-6.797461000	0.042679000	-0.012751000	C	-2.938373000	-0.326560000	-0.005529000
H	-5.967158000	-0.913238000	-1.248360000	C	-3.292238000	0.406463000	-1.278881000
H	-5.067411000	-0.574816000	1.673190000	C	-4.747635000	0.914035000	-1.220456000
H	-5.766930000	-2.038213000	0.964786000	C	-5.721759000	-0.226177000	-0.903632000
⁵TS_{hydr}				C	-5.333911000	-0.955437000	0.387732000
Fe	0.752642000	-0.807179000	0.063546000	H	-3.595817000	-1.927998000	1.284280000
O	-0.764032000	-1.551039000	-0.341448000	H	-3.802938000	-2.244845000	-0.448258000
O	1.649964000	-2.473658000	-0.685190000	H	-2.730339000	0.326548000	0.853598000
C	-0.843400000	3.137164000	-0.216135000	H	-1.741409000	-0.903272000	-0.185602000
N	-0.427446000	2.892916000	-1.519065000	H	-2.605087000	1.247527000	-1.454373000
C	-0.509402000	2.001522000	0.485429000	H	-3.187669000	-0.279556000	-2.139313000
C	0.118734000	1.651329000	-1.577125000	H	-4.825260000	1.686749000	-0.433866000
N	0.078281000	1.102300000	-0.379083000	H	-5.019052000	1.402355000	-2.172586000
C	-0.670705000	-0.858148000	2.602610000	H	-6.752340000	0.160909000	-0.830921000
O	0.478288000	-0.713122000	1.987807000	H	-5.716556000	-0.947072000	-1.742055000
O	-1.384759000	0.084911000	2.920241000	H	-5.438088000	-0.262899000	1.242284000
C	4.667943000	0.890244000	0.273838000	H	-6.021363000	-1.797218000	0.577711000
N	4.266441000	0.855065000	1.601091000	³IM_{hydr}			
C	3.613356000	0.352644000	-0.426268000	Fe	-0.749655000	0.640993000	-0.270895000
C	3.023158000	0.317659000	1.668258000	O	0.794414000	1.294825000	-0.928379000
N	2.610794000	0.003621000	0.454712000	O	-1.593991000	2.462792000	-0.489867000
C	1.808202000	-2.055718000	-1.874393000	C	0.747251000	-3.251782000	-0.177609000
O	1.515212000	-0.873367000	-2.184722000	N	0.572311000	-3.006541000	-1.533243000
C	2.346585000	-3.022333000	-2.904663000	C	0.312869000	-2.108097000	0.451039000
H	2.623294000	-2.495536000	-3.826817000	C	0.061496000	-1.759067000	-1.687446000
H	3.209050000	-3.569482000	-2.496970000	N	-0.104135000	-1.206432000	-0.501843000
H	1.565143000	-3.764743000	-3.131869000	C	0.583535000	1.319414000	2.239965000
C	-1.061042000	-2.297314000	2.876402000	O	-0.151743000	0.483440000	1.537031000
H	-0.233179000	-2.829587000	3.368993000	O	1.276729000	0.923561000	3.165354000
H	-1.971675000	-2.351442000	3.486839000	C	-4.639329000	-0.909960000	0.484098000
H	-1.223124000	-2.781329000	1.900158000	N	-4.084787000	-0.827314000	1.752281000
C	-1.520783000	4.397283000	0.200405000	C	-3.652880000	-0.452206000	-0.358895000
H	-0.889576000	5.285493000	0.026316000	C	-2.822327000	-0.340473000	1.647630000
H	-2.470581000	4.549018000	-0.340143000	N	-2.542349000	-0.106014000	0.380117000
H	-1.751278000	4.352718000	1.273335000	C	-1.890093000	2.145737000	-1.673958000
C	5.988968000	1.421685000	-0.165937000	O	-1.631324000	0.954478000	-2.049202000
H	6.120812000	2.481277000	0.112283000	C	-2.497443000	3.139634000	-2.622752000
H	6.827153000	0.853980000	0.272845000	H	-3.124537000	3.856625000	-2.075827000
H	6.073107000	1.349256000	-1.258775000	H	-1.680279000	3.699709000	-3.105660000
H	-0.534157000	3.524659000	-2.303228000	H	-3.075357000	2.627732000	-3.403799000
H	-0.690267000	1.735789000	1.528225000	C	0.518274000	2.784193000	1.849250000
H	0.524062000	1.168056000	-2.463648000	H	-0.525674000	3.131667000	1.840930000
H	4.810054000	1.171951000	2.394600000	H	1.118875000	3.383145000	2.545386000
H	3.494543000	0.196228000	-1.494227000	H	0.880209000	2.896186000	0.816662000
H	2.436266000	0.164580000	2.570632000	C	1.327182000	-4.517811000	0.352190000

H	0.732854000	-5.400314000	0.060404000	C	3.180412000	0.407411000	1.492998000
H	2.359499000	-4.674238000	-0.004401000	N	2.666651000	-0.028191000	0.357826000
H	1.357312000	-4.478975000	1.449362000	C	1.566940000	-2.304065000	-1.665143000
C	-6.021770000	-1.404396000	0.228074000	O	1.334104000	-1.146366000	-2.096409000
H	-6.158604000	-2.443511000	0.572952000	C	1.908254000	-3.433350000	-2.609781000
H	-6.780580000	-0.782225000	0.732467000	H	2.219022000	-3.042658000	-3.587428000
H	-6.232362000	-1.378987000	-0.849722000	H	2.691198000	-4.072330000	-2.177414000
H	0.813819000	-3.639570000	-2.285794000	H	1.009260000	-4.056215000	-2.744272000
H	0.298273000	-1.834755000	1.502337000	C	-0.962453000	-1.831010000	3.251557000
H	-0.169966000	-1.282486000	-2.637362000	H	-0.133850000	-2.362008000	3.743698000
H	-4.545062000	-1.078153000	2.618908000	H	-1.827362000	-1.752085000	3.922717000
H	-3.660175000	-0.345207000	-1.439778000	H	-1.229147000	-2.405984000	2.350154000
H	-2.129893000	-0.171033000	2.468896000	C	-1.299241000	4.502053000	-0.129952000
C	3.831695000	1.191101000	0.823658000	H	-0.659580000	5.328975000	-0.482854000
C	3.221827000	-0.149458000	0.568292000	H	-2.294262000	4.627063000	-0.590255000
C	3.556991000	-0.861054000	-0.703924000	H	-1.419566000	4.608265000	0.956530000
C	5.069825000	-0.817484000	-1.001449000	C	6.056276000	1.101908000	-0.658109000
C	5.618687000	0.608678000	-0.880503000	H	6.259945000	2.178243000	-0.526030000
C	5.339903000	1.199885000	0.505893000	H	6.894604000	0.544765000	-0.206370000
H	3.630628000	1.505134000	1.858348000	H	6.057499000	0.890317000	-1.735958000
H	3.346857000	1.951467000	0.173026000	H	-0.598889000	3.268784000	-2.577537000
H	2.535958000	-0.577467000	1.300540000	H	-0.451722000	1.989281000	1.452354000
H	1.517835000	0.815787000	-0.493971000	H	0.351936000	0.863050000	-2.524651000
H	3.192463000	-1.900752000	-0.679492000	H	5.056053000	1.236631000	1.985374000
H	3.031583000	-0.374644000	-1.555600000	H	3.412486000	-0.129154000	-1.654203000
H	5.597107000	-1.467400000	-0.280102000	H	2.653964000	0.397991000	2.444360000
H	5.271716000	-1.226244000	-2.006508000	C	-4.061233000	-1.039298000	0.804716000
H	6.701516000	0.617615000	-1.091420000	C	-3.391338000	0.251354000	0.453726000
H	5.143634000	1.246006000	-1.649620000	C	-3.428618000	0.710184000	-0.969723000
H	5.873781000	0.602189000	1.266354000	C	-4.833745000	0.563757000	-1.586151000
H	5.735480000	2.227106000	0.573744000	C	-5.407855000	-0.834585000	-1.334225000
⁵IM' _{hydr}				C	-5.457673000	-1.154979000	0.163627000
Fe	0.773677000	-0.777977000	0.193830000	H	-4.114057000	-1.161800000	1.897793000
O	-0.861306000	-1.479288000	-0.020662000	H	-3.444829000	-1.886660000	0.433774000
O	1.502708000	-2.559708000	-0.421797000	H	-2.830069000	0.797814000	1.214631000
C	-0.712174000	3.167770000	-0.438021000	H	-1.523653000	-0.782337000	0.128134000
N	-0.438478000	2.738007000	-1.730195000	H	-3.068617000	1.747593000	-1.055357000
C	-0.355815000	2.115056000	0.372976000	H	-2.727840000	0.093796000	-1.575382000
C	0.050155000	1.473754000	-1.676133000	H	-5.505930000	1.315057000	-1.133947000
N	0.109176000	1.083808000	-0.416788000	H	-4.797502000	0.778237000	-2.667920000
C	-0.509097000	-0.463893000	2.781214000	H	-6.414425000	-0.918337000	-1.777670000
O	0.618816000	-0.459073000	2.112618000	H	-4.775471000	-1.584109000	-1.845413000
O	-1.166532000	0.548660000	2.993740000	H	-6.145346000	-0.447086000	0.660293000
C	4.745838000	0.706613000	-0.068778000	H	-5.867205000	-2.165506000	0.328620000
N	4.440532000	0.858176000	1.275778000	³PC' _{hydr}			
C	3.618078000	0.149887000	-0.625067000	Fe	0.569764000	-0.403722000	-0.683358000

O	-1.312579000	-0.327835000	-1.479906000	H	-2.362994000	-0.626526000	0.214288000
O	0.663654000	1.180073000	-1.904790000	H	-1.130261000	0.421100000	-2.078438000
C	-0.711052000	0.551517000	3.355753000	H	-1.853966000	1.807431000	0.044430000
N	-0.084321000	1.728023000	2.971629000	H	-2.813265000	1.917629000	-1.444877000
C	-0.610933000	-0.276149000	2.260304000	H	-3.879636000	1.171159000	1.339546000
C	0.364811000	1.587061000	1.695600000	H	-4.175414000	2.698323000	0.496661000
N	0.054118000	0.384028000	1.245544000	H	-6.129114000	1.117534000	0.274779000
C	-0.484857000	-3.072393000	-0.304951000	H	-5.421824000	1.512288000	-1.297805000
O	0.520018000	-2.364585000	-0.704557000	H	-4.911699000	-1.050845000	0.321613000
O	-1.372699000	-2.694288000	0.461855000	H	-5.857529000	-0.933827000	-1.166863000
C	4.626876000	-0.028222000	0.247832000				
N	4.442814000	-1.402545000	0.216160000	⁵ PC _{hydr}			
C	3.394226000	0.502985000	-0.051817000	Fe	0.600727000	-0.553326000	0.331220000
C	3.146882000	-1.661940000	-0.092628000	O	-1.385549000	-1.407858000	0.501268000
N	2.492097000	-0.524982000	-0.258938000	O	0.834615000	-2.723628000	-0.273238000
C	1.080524000	2.393052000	-1.783904000	C	-0.949565000	3.326209000	-0.950327000
O	1.565269000	2.891300000	-0.761247000	N	-0.416001000	2.812832000	-2.124539000
C	0.920510000	3.237181000	-3.042780000	C	-0.725831000	2.351757000	-0.004046000
H	1.340995000	4.239882000	-2.894052000	C	0.098243000	1.581697000	-1.863216000
H	1.415385000	2.739668000	-3.891169000	N	-0.076588000	1.283344000	-0.589753000
H	-0.148274000	3.319838000	-3.298381000	C	-0.326815000	0.198610000	3.026782000
C	-0.505830000	-4.490016000	-0.866425000	O	0.663231000	-0.226880000	2.314226000
H	0.456092000	-4.991075000	-0.675166000	O	-1.297812000	0.831695000	2.605392000
H	-1.326081000	-5.070081000	-0.424157000	C	4.848491000	0.344669000	-0.311169000
H	-0.631437000	-4.444438000	-1.960205000	N	4.690377000	0.555305000	1.050101000
C	-1.325854000	0.354697000	4.699339000	C	3.600138000	-0.033168000	-0.752978000
H	-0.584694000	0.446890000	5.512032000	C	3.393425000	0.305149000	1.378002000
H	-2.129220000	1.085207000	4.897118000	N	2.717685000	-0.050619000	0.304745000
H	-1.765781000	-0.650072000	4.760215000	C	1.008862000	-2.399483000	-1.479479000
C	5.937755000	0.613200000	0.550213000	O	0.933499000	-1.193458000	-1.856131000
H	6.308449000	0.343186000	1.554078000	C	1.356075000	-3.470672000	-2.495886000
H	6.714755000	0.328815000	-0.180079000	H	1.008405000	-3.185555000	-3.498368000
H	5.830647000	1.705848000	0.515195000	H	2.453422000	-3.574382000	-2.532071000
H	0.019075000	2.559119000	3.540696000	H	0.936670000	-4.441126000	-2.197648000
H	-0.976244000	-1.290881000	2.105591000	C	-0.225653000	-0.151301000	4.508366000
H	0.878982000	2.349882000	1.105040000	H	0.742081000	0.184438000	4.913424000
H	5.155148000	-2.101295000	0.386702000	H	-1.048847000	0.303771000	5.074530000
H	3.082399000	1.541955000	-0.146618000	H	-0.257263000	-1.246794000	4.623004000
H	2.697084000	-2.645652000	-0.197138000	C	-1.608901000	4.660549000	-0.869680000
C	-3.708976000	-0.726164000	-1.441658000	H	-0.918967000	5.480960000	-1.132774000
C	-2.517322000	-0.094142000	-0.731882000	H	-2.482242000	4.731319000	-1.540841000
C	-2.730945000	1.393105000	-0.472860000	H	-1.961066000	4.835534000	0.156008000
C	-4.011419000	1.619684000	0.338237000	C	6.148827000	0.520740000	-1.018471000
C	-5.227507000	0.984197000	-0.346036000	H	6.528083000	1.554017000	-0.936955000
C	-4.993440000	-0.503606000	-0.634685000	H	6.928696000	-0.152400000	-0.622696000
H	-3.507322000	-1.799618000	-1.575637000	H	6.024353000	0.294170000	-2.086286000
H	-3.811060000	-0.277953000	-2.447625000	H	-0.419123000	3.271188000	-3.027369000

H	-1.004588000	2.306799000	1.048611000
H	0.558686000	0.920983000	-2.594586000
H	5.418421000	0.837835000	1.694712000
H	3.271133000	-0.303529000	-1.753344000
H	2.965446000	0.375449000	2.375972000
C	-3.777873000	-1.324890000	0.961709000
C	-2.611568000	-0.772004000	0.149835000
C	-2.869265000	-0.851575000	-1.352078000
C	-4.165914000	-0.122919000	-1.719990000
C	-5.354428000	-0.659538000	-0.912631000
C	-5.080287000	-0.603126000	0.595417000
H	-3.544725000	-1.206958000	2.030690000
H	-3.879701000	-2.408099000	0.758389000
H	-2.457777000	0.274294000	0.446940000
H	-1.322476000	-2.319017000	0.174299000
H	-2.002730000	-0.439924000	-1.891274000
H	-2.949853000	-1.917194000	-1.642516000
H	-4.040256000	0.955031000	-1.509856000
H	-4.361669000	-0.210779000	-2.801531000
H	-6.269886000	-0.095154000	-1.156879000
H	-5.545342000	-1.707904000	-1.207701000
H	-5.001808000	0.453028000	0.910413000
H	-5.925922000	-1.032744000	1.157025000

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