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Electronic Supplementary Information

What Drives the H-abstraction Reaction in Bio-mimetic Oxoiron-bTAML Complexes? A Computational Investigation

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Calculation of* p*K*a *values: The p*K*a for a molecule can be calculated from the solution phase free energy of the deprotonation reaction.[1]

$$AH \leftrightharpoons A^- + H^+$$

$$pKa = \Delta G^*_{aq} / 2.303\ RT$$

whereΔG_{aq}^* = $G_{aq}^*(A^-)$ + $G_{aq}^*(H^+)$ − $G_{aq}^*(AH)$ and A= Iron-oxo bTAML complexes and AH^+= Protonated Iron-oxo bTAML complexes. The calculated Gibbs free energies include ZPVE, thermal corrections and entropies computed by standard statistical thermodynamic methods at 298.15 K using the unscaled frequencies and the ideal gas/rigid rotor/harmonic oscillator approximations.

$$G^*_{aq}(H^+) = G^o_g(H^+) + \Delta G_{aq,solv}(H^+) + \Delta G^{1\ atm \rightarrow 1M}$$

$\Delta G_{aq,solv}(H^+)$= -265.9 kcal/mol was taken from the literature and $G^o_g(H^+)$ was calculated from $G^o_g = H^o_g - TS^o_g$ where E_{0K}=0, $H^o g$ = 1.48 Kcal/mol and $S^o g$ = 26.05 cal/(mole.k). $\Delta G^{1\ atm \rightarrow 1M}$ corresponds to 1.89 Kcal/mol.

Calculation of E^o values: The resulting standard reduction potential relative to the Standard Hydrogen Electrode (SHE) can be calculated according to the following expression[2]

$E^o_{rel,SHE}(A,B) = -[\Delta G^*(A\text{-}B)/n_e F] - E^o_{abs}(SHE)$; where $E^o_{abs}(SHE)$ = 4.28 V and A/B are the redox couple.

References

1. B. Thapa and H. B. Schlegel, *J. Phys. Chem. A.,* 2016, **120**, 5726.

2. A.V. Marenich, J. Ho, M.L. Coote, C.J. Cramer and D.G. Truhlar, *Phys. Chem. Chem. Phys.,* 2014, **16**, 15068.

Table S1.Thermochemical analyses of bTAML complexes (1a-1d). Energies are reported in kcal/mol. E^o are reported in Volts (V).

Catalyst	E^o ($Fe^{V/IV}$) calc	pK_a (Fe^{IV}-OH) calc	ΔG_{HAT} (BP86/TZVP/LANL2DZ-Fe)	ΔG_{HAT} (M06-L/6-31G*/LANL2DZ-Fe)	ΔG_{HAT} (PBE/6-31G*/LANL2DZ-Fe)
1a	-1.72	18.62	0.41	-3.3	1.07
1b	-1.68	17.83	0.21	-4.4	1.32
1c	-1.60	17.11	0.26	-4.6	2.06
1d	-1.58	16.49	0.41	-4.9	2.09

Table S2.Thermochemical analyses of bTAML complex (2). Energies are reported in kcal/mol. E^o are reported in Volts (V).

Catalyst	E^o ($Fe^{III/IV}$) calc	pK_a (Fe^{III}-OH) calc	ΔG_{HAT} (BP86/TZVP/LANL2DZ-Fe)	ΔG_{HAT} (M06-L/6-31G*/LANL2DZ-Fe)	ΔG_{HAT} (PBE/6-31G*/LANL2DZ-Fe)
2	-3.40	54.35	14.1	8.0	16.4

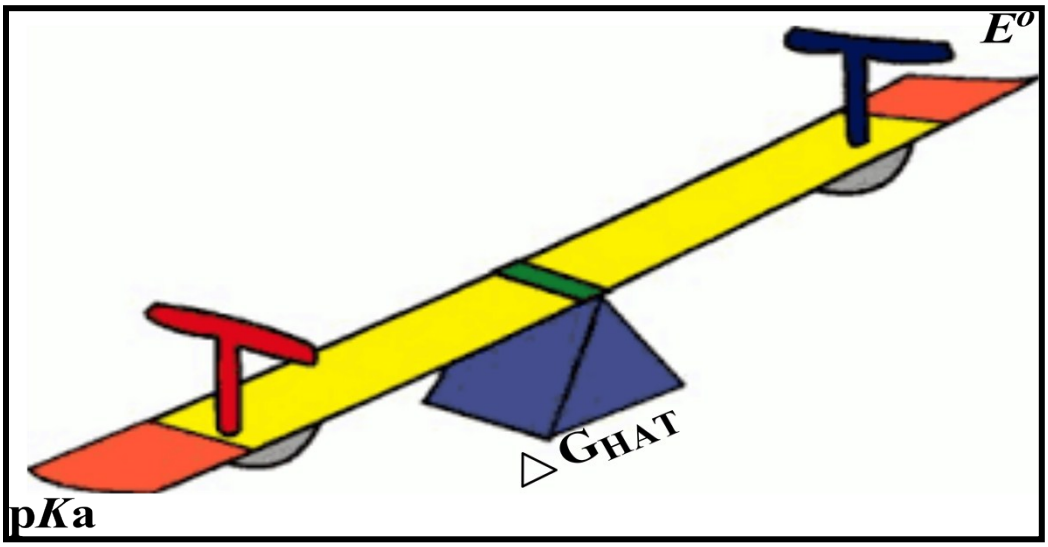
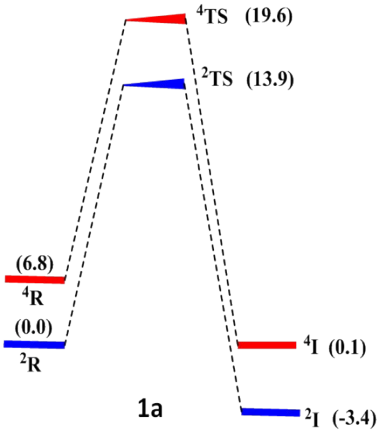
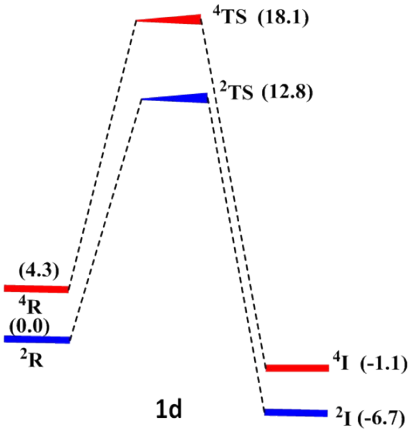
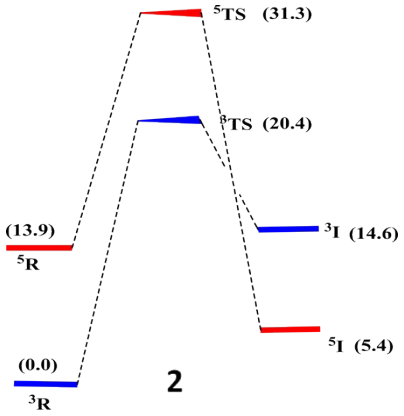
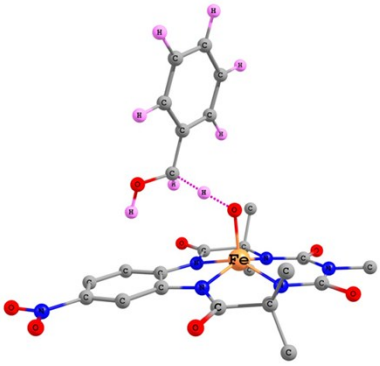


Fig S1. ***SEE SAW RELATIONSHIP*** **(1a-1d).**

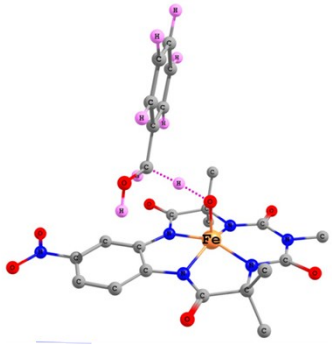

4TS (19.6)
2TS (13.9)
(6.8)
4R
(0.0)
2R
4I (0.1)
2I (-3.4)
1a


4TS (18.1)
2TS (12.8)
(4.3)
4R
(0.0)
2R
4I (-1.1)
2I (-6.7)
1d

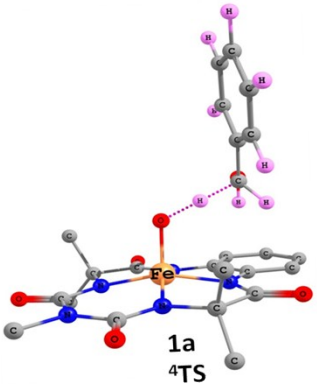

5TS (31.3)
3TS (20.4)
(13.9)
5R
3I (14.6)
5I (5.4)
(0.0)
3R
2



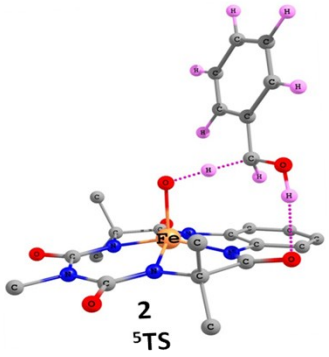
1d
^{2}TS



1d
^{4}TS



1a
^{4}TS



2
^{5}TS

R = Reactant (Catalyst + Substrate)
I = Intermediate formed after C-H abstraction.

Some hydrogen was omitted for clarity.

Color code: *Fe*=red*; N*=Blue*; C*=Ass*; 0*=Red*; H* = Pink
All the energy values in the profiles are expressed in kcal/mol

Fig S2. Gibb's free energy HAT reactions profile of b-TAML complexes with benzyl alcohol at M06-L/6-311G*/LANL2DZ(Fe)//M06-L/6-311G*/LANL2DZ(Fe),C-PCM (acetonitrile) level of theory

Table S3. Mulliken and Natural Population Analysis (NPA) charges of iron in the bTAML complexes(1a & 1d) in acetonitrile medium (C-PCM) at different levels of theory

Catalyst	Mulliken			NPA	
	M06-L/6-31G*/LANL2DZ-Fe	BP86/TZVP/LANL2DZ-Fe	PBE/6-31G*/LANL2DZ-Fe	M06-L/6-31G*/LANL2DZ-Fe	PBE/6-31G*/LANL2DZ-Fe
1a	0.948	0.613	0.621	0.403	0.243
1d	0.967	0.621	0.639	0.409	0.245

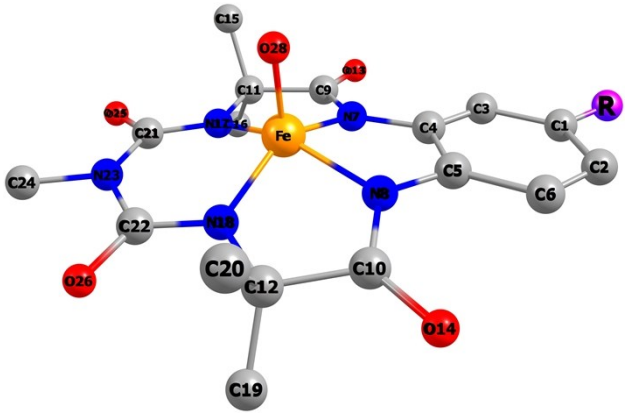
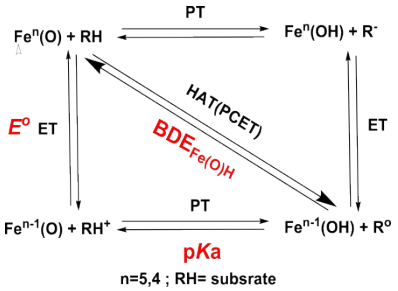
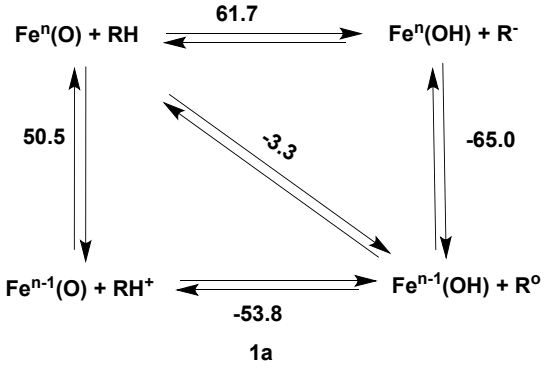


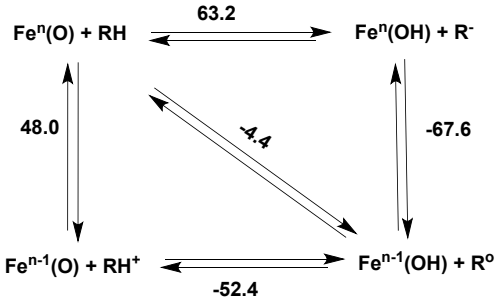
Table S4. Relative energies of the EAOs of the reported complexes at BP86/def2-TZVPP,C-PCM (acetonitrile) level of theory. All energies are reported in kcal/mol.

Catalyst	1
a	0.0
b	-1.3
c	-2.9
d	-4.1

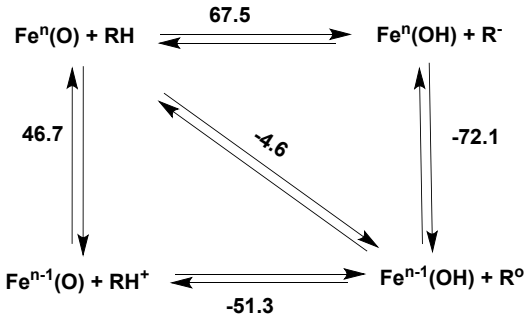




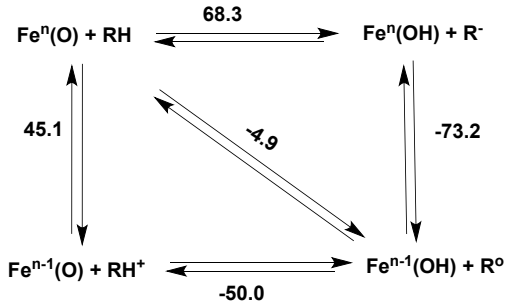
1a



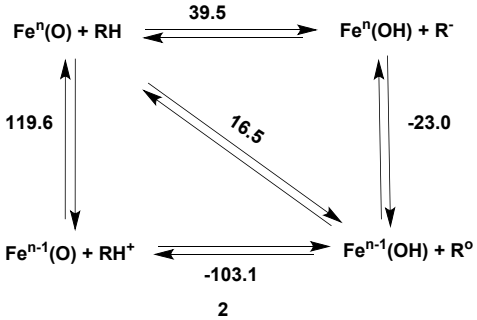
1b



1c



1d



2

Fig S3. Thermochemical Square Diagram with corresponding Gibb's free energy change value (ΔG) of the associated proton and electron transfer processes involved during HAT reaction of the reported complexes with benzyl alcohol at M06-L/6-31G*/LANL2DZ(Fe)//M06-L/6-31G*/LANL2DZ(Fe) /C-PCM (acetonitrile) level of theory for S=1/2 (for 1a-1d) and S=1 (for 2). All energies are reported in kcal/mol.

XYZ OF ALL REPORTED STRUCTURES

(The % of spin contamination are provided in parenthesis corresponding to the structures reported

	X	Y	Z
Encounter Complex of 1a with Benzyl Alcohol (0.026 %)			
C	-4.863317	-0.261359	-1.882476
C	-4.189881	-0.790213	-0.770107
C	-4.281675	-2.167944	-0.511838
C	-5.035126	-2.996444	-1.340527
C	-5.709601	-2.461130	-2.441696
C	-5.620282	-1.091980	-2.707372
C	-3.351071	0.069500	0.104741
O	-0.356883	-0.535261	-0.870938
Fe	0.917362	0.061375	0.050971
N	1.400995	-1.381395	1.148984
C	2.217956	-2.412495	0.803296
O	2.366057	-3.442440	1.477456
N	0.011802	0.689560	1.564601
C	-0.227111	-0.217473	2.557338
C	0.598098	-1.512568	2.386731
C	-0.394813	-2.692593	2.310767
C	-0.455654	2.006927	1.480362
C	-1.346847	2.658420	2.348056
C	-1.676982	3.997773	2.104776
C	-1.130458	4.679853	1.014535
C	-0.247558	4.042347	0.137735
C	0.091744	2.701081	0.361487
N	0.949810	1.897234	-0.384775
C	1.761831	2.283452	-1.410259
C	2.665315	1.128725	-1.902220
C	4.119128	1.641424	-1.820105
N	2.434038	-0.039476	-1.014712
C	3.168206	-1.172438	-1.238149
O	4.021343	-1.280042	-2.129051
N	2.939861	-2.298137	-0.415124
C	3.735674	-3.470905	-0.791299
O	1.819512	3.408402	-1.908988
O	-1.000956	-0.058372	3.504248
C	1.489398	-1.623484	3.644838
C	2.264640	0.823644	-3.362309
H	-2.260525	-0.107248	-0.214587

H	-0.981485	-2.626369	1.386983
H	-1.076442	-2.650748	3.166547
H	0.150492	-3.637404	2.309240
H	2.044522	-2.561686	3.625680
H	0.858402	-1.573477	4.537878
H	2.201162	-0.790027	3.674939
H	-1.746753	2.114800	3.194148
H	-2.367009	4.504601	2.775127
H	3.357599	-4.322469	-0.231632
H	1.237039	0.444702	-3.399879
H	2.317945	1.746133	-3.949975
H	2.936052	0.073201	-3.783145
H	4.802893	0.915267	-2.259633
H	4.184817	2.596777	-2.349412
H	4.401560	1.806835	-0.773405
H	0.186255	4.555021	-0.710646
H	4.796289	-3.322817	-0.555754
H	3.650331	-3.632401	-1.866785
O	-3.636314	1.417204	-0.037464
H	-3.326084	-0.264677	1.151824
H	-3.757493	-2.586385	0.344170
H	-5.097260	-4.060511	-1.126503
H	-6.298203	-3.106922	-3.088801
H	-6.141584	-0.669603	-3.563242
H	-4.789537	0.802104	-2.082305
H	-3.084124	1.915438	0.594701
H	-1.397575	5.718974	0.836476

Encounter Complex of 2 with Benzyl Alcohol (0.05 %)

C	-4.434047	0.226021	-1.973716
C	-4.345446	-0.591774	-0.825497
C	-5.119921	-1.770844	-0.801773
C	-5.944297	-2.109840	-1.874114
C	-6.025248	-1.288707	-3.002532
C	-5.257506	-0.116421	-3.040609
C	-3.446420	-0.232604	0.277771
O	-0.482537	-0.425694	-0.778339
Fe	0.980040	0.064565	0.069103
N	1.479377	-1.504439	1.005283
C	2.312735	-2.469152	0.571035
O	2.550321	-3.536737	1.175897

N	0.199124	0.595083	1.741094
C	-0.186287	-0.454963	2.485265
C	0.678833	-1.725702	2.230468
C	-0.271864	-2.930690	2.077811
C	-0.270765	1.912467	1.754623
C	-1.105410	2.508209	2.708592
C	-1.418208	3.869860	2.604754
C	-0.904971	4.634615	1.555100
C	-0.077951	4.054605	0.584931
C	0.243068	2.692210	0.668091
N	1.043617	1.953862	-0.204372
C	1.766157	2.396943	-1.259317
C	2.587111	1.257109	-1.938371
C	4.056409	1.732920	-1.963608
N	2.416092	0.014795	-1.151613
C	3.113550	-1.090920	-1.492679
O	3.897950	-1.177222	-2.459824
N	2.971114	-2.261081	-0.685866
C	3.759379	-3.391612	-1.171319
O	1.829443	3.560039	-1.688487
O	-1.135346	-0.483829	3.302530
C	1.573494	-1.893807	3.482565
C	2.044674	1.092835	-3.375553
H	-2.358625	-0.422912	-0.056960
H	-0.921733	-2.782625	1.209803
H	-0.903396	-3.019622	2.968142
H	0.316620	-3.840123	1.939392
H	2.171995	-2.801374	3.383267
H	0.947300	-1.949697	4.381308
H	2.247268	-1.033521	3.578649
H	-1.497195	1.894119	3.510845
H	3.470728	-4.266127	-0.592660
H	1.005187	0.748813	-3.337265
H	2.080830	2.055637	-3.898962
H	2.644647	0.351594	-3.909484
H	4.672097	1.020113	-2.514136
H	4.103006	2.724552	-2.426005
H	4.440129	1.811731	-0.938315
H	0.329362	4.629235	-0.237712
H	-1.153942	5.692904	1.480017
H	4.837738	-3.216490	-1.051290
H	3.570624	-3.540550	-2.237263
H	-3.395302	0.851245	0.460407
O	-3.696849	-0.976417	1.436934

H -5.060786 -2.404870 0.076407
H -6.533011 -3.025936 -1.827653
H -6.668601 -1.556301 -3.838953
H -5.302180 0.534100 -3.913017
H -3.831196 1.130391 -2.019026
H -3.053767 -0.723878 2.133177
H -2.070373 4.327729 3.347723

Optimized coordinates for electronic structures of bTAML complexes (1a-1d) at BP86/def2-TZVPP/C-PCM (acetonitrile) level of theory:

1a (0.013 %)

C -4.435456 -0.259681 -0.050586
C -2.839764 -2.096170 -0.152585
C -1.787909 -1.172863 -0.029812
C -2.069693 0.217530 0.076516
C -3.397989 0.671836 0.063344
N -0.405973 -1.435474 -0.020048
N -0.900717 0.978025 0.144150
C 0.189470 -2.660822 -0.217961
C -0.774846 2.296209 -0.161285
C 1.725552 -2.598607 -0.200815
C 0.705233 2.732022 -0.245576
O -0.427171 -3.718040 -0.384566
O -1.705444 3.086412 -0.378160
C 2.205784 -3.466019 0.984233
C 2.200933 -3.182235 -1.550548
N 2.102316 -1.176879 -0.031825
N 1.539066 1.495978 -0.139104
C 0.883513 3.439765 -1.603916
C 0.954291 3.694364 0.936816
C 3.415529 -0.849926 -0.094567
C 2.910439 1.651280 -0.191968
N 3.740780 0.534224 -0.006093
C 5.175125 0.847512 0.066155
O 4.350713 -1.663893 -0.221727
O 3.447596 2.759550 -0.364260
Fe 0.689951 -0.018198 0.500745
O 0.750223 -0.013311 2.109714
H -2.616815 -3.155921 -0.234595
H -3.598515 1.737500 0.140094
H -4.976753 -2.345417 -0.239442
H 1.855781 -3.043338 1.936663

H	3.300620	-3.506497	0.992470
H	1.802784	-4.482843	0.883051
H	1.748293	-4.172995	-1.689034
H	3.291442	-3.271117	-1.563049
H	1.885249	-2.535583	-2.381976
H	0.841802	3.165732	1.894283
H	0.212962	4.504366	0.898353
H	1.961634	4.119681	0.879051
H	0.760899	2.725178	-2.430461
H	1.873399	3.899894	-1.673372
H	0.108020	4.211389	-1.697245
H	5.688586	-0.017287	0.491980
H	5.315833	1.731677	0.695398
H	5.595477	1.057320	-0.928615
H	-5.469592	0.088747	-0.051609

1b (0.013 %)

C	-4.604984	3.523462	-0.256057
C	-3.233004	3.656459	-0.027778
C	-5.240740	2.280734	-0.297110
C	-4.459838	1.132242	-0.091539
C	-3.060928	1.246421	0.142176
C	-2.454812	2.511440	0.168990
N	-4.888900	-0.204496	-0.111281
N	-2.456765	-0.002635	0.278934
C	-6.155444	-0.646616	-0.424241
C	-1.142590	-0.288875	0.080421
C	-6.280976	-2.178182	-0.409075
C	-0.885482	-1.810360	0.010712
O	-7.106725	0.095359	-0.686017
O	-0.231798	0.539421	-0.062414
C	-7.316793	-2.541968	0.678426
C	-6.775771	-2.590162	-1.813669
N	-4.937977	-2.721291	-0.100885
N	-2.218170	-2.488941	0.030741
C	-0.128493	-2.071841	-1.307269
C	-0.030284	-2.178283	1.242789
C	-4.768670	-4.065735	-0.127828
C	-2.228294	-3.869872	-0.014015
N	-3.449723	-4.553470	0.095661
C	-3.324956	-6.014201	0.204909
O	-5.673818	-4.897577	-0.330080
O	-1.185195	-4.539264	-0.109967

Fe	-3.667902	-1.458221	0.537778
O	-3.815687	-1.502532	2.139430
H	-6.307390	2.193818	-0.476630
H	-1.384631	2.590794	0.341710
H	-6.951646	-2.248262	1.672654
H	-7.498253	-3.622339	0.670215
H	-8.257381	-2.010885	0.479240
H	-7.695541	-2.036874	-2.044819
H	-6.976574	-3.665344	-1.842884
H	-6.021009	-2.346328	-2.574961
H	-0.600761	-2.023717	2.169780
H	0.853320	-1.525823	1.266423
H	0.290140	-3.223799	1.189868
H	-0.766497	-1.838283	-2.171607
H	0.186040	-3.117785	-1.367187
H	0.752570	-1.417640	-1.342164
H	-4.264521	-6.406555	0.600581
H	-2.493222	-6.249490	0.875506
H	-3.128830	-6.480755	-0.771960
H	-2.775038	4.644486	0.001720
Cl	-5.576117	4.970953	-0.491457

1c (0.013 %)

C	-4.570068	3.471133	-0.269800
C	-3.183904	3.586688	-0.035469
C	-5.198117	2.207569	-0.305162
C	-4.422284	1.064594	-0.094081
C	-3.021205	1.181903	0.145784
C	-2.409581	2.447876	0.168413
N	-4.847886	-0.273652	-0.110000
N	-2.420179	-0.059069	0.294769
C	-6.114391	-0.716888	-0.424597
C	-1.099109	-0.345489	0.116442
C	-6.241115	-2.247819	-0.393977
C	-0.845677	-1.866519	0.031125
O	-7.062228	0.025325	-0.695378
O	-0.186930	0.481696	-0.001638
C	-7.269138	-2.598779	0.705382
C	-6.746042	-2.674427	-1.790365
N	-4.895779	-2.787658	-0.089048
N	-2.178806	-2.546053	0.038477
C	-0.082999	-2.111837	-1.287334
C	0.003516	-2.248520	1.263216

C	-4.724948	-4.133015	-0.110898
C	-2.185376	-3.928061	-0.018162
N	-3.402628	-4.617032	0.095255
C	-3.270474	-6.078074	0.195400
O	-5.632041	-4.965112	-0.298500
O	-1.140307	-4.591185	-0.127165
Fe	-3.630632	-1.523601	0.547510
O	-3.771959	-1.570414	2.147159
H	-6.263979	2.117549	-0.489725
H	-1.340235	2.522481	0.346473
H	-6.897105	-2.293442	1.693582
H	-7.450301	-3.679282	0.710746
H	-8.211328	-2.070377	0.506380
H	-7.664333	-2.118897	-2.022153
H	-6.952959	-3.748729	-1.805655
H	-5.994743	-2.443545	-2.559099
H	-0.570931	-2.104172	2.189439
H	0.887351	-1.596914	1.297878
H	0.323348	-3.293557	1.199370
H	-0.716305	-1.864830	-2.151365
H	0.228557	-3.157845	-1.359361
H	0.800328	-1.460124	-1.308776
H	-4.207028	-6.476821	0.591734
H	-2.435423	-6.313750	0.861843
H	-3.075507	-6.536701	-0.785383
H	-2.721327	4.573036	-0.009111
C	-5.354339	4.646146	-0.470098
N	-5.993832	5.610273	-0.635104

1d (0.013 %)

C	-4.647015	3.334459	-0.263492
C	-3.267966	3.424300	-0.036980
C	-5.258086	2.084026	-0.299209
C	-4.479828	0.927754	-0.098540
C	-3.075252	1.041168	0.134353
C	-2.463180	2.295679	0.162454
N	-4.905010	-0.400623	-0.113093
N	-2.472978	-0.205216	0.275927
C	-6.175549	-0.847514	-0.427932
C	-1.158520	-0.490382	0.070212
C	-6.299244	-2.378611	-0.400223
C	-0.902662	-2.012256	0.011148
O	-7.122363	-0.107670	-0.698696

O	-0.252630	0.338924	-0.084410
C	-7.333342	-2.732524	0.692411
C	-6.796962	-2.802219	-1.800741
N	-4.955662	-2.920238	-0.089464
N	-2.236518	-2.689577	0.034898
C	-0.144174	-2.283506	-1.303611
C	-0.050188	-2.370401	1.248557
C	-4.788018	-4.266290	-0.106691
C	-2.248220	-4.072236	-0.001694
N	-3.468813	-4.754110	0.113371
C	-3.343968	-6.214650	0.226945
O	-5.695283	-5.096650	-0.298515
O	-1.204632	-4.739549	-0.094862
Fe	-3.683007	-1.660432	0.542034
O	-3.825004	-1.705684	2.141081
H	-6.325135	1.990628	-0.474900
H	-1.396289	2.390250	0.334061
H	-5.229751	4.241899	-0.406221
H	-6.971943	-2.421406	1.682606
H	-7.504948	-3.814409	0.698753
H	-8.278089	-2.212489	0.484495
H	-7.707690	-2.238151	-2.041559
H	-7.015459	-3.874208	-1.815981
H	-6.036819	-2.580473	-2.563328
H	-0.621757	-2.207168	2.173333
H	0.834184	-1.718964	1.267210
H	0.268773	-3.416773	1.204964
H	-0.780777	-2.057354	-2.170760
H	0.172359	-3.329167	-1.354980
H	0.735706	-1.627941	-1.340633
H	-4.286470	-6.605964	0.616326
H	-2.517071	-6.447781	0.904322
H	-3.140457	-6.681520	-0.748006
N	-2.641127	4.745720	0.002529
O	-1.417123	4.813208	0.206416
O	-3.358371	5.746427	-0.169951

Coordinates of optimized transition states (TS)

TS of 1a

^{2}TS (3.2 %)

C	-4.124577000	-0.101369000	-2.432928000

C	-3.651678000	-0.365751000	-1.140430000
C	-4.046287000	-1.551804000	-0.503067000
C	-4.890016000	-2.447466000	-1.141320000
C	-5.357880000	-2.176171000	-2.425889000
C	-4.973073000	-0.999359000	-3.064577000
C	-2.722540000	0.531251000	-0.460987000
O	-0.377342000	-0.307044000	-1.029361000
Fe	0.841206000	0.021285000	0.089205000
N	1.042682000	-1.599880000	1.005181000
C	1.890921000	-2.609737000	0.702979000
O	1.850273000	-3.730406000	1.211244000
N	-0.261185000	0.492815000	1.529853000
C	-0.839321000	-0.566131000	2.165252000
C	-0.052913000	-1.873307000	1.955152000
C	-1.018385000	-2.917624000	1.395067000
C	-0.662725000	1.824582000	1.556122000
C	-1.668299000	2.396572000	2.341132000
C	-1.930000000	3.760548000	2.223328000
C	-1.201436000	4.551932000	1.338586000
C	-0.194085000	4.000345000	0.548835000
C	0.081657000	2.632428000	0.647775000
N	1.025044000	1.899565000	-0.053682000
C	2.019214000	2.373479000	-0.850893000
C	2.935431000	1.237877000	-1.352615000
C	4.367924000	1.642399000	-1.005095000
N	2.518347000	-0.018741000	-0.686472000
C	3.264686000	-1.140003000	-0.918218000
O	4.241415000	-1.172330000	-1.664783000
N	2.892909000	-2.338269000	-0.272584000
C	3.753654000	-3.459515000	-0.622042000
O	2.213123000	3.543503000	-1.157138000
O	-1.868184000	-0.523800000	2.833708000
C	0.459176000	-2.283222000	3.339490000
C	2.741076000	1.141488000	-2.867347000
H	-1.521096000	0.026190000	-0.723237000
H	-1.335913000	-2.637729000	0.385320000
H	-1.903869000	-2.985619000	2.034772000
H	-0.530839000	-3.891727000	1.345036000
H	0.947227000	-3.255659000	3.293105000
H	-0.380079000	-2.325458000	4.040195000
H	1.180335000	-1.549716000	3.714761000
H	-2.230820000	1.764134000	3.017871000
H	-2.719404000	4.204414000	2.826732000
H	3.369576000	-4.342989000	-0.121804000

H	1.717551000	0.832809000	-3.103274000
H	2.918219000	2.120502000	-3.323261000
H	3.433123000	0.413372000	-3.292328000
H	5.089201000	0.972174000	-1.469149000
H	4.537220000	2.666483000	-1.348488000
H	4.521589000	1.621054000	0.078940000
H	0.386552000	4.599724000	-0.142764000
H	4.784786000	-3.273389000	-0.307405000
H	3.765597000	-3.602578000	-1.704471000
O	-2.708554000	1.811176000	-0.963425000
H	-2.746536000	0.472356000	0.636363000
H	-3.684993000	-1.754886000	0.504363000
H	-5.188725000	-3.362502000	-0.633713000
H	-6.019473000	-2.879865000	-2.927265000
H	-5.336917000	-0.782492000	-4.067426000
H	-3.817895000	0.817764000	-2.924605000
H	-2.097192000	2.339998000	-0.428453000
H	-1.422134000	5.614355000	1.252953000

^{4}TS (0.016 %)

C	-4.248788000	-0.399950000	-2.322722000
C	-3.604207000	-0.762182000	-1.132007000
C	-3.701208000	-2.090213000	-0.689813000
C	-4.424088000	-3.025552000	-1.413331000
C	-5.066611000	-2.654903000	-2.593438000
C	-4.975810000	-1.338765000	-3.040663000
C	-2.794523000	0.192848000	-0.377486000
O	-0.356898000	-0.335755000	-0.981752000
Fe	0.869498000	0.106386000	0.172187000
N	1.430835000	-1.438338000	1.042775000
C	2.374354000	-2.311144000	0.600660000
O	2.545473000	-3.437048000	1.065921000
N	-0.219418000	0.374223000	1.682549000
C	-0.432678000	-0.719965000	2.471148000
C	0.497928000	-1.895808000	2.097769000
C	-0.393931000	-3.021754000	1.569548000
C	-0.824560000	1.618492000	1.759866000
C	-1.850843000	2.019969000	2.622437000
C	-2.342996000	3.318691000	2.537839000
C	-1.827430000	4.217976000	1.603573000
C	-0.806156000	3.841531000	0.735320000
C	-0.290010000	2.541035000	0.806815000
N	0.715324000	1.985032000	0.036786000
C	1.445413000	2.581435000	-0.950643000
C	2.436193000	1.598371000	-1.617531000

C	3.814517000	2.259201000	-1.562952000
N	2.381491000	0.321015000	-0.874177000
C	3.273461000	-0.659097000	-1.188734000
O	4.121985000	-0.564216000	-2.074121000
N	3.215694000	-1.875206000	-0.463319000
C	4.208030000	-2.841233000	-0.915597000
O	1.359985000	3.748867000	-1.307655000
O	-1.264816000	-0.814456000	3.365358000
C	1.212796000	-2.311460000	3.383932000
C	1.978131000	1.401463000	-3.063562000
H	-1.571359000	-0.072888000	-0.675493000
H	-0.845060000	-2.725011000	0.616695000
H	-1.192240000	-3.237615000	2.286996000
H	0.196967000	-3.923511000	1.402708000
H	1.781644000	-3.226996000	3.232931000
H	0.470314000	-2.460890000	4.172691000
H	1.901698000	-1.525822000	3.711415000
H	-2.243932000	1.303230000	3.334464000
H	-3.146822000	3.628751000	3.202667000
H	4.104288000	-3.735677000	-0.309912000
H	0.998458000	0.915150000	-3.088333000
H	1.900512000	2.370463000	-3.566289000
H	2.695116000	0.775164000	-3.597680000
H	4.538863000	1.703259000	-2.154971000
H	3.730210000	3.281079000	-1.942151000
H	4.178065000	2.310398000	-0.531152000
H	-0.393994000	4.526127000	0.003134000
H	-2.230702000	5.227149000	1.543519000
H	5.215942000	-2.430611000	-0.815777000
H	4.058426000	-3.079254000	-1.971741000
O	-3.048350000	1.508499000	-0.711519000
H	-2.768234000	0.002250000	0.706231000
H	-3.203847000	-2.379235000	0.235080000
H	-4.489408000	-4.051066000	-1.055286000
H	-5.633036000	-3.389455000	-3.162478000
H	-5.475629000	-1.043073000	-3.961527000
H	-4.171605000	0.627810000	-2.665950000
H	-2.479994000	2.076092000	-0.171346000

TS of 1d

^{2}TS (3.28 %)

C	1.385623000	4.057863000	-2.120355000
C	0.673247000	3.728899000	-0.959222000
C	-0.446792000	4.498141000	-0.612734000
C	-0.835450000	5.571990000	-1.398307000

C	-0.116394000	5.897196000	-2.546685000
C	0.994256000	5.135656000	-2.901097000
C	1.051624000	2.576157000	-0.142566000
O	-0.687130000	0.832175000	-0.818883000
Fe	-0.819724000	-0.590376000	0.074270000
N	-2.192184000	-0.231029000	1.299684000
C	-3.520750000	-0.406434000	1.096468000
O	-4.400962000	0.070868000	1.811273000
N	0.319553000	-0.130754000	1.499017000
C	-0.239233000	0.645076000	2.477939000
C	-1.777085000	0.642209000	2.416020000
C	-2.228669000	2.084887000	2.176072000
C	1.654045000	-0.432986000	1.315831000
C	2.738570000	-0.009096000	2.099387000
C	4.023829000	-0.412964000	1.763239000
C	4.216046000	-1.233400000	0.654775000
C	3.165198000	-1.675293000	-0.147292000
C	1.873346000	-1.271505000	0.178024000
N	0.696473000	-1.585516000	-0.473047000
C	0.517576000	-2.508129000	-1.460448000
C	-0.972808000	-2.658320000	-1.831223000
C	-1.291092000	-4.151874000	-1.781845000
N	-1.767568000	-1.866080000	-0.861518000
C	-3.131241000	-1.939131000	-0.944586000
O	-3.729368000	-2.604255000	-1.786748000
N	-3.900570000	-1.202616000	-0.020088000
C	-5.334010000	-1.352326000	-0.231892000
O	1.393795000	-3.161381000	-2.007265000
O	0.379220000	1.292506000	3.313116000
C	-2.255958000	0.135029000	3.778632000
C	-1.141487000	-2.101944000	-3.247155000
H	0.153460000	1.658472000	-0.481814000
H	-1.951651000	2.398699000	1.164234000
H	-1.750835000	2.754392000	2.898486000
H	-3.312848000	2.159466000	2.269042000
H	-3.337894000	0.219158000	3.860874000
H	-1.778818000	0.721327000	4.569162000
H	-1.977288000	-0.914637000	3.918232000
H	2.551074000	0.628729000	2.955019000
H	4.884679000	-0.098998000	2.342747000
H	-5.845605000	-0.760395000	0.520677000
H	-0.918733000	-1.030279000	-3.267853000
H	-0.451278000	-2.610000000	-3.927781000
H	-2.165674000	-2.254567000	-3.590814000

H	-2.271030000	-4.361427000	-2.206383000
H	-0.521765000	-4.690981000	-2.340847000
H	-1.274587000	-4.516464000	-0.749456000
H	3.345080000	-2.313367000	-1.002514000
H	-5.628138000	-2.402025000	-0.149667000
H	-5.607558000	-1.015541000	-1.234595000
O	2.300227000	2.086880000	-0.438175000
H	0.843468000	2.668808000	0.933756000
H	-1.009641000	4.247398000	0.285060000
H	-1.705467000	6.160409000	-1.114291000
H	-0.422759000	6.739873000	-3.163247000
H	1.560137000	5.384631000	-3.796933000
H	2.251517000	3.460213000	-2.389689000
H	2.529902000	1.403729000	0.208666000
N	5.581011000	-1.638449000	0.312695000
O	5.740890000	-2.358705000	-0.666876000
O	6.497544000	-1.236082000	1.028037000

^{4}TS (0.016 %)

C	2.294536000	3.156764000	-2.756890000
C	2.042164000	2.816642000	-1.420894000
C	1.854097000	3.843531000	-0.483722000
C	1.919068000	5.172728000	-0.871398000
C	2.174670000	5.502076000	-2.201161000
C	2.364410000	4.488546000	-3.138369000
C	1.920527000	1.424810000	-0.993327000
O	-0.563666000	0.781258000	-1.069049000
Fe	-1.083629000	-0.370314000	0.129598000
N	-1.900514000	0.527166000	1.530201000
C	-3.200854000	0.926144000	1.581835000
O	-3.648851000	1.700632000	2.424122000
N	0.429265000	-0.413415000	1.242885000
C	0.438903000	0.483622000	2.274583000
C	-0.949555000	1.122261000	2.498355000
C	-0.802157000	2.625058000	2.253533000
C	1.461155000	-1.230839000	0.811312000
C	2.762029000	-1.292110000	1.303956000
C	3.647580000	-2.192987000	0.714225000
C	3.279632000	-3.021309000	-0.345809000
C	1.987036000	-2.969014000	-0.842727000
C	1.058746000	-2.083337000	-0.270774000
N	-0.256571000	-1.903472000	-0.623299000
C	-0.958469000	-2.533492000	-1.616549000
C	-2.406055000	-2.002855000	-1.733626000

C	-3.327115000	-3.220614000	-1.635732000
N	-2.628043000	-1.029286000	-0.642062000
C	-3.881960000	-0.525966000	-0.456279000
O	-4.848875000	-0.812067000	-1.158986000
N	-4.083484000	0.397202000	0.597479000
C	-5.461095000	0.868268000	0.669792000
O	-0.533338000	-3.413605000	-2.349126000
O	1.410221000	0.786864000	2.953702000
C	-1.329167000	0.831298000	3.951229000
C	-2.534076000	-1.323518000	-3.098163000
H	0.671718000	1.155461000	-0.992324000
H	-0.591960000	2.817732000	1.195963000
H	0.023020000	3.021416000	2.853399000
H	-1.724290000	3.143235000	2.518919000
H	-2.240365000	1.359823000	4.225719000
H	-0.509376000	1.142313000	4.604616000
H	-1.492034000	-0.241292000	4.098790000
H	3.076066000	-0.654132000	2.120078000
H	-5.532516000	1.570678000	1.493694000
H	-1.882189000	-0.446559000	-3.148072000
H	-2.245148000	-2.020561000	-3.890533000
H	-3.565755000	-1.004865000	-3.257277000
H	-4.356355000	-2.950581000	-1.863381000
H	-2.980003000	-3.982860000	-2.338151000
H	-3.296523000	-3.649533000	-0.628638000
H	1.668543000	-3.601477000	-1.662511000
H	4.019113000	-3.693791000	-0.766295000
H	-6.145143000	0.030761000	0.828317000
H	-5.748862000	1.350025000	-0.267489000
O	2.522131000	0.527665000	-1.854707000
H	2.164805000	1.259941000	0.066417000
H	1.667494000	3.584111000	0.557690000
H	1.775051000	5.958111000	-0.132385000
H	2.225695000	6.545423000	-2.505778000
H	2.566398000	4.741561000	-4.177525000
H	2.439979000	2.360207000	-3.481230000
H	2.392216000	-0.364128000	-1.503231000
N	5.017035000	-2.265830000	1.219192000
O	5.785113000	-3.067383000	0.687997000
O	5.330597000	-1.526321000	2.147360000

TS of 2

^{3}TS (0.29 %)

C	-3.85943800	0.44452400	-1.96705300

C	-3.73818500	-0.69680900	-1.14691800
C	-4.38893900	-1.87321300	-1.56532600
C	-5.11852300	-1.90310800	-2.74806300
C	-5.22426100	-0.76850200	-3.54974400
C	-4.58653000	0.40817100	-3.14503600
C	-2.90871200	-0.65003100	0.04130900
O	-0.50343200	-0.38831300	-0.87028700
Fe	0.86439400	0.10013700	0.13467400
N	1.60817300	-1.54289900	0.67211900
C	2.57503500	-2.22250600	0.02875800
O	2.94843700	-3.37165200	0.30488700
N	-0.07557600	0.01625900	1.79428700
C	-0.24693500	-1.23316100	2.25267100
C	0.80195600	-2.23032900	1.70362400
C	0.03757300	-3.41070500	1.10361300
C	-0.79727700	1.17196900	2.09382000
C	-1.78899500	1.32646800	3.06487300
C	-2.39708300	2.56981400	3.24150900
C	-2.02230700	3.65617400	2.45631800
C	-1.03376900	3.52155200	1.48065100
C	-0.41416200	2.28437500	1.28526700
N	0.57672200	1.96678100	0.35521400
C	1.25977800	2.79872600	-0.46071500
C	2.34123400	2.06004200	-1.29172100
C	3.67570600	2.72125100	-0.93799400
N	2.31834000	0.62306500	-0.93652000
C	3.24984200	-0.19716300	-1.46242600
O	4.12663100	0.14235900	-2.26951000
N	3.21553700	-1.57236000	-1.07224100
C	4.17715800	-2.41280000	-1.77312800
O	1.11254400	4.01974300	-0.57060700
O	-1.14352400	-1.62726900	3.02132000
C	1.64525300	-2.67599100	2.90108600
C	2.01239500	2.27366900	-2.76960900
H	-1.54620900	-0.55904700	-0.43831100
H	-0.56058700	-3.07716500	0.24994600
H	-0.64237900	-3.83894000	1.84536000
H	0.73281000	-4.18119500	0.76810300
H	2.35190000	-3.45026400	2.60353600
H	0.99745500	-3.06735200	3.69133200
H	2.21053400	-1.83290600	3.31270800
H	-2.07597300	0.47035900	3.66568100
H	3.81046700	-3.43615000	-1.79066000
H	1.05058900	1.81641400	-3.02623000

H	1.94661300	3.34269100	-2.99303200
H	2.78455500	1.82689200	-3.39757700
H	4.47945300	2.33591400	-1.56389900
H	3.59638200	3.80285600	-1.07640000
H	3.93488400	2.53381000	0.10983300
H	-0.73397600	4.36167500	0.86455900
H	-2.50426400	4.62158800	2.59789700
H	5.16149300	-2.41632900	-1.28766900
H	4.30447300	-2.03750500	-2.78503400
H	-2.91283100	0.31990700	0.56250700
O	-3.09435100	-1.73602500	0.89677000
H	-4.31629900	-2.76165600	-0.94340900
H	-5.61547400	-2.82491500	-3.04692400
H	-5.79594100	-0.79579900	-4.47437600
H	-4.66451000	1.30559600	-3.75640700
H	-3.36311200	1.36682100	-1.66220400
H	-2.50942200	-1.63426600	1.66774300
H	-3.17258300	2.68422500	3.99620400

^{5}TS (0.012 %)

C	-3.502512000	1.052985000	-1.787760000
C	-3.574674000	-0.303146000	-1.431770000
C	-4.550762000	-1.102675000	-2.037501000
C	-5.444214000	-0.556870000	-2.953243000
C	-5.377423000	0.792501000	-3.287638000
C	-4.395953000	1.592825000	-2.698875000
C	-2.598775000	-0.840349000	-0.472550000
O	-0.363241000	-0.088743000	-1.394807000
Fe	0.866101000	0.043107000	0.153371000
N	1.924873000	-1.522336000	-0.009466000
C	3.033994000	-1.660780000	-0.750553000
O	3.583560000	-2.739897000	-1.022412000
N	-0.053042000	-0.947746000	1.505038000
C	-0.000229000	-2.277492000	1.324268000
C	1.201945000	-2.724590000	0.448189000
C	0.631649000	-3.491479000	-0.747234000
C	-0.908662000	-0.197385000	2.309016000
C	-1.831594000	-0.676242000	3.240378000
C	-2.597138000	0.223965000	3.984455000
C	-2.444162000	1.594943000	3.803346000
C	-1.527114000	2.095233000	2.877442000
C	-0.753785000	1.213111000	2.116795000
N	0.196501000	1.532298000	1.155710000

C	0.680755000	2.751677000	0.826470000
C	1.825778000	2.664779000	-0.228409000
C	2.975265000	3.524682000	0.299176000
N	2.196389000	1.247893000	-0.412759000
C	3.275924000	0.928898000	-1.152068000
O	4.004115000	1.736259000	-1.747685000
N	3.630920000	-0.454418000	-1.266263000
C	4.819044000	-0.651616000	-2.075743000
O	0.306624000	3.846140000	1.256354000
O	-0.819180000	-3.117040000	1.745882000
C	2.057832000	-3.641369000	1.327244000
C	1.278163000	3.240306000	-1.537538000
H	-1.476304000	-0.578257000	-0.987377000
H	0.044804000	-2.809443000	-1.371066000
H	-0.019943000	-4.303277000	-0.406193000
H	1.448381000	-3.901077000	-1.346057000
H	2.870683000	-4.072936000	0.743228000
H	1.433918000	-4.437744000	1.747412000
H	2.494158000	-3.073772000	2.157328000
H	-1.942137000	-1.749721000	3.356414000
H	-3.324290000	-0.155839000	4.702742000
H	5.029154000	-1.717556000	-2.096658000
H	0.462837000	2.608086000	-1.905565000
H	0.897740000	4.256897000	-1.382787000
H	2.070526000	3.260066000	-2.290786000
H	3.755641000	3.633559000	-0.453349000
H	2.584469000	4.505062000	0.588545000
H	3.419591000	3.062060000	1.188188000
H	-1.393799000	3.160418000	2.721710000
H	-3.051054000	2.291597000	4.383111000
H	5.673143000	-0.104472000	-1.661713000
H	4.669840000	-0.277836000	-3.094689000
H	-2.548653000	-0.242245000	0.447013000
O	-2.764844000	-2.197268000	-0.238568000
H	-4.594511000	-2.154767000	-1.768298000
H	-6.202256000	-1.193158000	-3.411718000
H	-6.076126000	1.217883000	-4.007621000
H	-4.322190000	2.647082000	-2.963735000
H	-2.710926000	1.661970000	-1.351619000
H	-2.197180000	-2.470283000	0.504576000