supplementary information

In situ synthesis of iron(III) complexes with amino acid Schiff base ligand: experimental and theoretical evidences

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Infrared Spectra

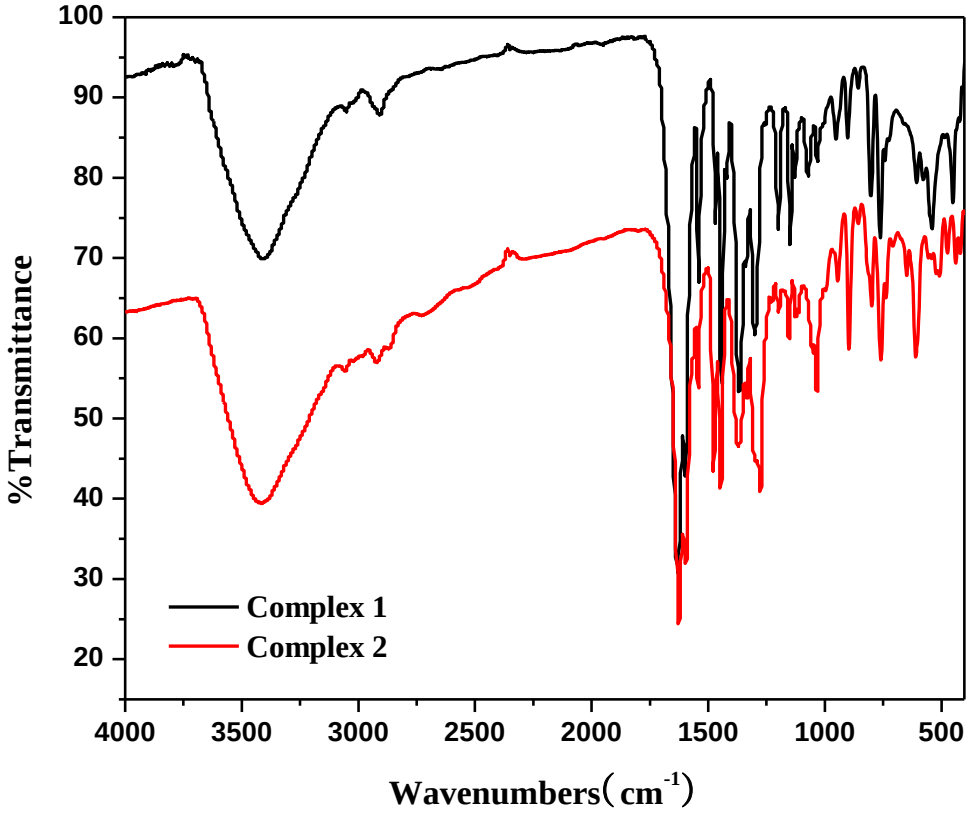


Fig. S1. IR spectrum picture of complexes **1** and **2**.

Crystal Structures

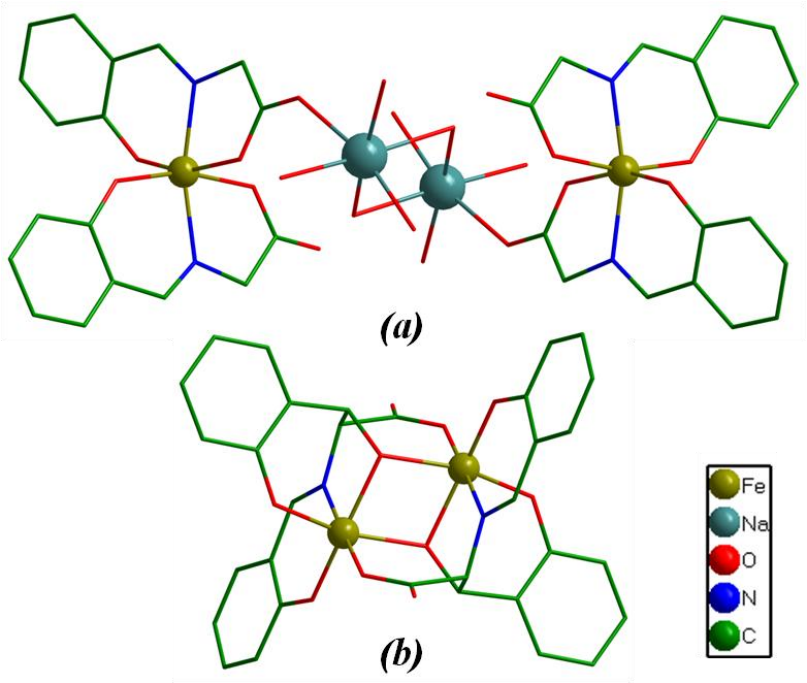
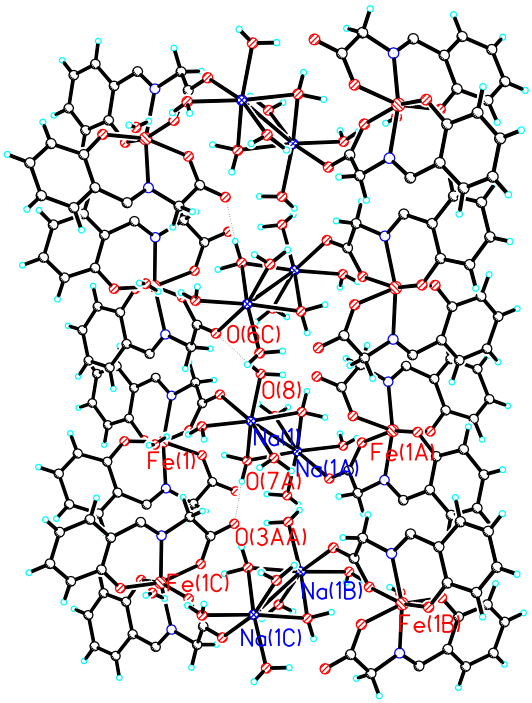
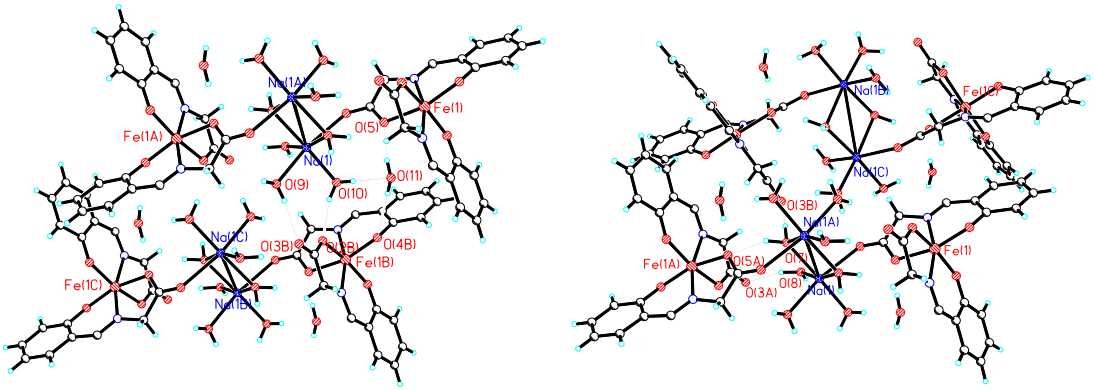


Fig. S2 The line drawings of the molecular structure of complexes **1** and **2**.



O6C···H08A–O8: 1.985Å, 2.828Å, 162.7°
O3AA···H70C–O7A: 1.837Å, 2.778Å, 166.8°

Fig. S3 1D H-bonding details in complex **1**.



O3B···H09A—O9: 2.149, 2,986, 164.1
O11···H00A—O10: 1.832, 2.670, 168.3
O2B···H00B—O10: 2.013, 2.871, 161.9
O5···H01A—O11: 1.929, 2.753, 163.4
O4B···H01B—O11: 2.479, 3.347, 179.3

O5A···H70B—O7: 2.019, 2.996, 158.1
O3A···H08B—O8: 1.864, 2.817, 162.1

Fig. S4 3D H-bonding details in complex **1**.

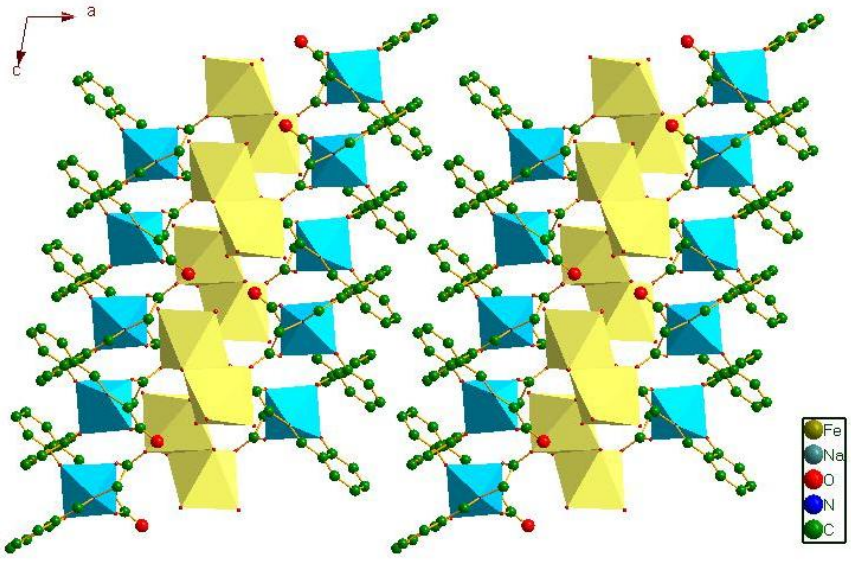


Fig. S5 The 3D structure picture of complex **1,** view down from b axis.

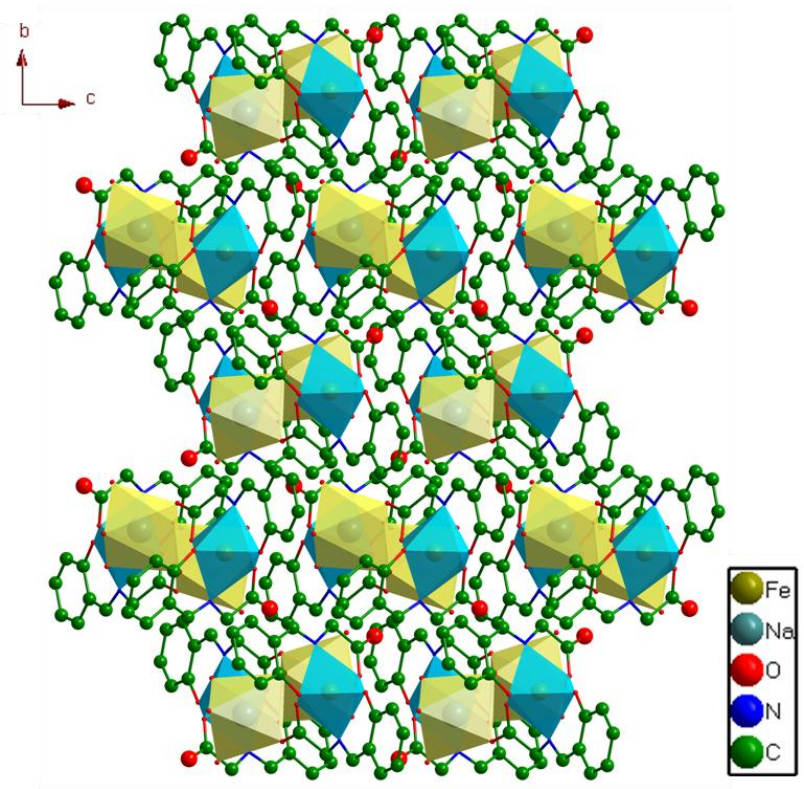
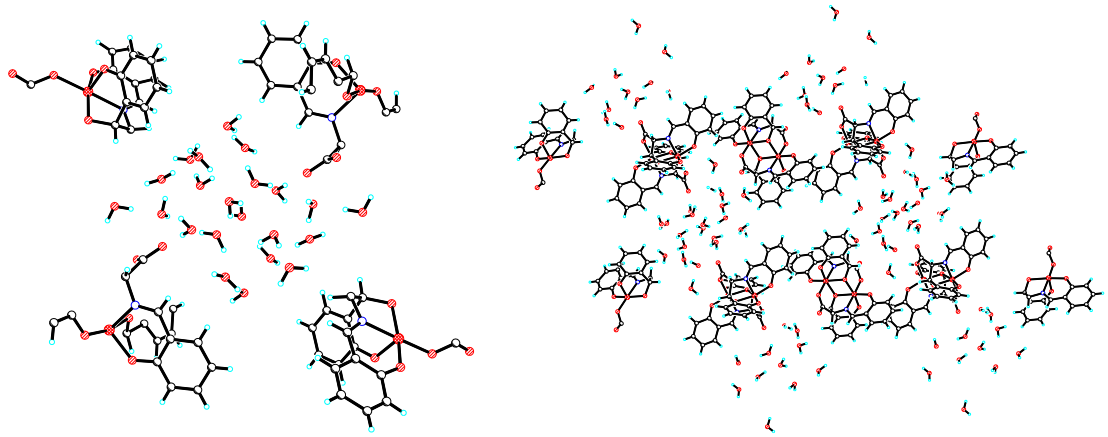


Fig. S6 The 3D structure picture of complex **1,** view down from a axis.



O15…H11F−O11A: 1.976, 2.826, 179.6

O3…H5CA−O5A: 1.998, 2.848, 179.5

O8…H24C−O24: 1.805, 2.657, 179.0

O22…H17B−O17A: 1.915, 2.743, 164.1

O12A…H9D−O9: 2.052, 2.901, 176.6

O12…H23C−O23:2.279, 3.129, 179.7

Fig. S7 3D H-bonding details in complex **2**.

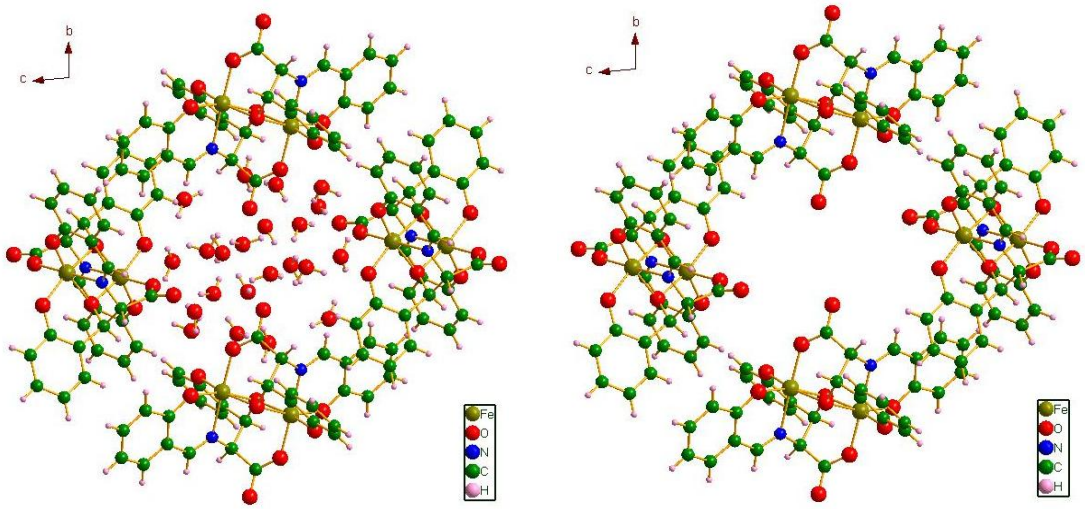


Fig. S8 The 1D structure picture of complex **2,** view down from a axis. Every four complex can form a hole, and the hole is filled with some water molecules.

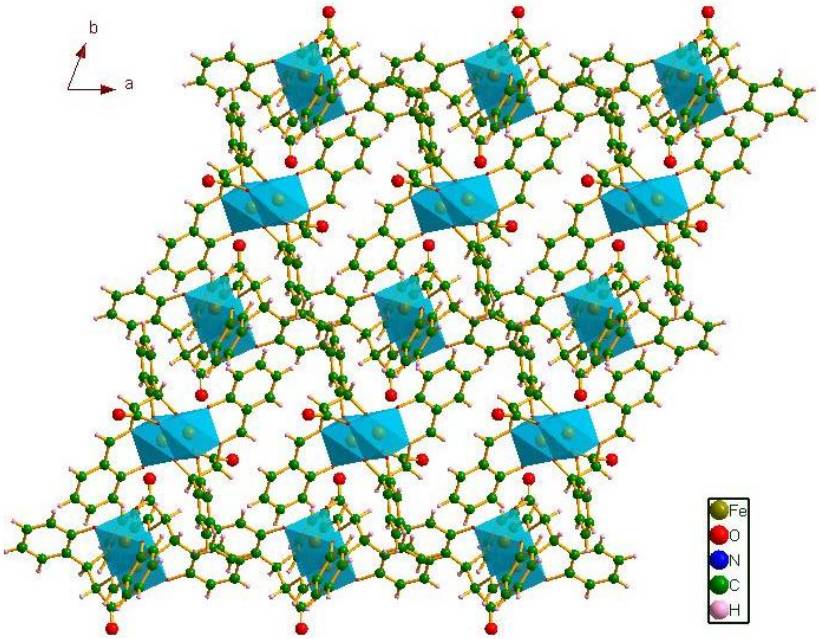


Fig. S9 The 3D structure picture of complex **2,** view down from b axis.

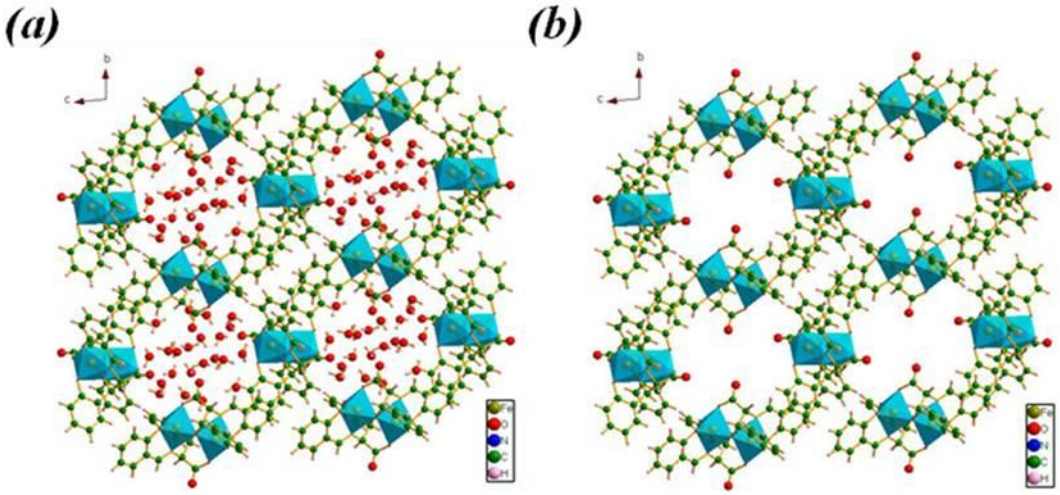


Fig. S10 The 3D structure picture of complex **2,** view down from a axis.

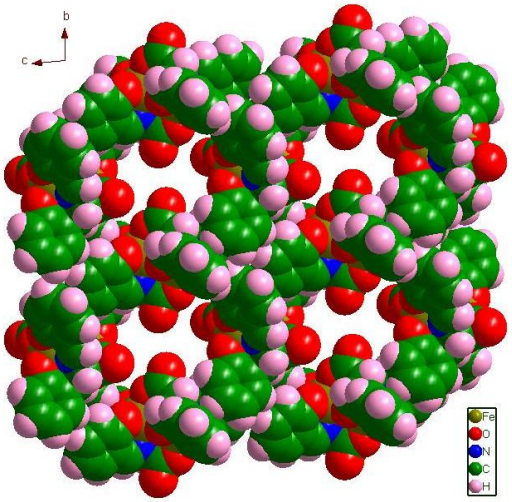


Fig. S11 The 3D Space-filling picture of complex **2,** view down from a axis.

Table S1 Selected Bond Distances (Å) and Angles (deg) for **1**

Fe(1)-O(1)	1.930(4)	Na(1)-O(10)	2.346(5)
Fe(1)-O(4)	1.933(4)	Na(1)-O(9)	2.377(4)
Fe(1)-O(2)	2.038(4)	Na(1)-O(8)	2.393(4)
Fe(1)-O(5)	2.094(3)	Na(1)-O(7)	2.434(5)
Fe(1)-N(2)	2.092(4)	Na(1)-O(7)[a]	2.459(4)
Fe(1)-N(1)	2.124(4)	Na(1)-O(6)	2.534(4)
O(7)-Na(1)[a]	2.459(4)	Na(1)-Na(1)[a]	3.686(5)
O(1)-Fe(1)-O(4)	92.31(18)	O(2)-Fe(1)-N(1)	77.84(16)
O(4)-Fe(1)-O(2)	89.28(17)	O(5)-Fe(1)-N(1)	88.81(14)
O(1)-Fe(1)-O(5)	95.01(17)	O(9)-Na(1)-O(8)	95.83(17)
O(1)-Fe(1)-N(2)	101.48(15)	O(9)-Na(1)-O(7)	90.81(17)
O(4)-Fe(1)-N(2)	86.21(15)	O(10)-Na(1)-O(6)	85.95(16)
O(2)-Fe(1)-N(2)	94.75(16)	O(8)-Na(1)-O(6)	96.88(14)
O(5)-Fe(1)N(2)	76.76(14)	O(7)-Na(1)-O(6)	95.59(16)

[a] Symmetry code: -x+1,-y+1,-z+1

Table S2 Geometries (Distances in (Å) and Angles in (°)) of the Hydrogen Bonds in **1**

D…H−A	D…H	D…A	D…H−A
O3[d]…H70[a]−O7	1.837	2.778	166.8
O5[a]…H70[b]−O7	2.019	2.996	158.1
O6[c]…H08[a]−O8	1.988	2.828	162.7
O3[a]…H08[b]−O8	1.864	2.817	162.1
O3[b]…H09[a]−O9	2.149	2.986	164.1
O8[c]…H09[b]−O9	2.149	2.986	164.1
O11…H00[a]−O10	1.832	2.670	168.3
O2[b]…H00[b]−O10	2.013	2.871	161.9
O5…H01[a]−O11	1.929	2.753	163.4
O4[b]…H01[b]−O11	2.497	3.347	179.3

[a] Symmetry code: -x+1, -y+1, -z+1; [b] Symmetry code: x, y, z+1; [c] Symmetry code: x, -y+1/2, z+1/2; [d] Symmetry code: -x+1, y-1/2, -z+1/2

Table S3 Selected Bond Distances (Å) and Angles (°) for **2**

Fe(1)-O(3)	1.927(4)	Fe(1)#1-O(6)	2.005(4)
Fe(1)-O(21)	1.947(4)	Fe(2)-O(1)	1.931(4)
Fe(1)-O(6) [a]	2.005(4)	Fe(2)-O(19)	2.006(4)
Fe(1)-O(18) [a]	2.016(4)	Fe(2)-O(2)	2.056(4)
Fe(1)-O(18)	2.037(4)	Fe(2)-O(2) [b]	2.056(4)
Fe(1)-N(2)	2.113(5)	Fe(2)-N(1)	2.109(5)
Fe(2)-O(4)	1.937(4)	O(18)-Fe(1) [a]	2.016(4)
O(3)-Fe(1)-O(18)	97.35(16)	O(4)-Fe(2)-O(2)	87.32(16)
O(21)-Fe(1)-O(18)	168.16(16)	O(1)-Fe(2)-O(2)	164.82(17)
O(3)-Fe(1)-N(2)	87.70(17)	O(19)-Fe(2)-O(2)	98.87(16)
O(21)-Fe(1)-N(2)	88.96(18)	O(4)-Fe(2)-N(1)	90.20(18)
O(18)-Fe(1)-N(2)	90.31(16)	O(1)-Fe(2)-N(1)	87.88(18)
O(4)-Fe(2)-O(1)	99.89(17)	O(19)-Fe(2)-N(1)	177.47(17)
O(4)-Fe(2)-O(19)	89.05(17)	O(2)-Fe(2)-N(1)	78.69(16)

[a] Symmetry code: -x,-y+1,-z+2 [b] Symmetry code: -x,-y,-z+1

Table S4 Geometries (Distances in (Å) and Angles in (°)) of Some Important Hydrogen Bonds in **2**

D…H−A	D…H	D…A	D…H−A
O15…H11F−O11A	1.976	2.826	179.6
O22…H17B−O17A	1.915	2.743	164.1
O3…H5CA−O5A	1.998	2.848	179.5
O12[a]…H9D−O9	2.052	2.901	176.6
O8…H24C−O24	1.805	2.657	179.0
O12…H23C−O23	2.279	3.129	179.7

[a] Symmetry code: –x+1,-y+1,-z+1

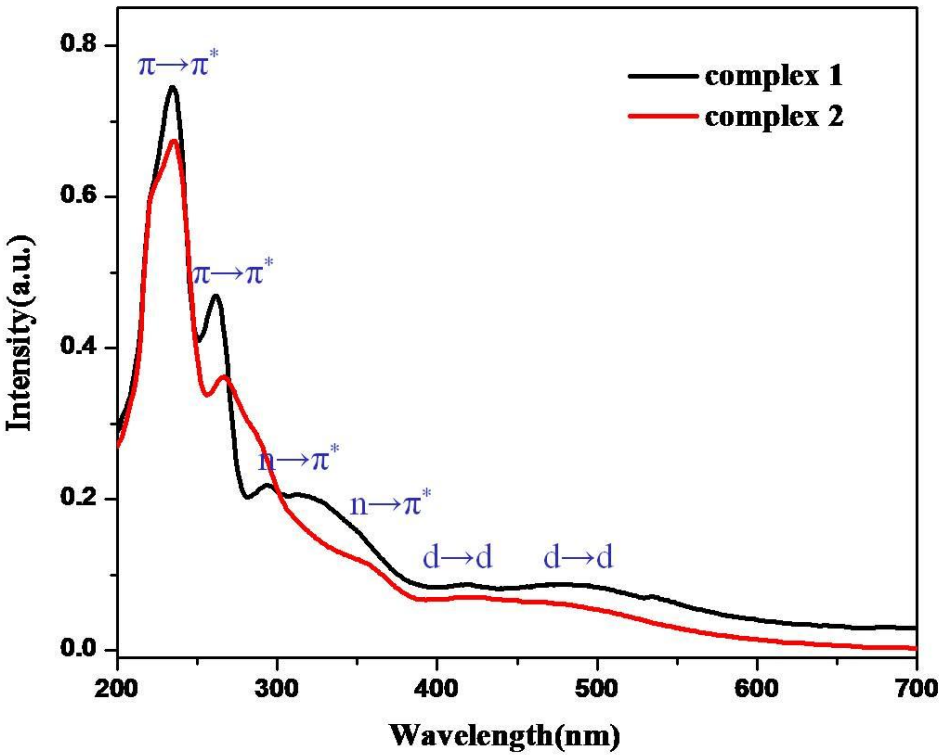


Fig. S12. UV-vis spectra of complexes **1** and **2**.

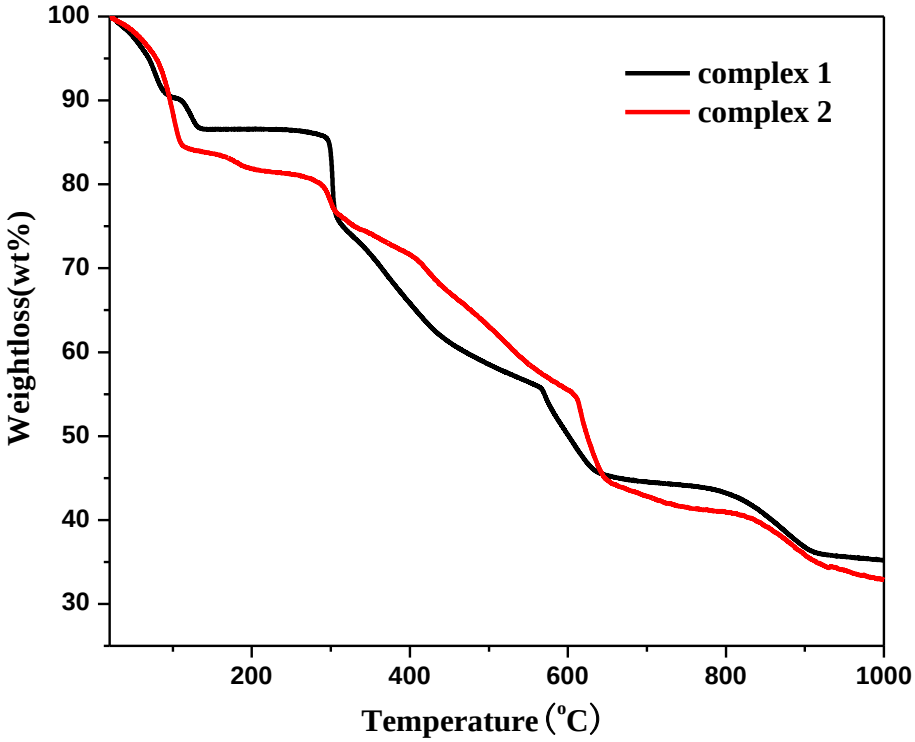
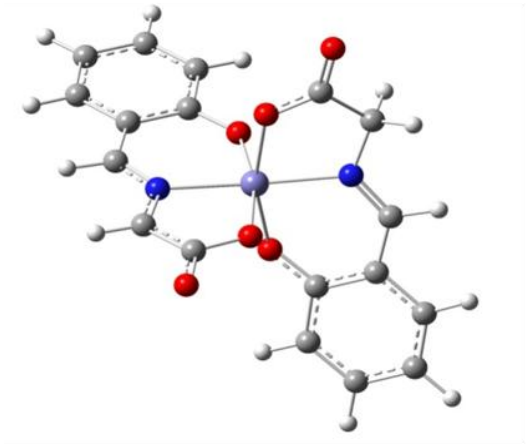


Fig. S13. TG curves for complexes **1** and **2**.



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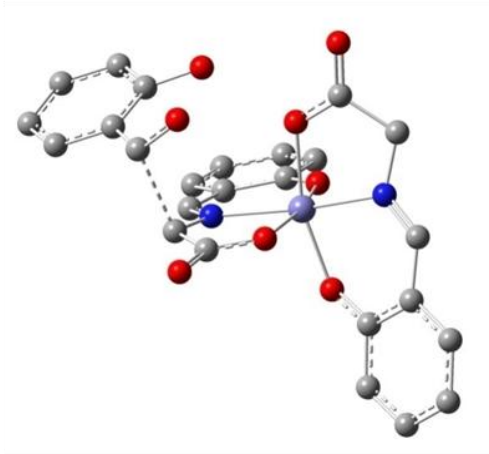
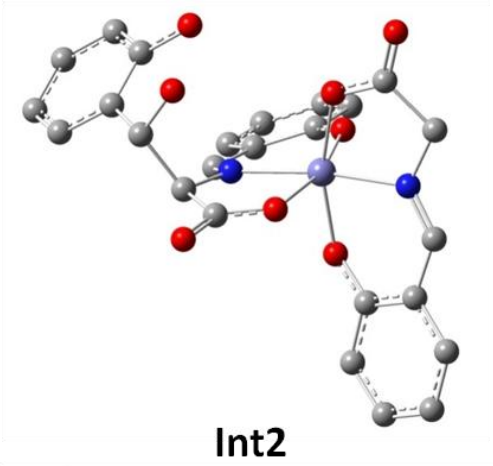


TS1



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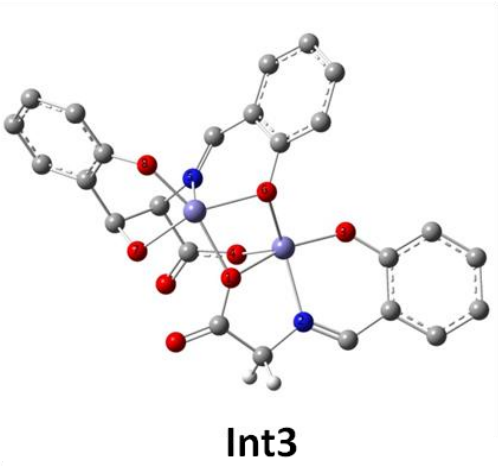

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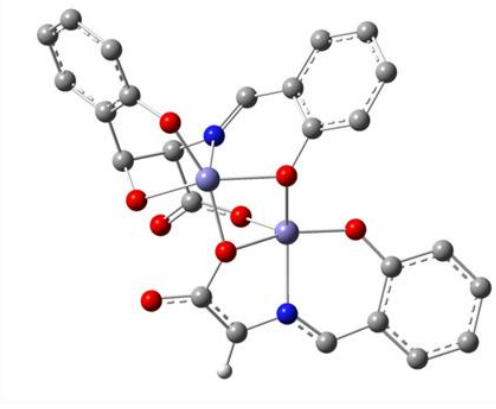

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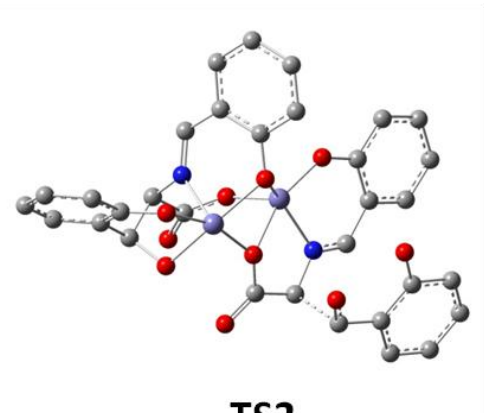

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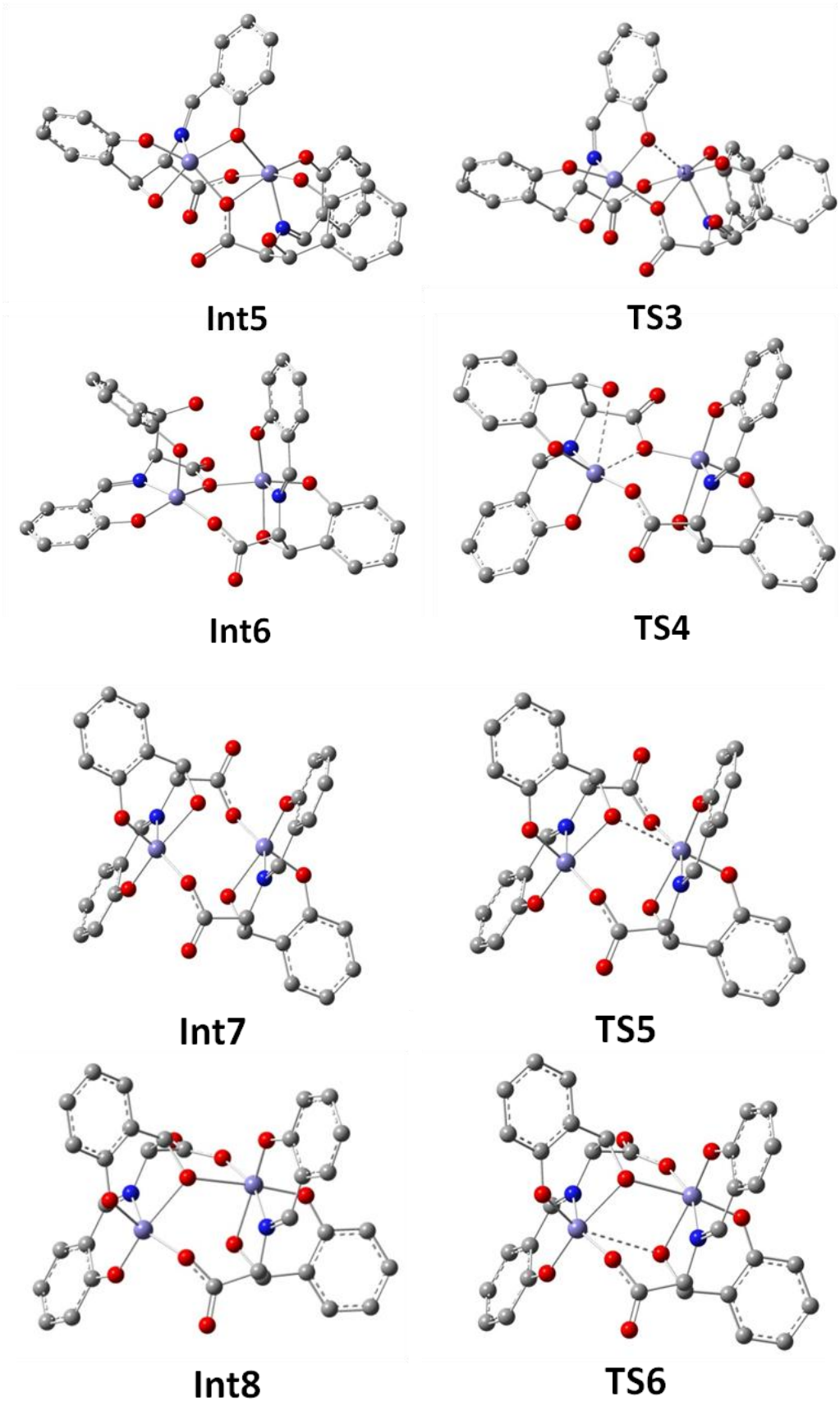
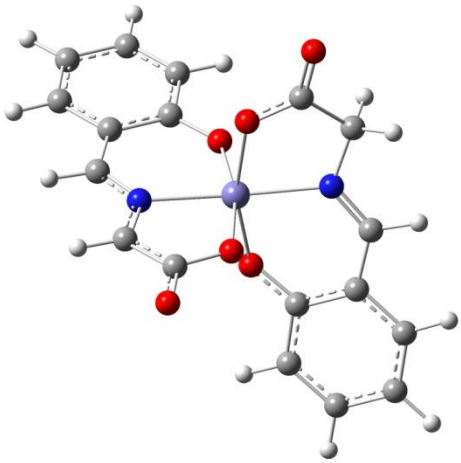


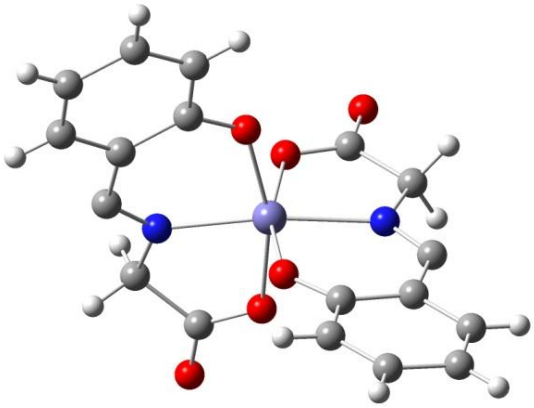
Fig. S14 The optimized structures of intermediates and transition states involved in the crystal transition process by DFT M06 method.

Theoretical Calculations

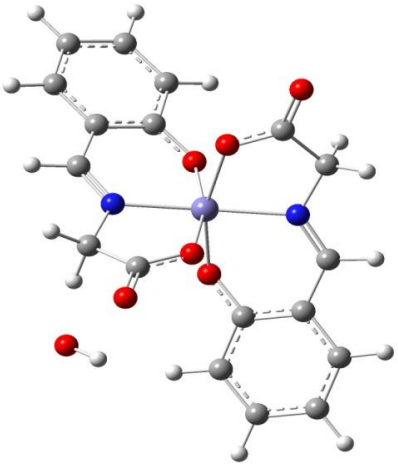
The optimized structures of all the intermediates and transition states involved in the crystal transition process by DFT M06 method. The x-ray structures of Crystal **1** (Com1) and Crystal **2** (Com2) are also shown for comparison.



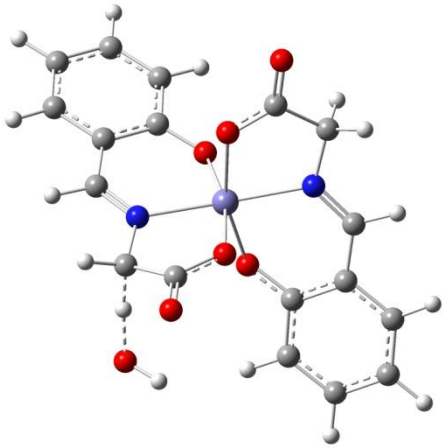
Com1



Com1 (x-ray)



Com1-OH$^-$ VW



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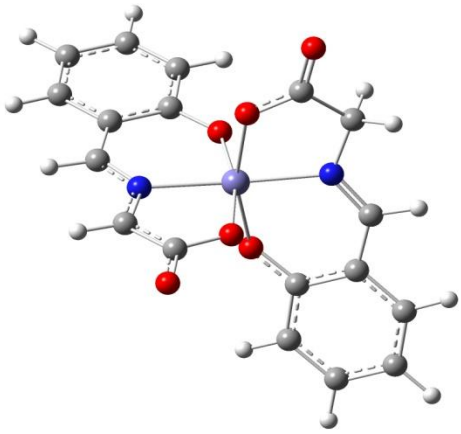

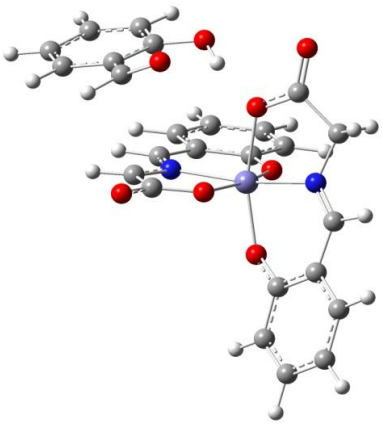

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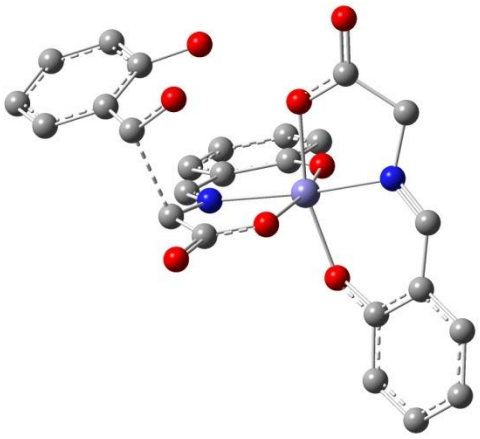
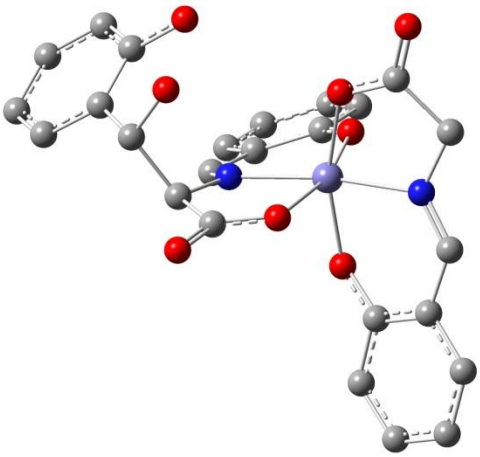
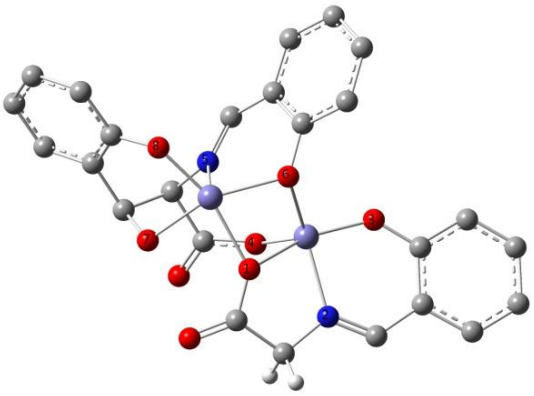


Int1-Sal VW



TS2



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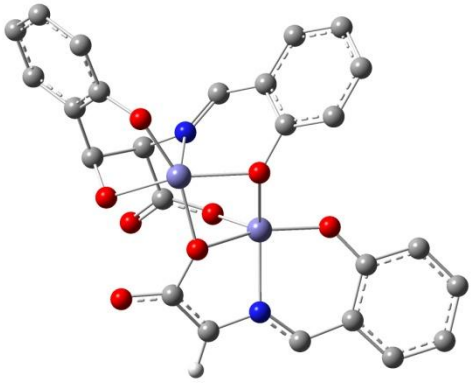

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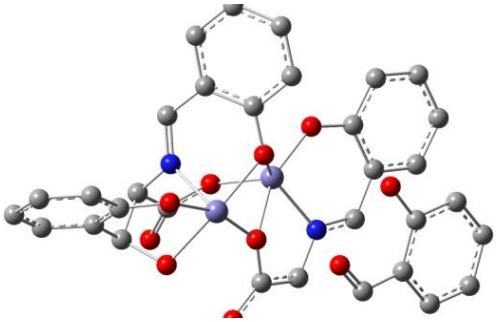

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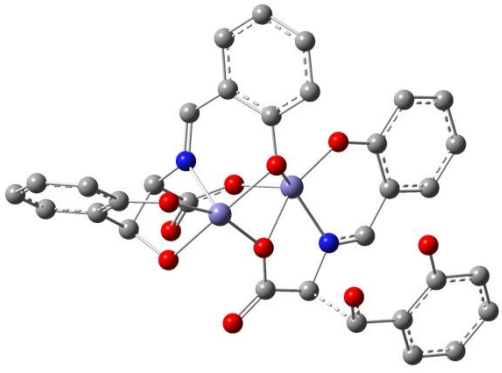
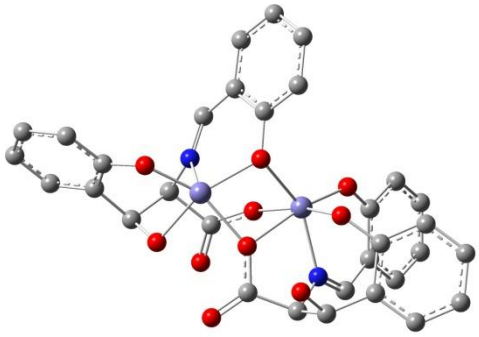


Int4-Sal VW

TS3



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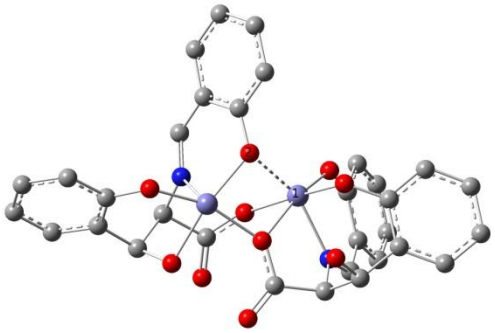

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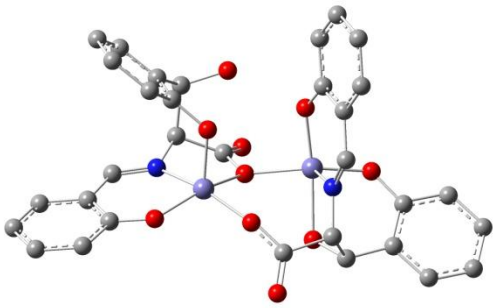

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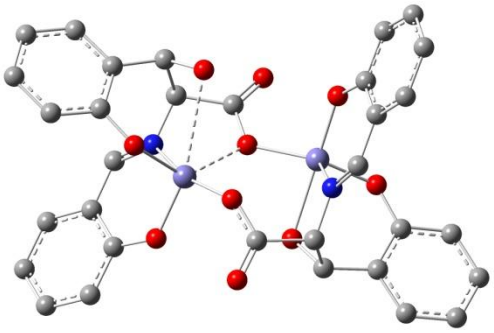

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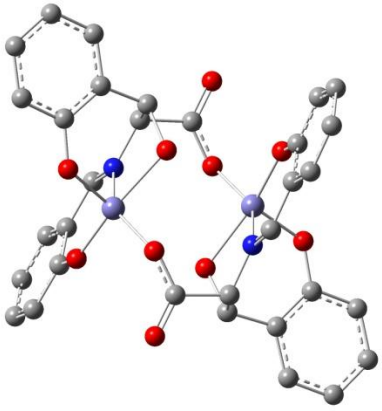

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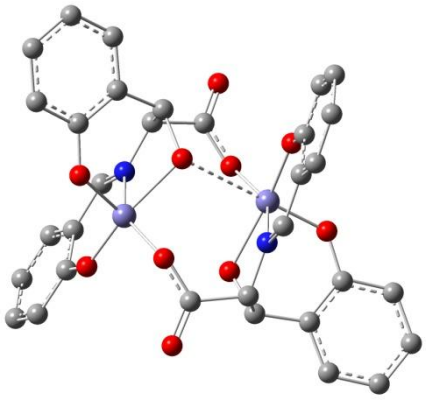
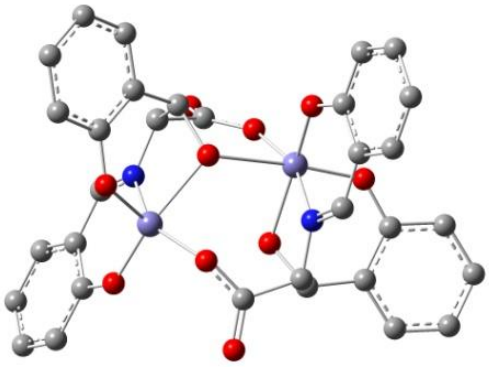
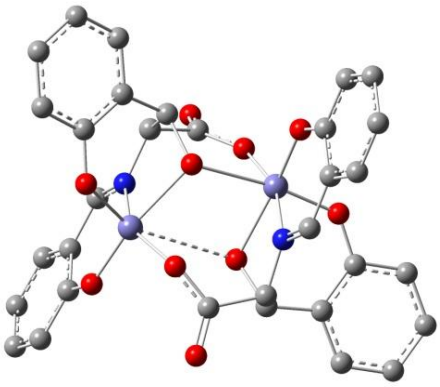


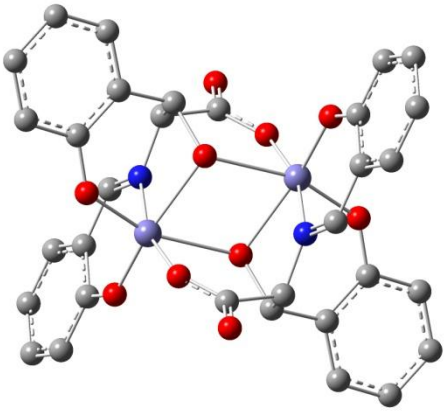
TS6



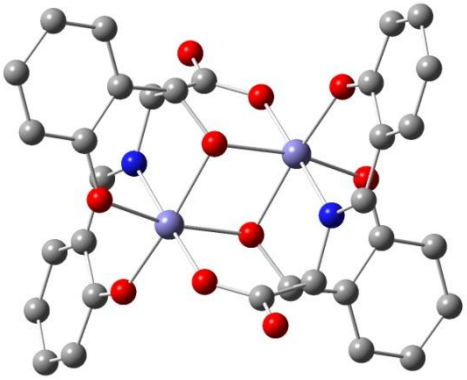
Int8



TS7

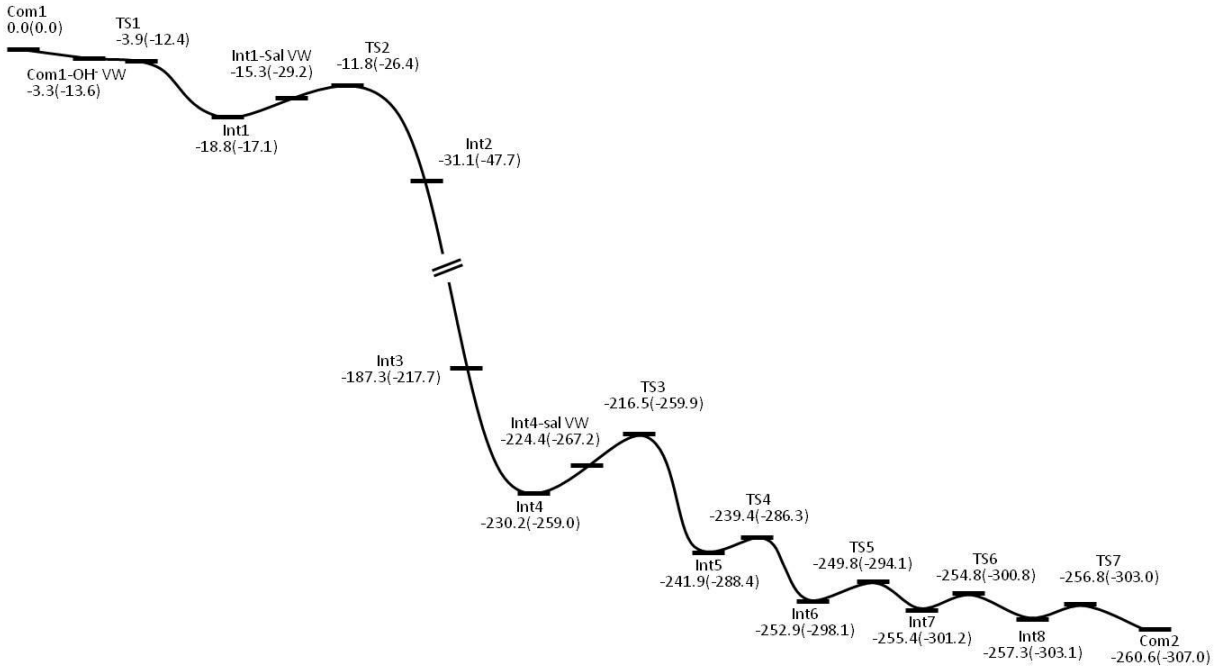


Com2



Com2 (Crystal)

Gibbs free energy profile of all the intermediates and transition states involved in the crystal transition process calculated by DFT M06 method. The relative electronic energies are shown in parenthesis. The Units for Gibbs free energy and electronic energy is kcal·mol^{-1}.



The optimized geometries for the structures depicted in Figure 5 by the M06/cep-121G method.

Com1

Fe,0,0.0387671711,-0.1880368561,0.2549971829
O,0,-1.2647511543,0.5640055102,-0.9812920387
O,0,1.0181483634,-1.3863572846,1.6046481891
O,0,1.2483408232,-3.498315392,2.4809173635
O,0,1.3508707024,-0.6500423376,-1.1080326221
O,0,-0.9508558292,0.683747138,1.8284450414
O,0,-1.1857937709,2.5483022393,3.1510892268
N,0,-1.144739714,-1.9335002869,0.2237778709
N,0,1.2230950798,1.5188518594,0.6195228885
C,0,-2.5730539,0.3158410374,-1.1432901871
C,0,-3.4028032515,1.2960227915,-1.7708534772
H,0,-2.9351327898,2.2295923112,-2.0853101026
C,0,-4.7715071018,1.0616114455,-1.9675300939
C,0,-5.3709143078,-0.1632779253,-1.5580756118
H,0,-6.433673001,-0.3386595243,-1.7185691464
C,0,-4.5718393602,-1.1400236648,-0.9509052624
H,0,-5.0085037389,-2.0910351381,-0.6361684729
C,0,-3.1781274641,-0.9267300471,-0.7251269624
C,0,-2.4143559733,-2.0022279163,-0.1090187019
C,0,-0.4806428788,-3.1147060283,0.809582983
H,0,-0.0432705112,-3.7296024285,0.0049883056
H,0,-1.1737447015,-3.7533643173,1.3790353782

C,0,0.6797665977,-2.6563127585,1.7196327218
C,0,3.2621307578,0.745364377,-0.5176999487
C,0,2.4945709419,1.6582391786,0.3172253045
C,0,0.5561722004,2.5414692732,1.4496189947
H,0,0.126309719,3.3223705867,0.7998915868
H,0,1.2458431868,3.0342132963,2.152550159
C,0,-0.6120148189,1.8952696241,2.2258108513
H,0,-5.3830706303,1.8292707082,-2.4435228555
H,0,-2.9679851239,-2.9366166259,0.0790461073
H,0,3.0470261723,2.5269373782,0.711072054
C,0,4.6569827455,1.0022310754,-0.6830238483
H,0,5.0914197562,1.8597687528,-0.1633599248
C,0,5.4598797995,0.1832601865,-1.4866855957
H,0,6.5234243509,0.3889860995,-1.5985917347
C,0,2.6599680086,-0.373453281,-1.2036110651
C,0,3.4937091773,-1.1915165103,-2.0274609436
C,0,4.86336965,-0.9204901499,-2.1598890931
H,0,5.4779635536,-1.5645401743,-2.7902443566
H,0,3.028274264,-2.0322132218,-2.5429661637

Com1-OH$^-$ VW

Fe,0,-0.0783533025,0.2709430121,0.1696109931
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O,0,-1.3149491245,3.6465767514,2.2908955124
O,0,-1.4882066471,0.6155434071,-1.1245395879
O,0,1.0529763326,-0.4980391052,1.6873650732
O,0,1.5376011975,-2.3427712317,2.9670796584
N,0,1.0431047617,2.0647256653,0.0190363616
N,0,-1.1241028414,-1.5030318495,0.6387683785
C,0,2.5222407646,-0.2448166931,-1.1402763755
C,0,3.3791228327,-1.3246296705,-1.5170548813
H,0,2.9135736371,-2.3017220635,-1.6758807188
C,0,4.7661279952,-1.1278500151,-1.6086800949
C,0,5.3499999514,0.1404117555,-1.3282873592
H,0,6.4265848208,0.282397667,-1.4140319581
C,0,4.5238482167,1.197049589,-0.9200676662
H,0,4.9546063963,2.1711302784,-0.6747470232
C,0,3.11307731,1.0252072625,-0.7950319089
C,0,2.3161233489,2.1406754045,-0.2980308199
C,0,0.3358122696,3.2471437942,0.5433902047
H,0,-0.1819684984,3.7640630915,-0.2823076921
H,0,1.0100959255,3.9729343393,1.0244327464

C,0,-0.7479761706,2.7870897053,1.5467978218
C,0,-3.2649641614,-0.8971844727,-0.4143984514
C,0,-2.3898249248,-1.7442814265,0.390915148
C,0,-0.3173904085,-2.4707600054,1.3997296347
H,0,0.1861115671,-3.1966260241,0.6811210574
H,0,-0.9135607172,-3.0453081087,2.1273874584
C,0,0.8296503808,-1.7387356646,2.0983463155
H,0,5.4069792178,-1.9636592883,-1.8937580223
H,0,2.8501438682,3.0958296947,-0.1629872091
H,0,-2.8534325784,-2.6545494943,0.8064972084
C,0,-4.6430457892,-1.2537675537,-0.5064303869
H,0,-4.9894319039,-2.1280549605,0.0507268718
C,0,-5.5420147399,-0.5118109413,-1.2858321787
H,0,-6.5922477365,-0.7955223238,-1.3397437818
C,0,-2.7791840507,0.2449480745,-1.1498067681
C,0,-3.7070464628,0.9827727766,-1.9477181849
C,0,-5.0598273388,0.6138972503,-2.0094827214
H,0,-5.7474712433,1.1986378864,-2.6221737996
H,0,-3.3271074463,1.8414724171,-2.5027021458
O,0,1.343489607,-4.1212092608,-0.4424679952
H,0,2.0789382493,-3.6408881261,0.0004022178

TS1

Fe,0,0.0552251059,-0.2358685419,0.2427859966
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O,0,0.9965348313,-1.4444572548,1.6334221002
O,0,1.1847003852,-3.5528025527,2.5297223387
O,0,1.4039149909,-0.709401034,-1.0759165687
O,0,-1.013266522,0.6310063162,1.7346686675
O,0,-1.2397950204,2.4478558326,3.1240749975
N,0,-1.153299694,-1.9779046832,0.2227058543
N,0,1.2262430947,1.4780109904,0.6555337024
C,0,-2.5167689544,0.2768540259,-1.1871322673
C,0,-3.321465308,1.2910151,-1.7956864261
H,0,-2.8189004196,2.2024516539,-2.1228189039
C,0,-4.7062298346,1.119818893,-1.9389853826
C,0,-5.3475084787,-0.0694015065,-1.4893905421
H,0,-6.4226851942,-0.1955722157,-1.6093265953
C,0,-4.5754583066,-1.0720651314,-0.8874510604
H,0,-5.0471848453,-1.9922067104,-0.5333754421
C,0,-3.1662974475,-0.9227600093,-0.7147498182
C,0,-2.4297603031,-2.0122714078,-0.0878482037
C,0,-0.5179512198,-3.1600266991,0.8343800464

H,0,-0.0799210582,-3.7944481308,0.0451948514
H,0,-1.2284314152,-3.779076696,1.404810643
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C,0,3.2730486621,0.7562055227,-0.5230885964
C,0,2.4855416078,1.6529797414,0.3215775364
C,0,0.5085292389,2.4686333913,1.4418085835
H,0,-0.0951633275,3.2519585845,0.668720546
H,0,1.1549493723,3.079741351,2.0921378293
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H,0,-5.2987151064,1.910742124,-2.4012405477
H,0,-3.0132629751,-2.921104689,0.1347732469
H,0,3.0158040254,2.5440464045,0.6981560194
C,0,4.6539641039,1.0560781175,-0.7124246543
H,0,5.0666315562,1.9317136133,-0.2043209256
C,0,5.4769325946,0.2595190248,-1.5242268076
H,0,6.5308168879,0.5049176475,-1.6515897908
C,0,2.7051319781,-0.3880735283,-1.1921610614
C,0,3.554088728,-1.1840332166,-2.0204747428
C,0,4.9138563843,-0.8684414485,-2.1801180679
H,0,5.5399662427,-1.4965005979,-2.8157974384
H,0,3.1085157622,-2.0440581467,-2.5226938853
O,0,-0.8833355729,4.0908538929,-0.1795997173
H,0,-1.8151145323,3.8609022783,0.0247063618

Int1

Fe,0,-0.0181501678,0.3855390098,0.1986172071
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O,0,-0.7408746453,2.336130494,0.1106974875
O,0,-0.6654103637,4.3623908609,-0.9731778718
O,0,-1.3787678324,-0.2070380102,-1.0329383396
O,0,1.0957812683,0.8715339375,1.7986329993
O,0,1.2240046795,0.8438230771,4.1086968121
N,0,1.3031417236,1.3013284616,-1.1905569104
N,0,-1.3282117398,-0.233331171,1.7789103484
C,0,2.3746065935,-1.3722692989,-0.3455127907
C,0,3.0554523771,-2.586984143,-0.0051241363
H,0,2.4760994344,-3.3670768368,0.4906868175
C,0,4.4157925129,-2.7618436961,-0.2936919799
C,0,5.163897068,-1.7392354611,-0.9447244528
H,0,6.2199098609,-1.8838257554,-1.169158084
C,0,4.5164119577,-0.5482034641,-1.2961428273
H,0,5.0671663537,0.2477346763,-1.8044047718
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H,0,1.6280184768,3.3267859724,-1.8549402386
C,0,-0.2709461329,3.164665666,-0.795272027
C,0,-3.2282614909,-0.9897599927,0.3527423488
C,0,-2.5505800309,-0.759897532,1.6229916027
C,0,-0.7408315968,-0.0211430401,3.0060375684
H,0,-1.2581401187,-0.2799141171,3.9358167644
C,0,0.572557839,0.583608495,3.02183356
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H,0,3.196381182,1.5895904441,-2.0182820313
H,0,-3.1118935763,-1.0392376921,2.5303056614
C,0,-4.5495431653,-1.5309468514,0.3730895195
H,0,-4.9982179093,-1.7521746576,1.3463038786
C,0,-5.2759558125,-1.7802160988,-0.8075848513
H,0,-6.2842627511,-2.1928243463,-0.7524217303
C,0,-2.6341314825,-0.7012838185,-0.9325295022
C,0,-3.379661121,-0.9569241036,-2.117807947
C,0,-4.6851366039,-1.4887141406,-2.0634674582
H,0,-5.2345913651,-1.6755871003,-2.9878407731
H,0,-2.9019691336,-0.7282849716,-3.0730417082

Int1-Sal VW

Fe,0,0.9654283574,0.1260266442,0.1583517502
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O,0,-0.0958892357,-0.7254028114,1.742492678
O,0,-0.0648771461,-1.5018218603,3.9013627855
O,0,0.2440499763,1.8606083592,0.5874949181
O,0,1.3556449871,-1.6976884328,-0.5937760047
O,0,0.6829416445,-3.3389035927,-2.0761261483
N,0,2.4563095633,-0.1131425104,1.6602901641
N,0,-0.6719574215,-0.1001421528,-1.2041579285
C,0,3.7152741256,0.6507491006,-0.9634561979
C,0,4.4786933486,0.9501630651,-2.1385480673
H,0,3.9446028482,1.3666210989,-2.9937146025
C,0,5.8595873213,0.7141405825,-2.1847139067
C,0,6.548620039,0.1757234433,-1.0603398559
H,0,7.6222235363,-0.0026524356,-1.1030314369
C,0,5.8230431003,-0.1162069942,0.1012716557
H,0,6.3312045113,-0.5243076014,0.9788785212
C,0,4.4136678736,0.10439614,0.1776849512
C,0,3.7479783668,-0.2058854701,1.4342504865

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C,0,-0.6067244553,-1.3107093361,-1.8604856544
H,0,-1.3307722897,-1.5799870428,-2.6354560064
C,0,0.5055397296,-2.1787189982,-1.5362426035
H,0,6.4130415372,0.9486117719,-3.0953904538
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C,0,-1.1220969683,3.8062363225,0.8970320806
C,0,-2.2656207206,4.5690951208,0.5824925775
H,0,-2.431500451,5.5272314663,1.0782851697
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H,0,-3.9517460245,-2.7365063803,-2.2445488444
C,0,-4.1412820125,-1.952805509,-1.5053730267
C,0,-5.2174830123,-1.0675067497,-1.6733707972
C,0,-3.2868106528,-1.8852617986,-0.3678584773
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H,0,-5.8677334724,-1.1449153962,-2.5440098374
C,0,-3.4968770016,-0.8405019327,0.5854108328
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C,0,-4.602947684,0.0357666813,0.4284931468
H,0,-6.2911318836,0.6141715637,-0.7906693761
O,0,-2.7164168311,-0.6362687643,1.6978175418
H,0,-2.1528001294,-3.5948258122,-1.1130903442
O,0,-1.665143577,-3.2390719182,0.8559347833
H,0,-4.7470420426,0.8126407076,1.1803876436
H,0,-1.7570272081,-0.9519500388,1.6511335837

TS2

26	0	0.921646	0.055596	0.287629
8	0	2.265860	0.938296	-0.858363
8	0	-0.006630	-0.876143	1.868182
8	0	0.166615	-1.837591	3.945081
8	0	0.199277	1.759539	0.850392

8	0	1.287128	-1.709018	-0.625266
8	0	0.616107	-3.196546	-2.253567
7	0	2.525803	-0.263811	1.653961
7	0	-0.756027	-0.084547	-1.027730
6	0	3.576519	0.709525	-0.989347
6	0	4.247308	1.120405	-2.186426
1	0	3.647721	1.599193	-2.961639
6	0	5.622761	0.908842	-2.354715
6	0	6.398063	0.285268	-1.335387
1	0	7.466538	0.125148	-1.473166
6	0	5.764250	-0.112335	-0.151722
1	0	6.339772	-0.584984	0.648348
6	0	4.363263	0.083251	0.048566
6	0	3.796437	-0.331345	1.323432
6	0	2.115125	-0.711634	3.000661
1	0	2.153298	0.137288	3.704017
1	0	2.766132	-1.505109	3.400482
6	0	0.654493	-1.204179	2.958357
6	0	-1.753051	2.139827	-0.556902
6	0	-1.675935	0.852536	-1.238290
6	0	-0.794434	-1.318354	-1.697749
1	0	-1.375441	-1.397793	-2.624968
6	0	0.425046	-2.127271	-1.567832
1	0	6.104437	1.227777	-3.280318
1	0	4.518711	-0.729083	2.055961
1	0	-2.450405	0.666328	-2.000778
6	0	-2.805838	3.032022	-0.919052
1	0	-3.504420	2.712473	-1.698037
6	0	-2.963223	4.284975	-0.301602
1	0	-3.777766	4.946050	-0.597827
6	0	-0.825140	2.546086	0.469998
6	0	-0.999412	3.818800	1.091173
6	0	-2.049683	4.675361	0.713235
1	0	-2.159152	5.644234	1.203434
1	0	-0.287899	4.104432	1.867987
1	0	-3.971025	-2.475402	-2.491791
6	0	-4.178293	-1.799794	-1.656128
6	0	-5.324056	-0.982878	-1.672011
6	0	-3.269617	-1.793233	-0.565682
6	0	-5.573720	-0.124943	-0.569889
1	0	-6.012999	-1.014093	-2.516185
6	0	-3.513578	-0.897997	0.516697
6	0	-2.091778	-2.712856	-0.589845
6	0	-4.676850	-0.084864	0.513133

1	0	-6.459389	0.511665	-0.560523
8	0	-2.688367	-0.771727	1.616757
1	0	-2.040425	-3.352462	-1.499252
8	0	-1.527127	-3.123885	0.502675
1	0	-4.837156	0.584889	1.359485
1	0	-1.786613	-1.202231	1.539629

Int2

26	0	0.970282	-0.219991	0.537490
8	0	1.899799	0.905416	-0.791473
8	0	0.585935	-1.392065	2.150587
8	0	1.348814	-2.380195	4.078139
8	0	0.239391	1.314904	1.485565
8	0	1.196863	-1.877382	-0.632074
8	0	0.331280	-3.227453	-2.274076
7	0	2.901580	-0.441634	1.414347
7	0	-0.804298	-0.196098	-0.615195
6	0	3.154005	0.880684	-1.256586
6	0	3.450848	1.482609	-2.521744
1	0	2.625920	1.938205	-3.070740
6	0	4.755268	1.477274	-3.035222
6	0	5.827156	0.883346	-2.309079
1	0	6.837893	0.886655	-2.714625
6	0	5.560680	0.302588	-1.063105
1	0	6.368189	-0.149543	-0.481799
6	0	4.241080	0.283591	-0.517684
6	0	4.055781	-0.301146	0.800384
6	0	2.887921	-1.012825	2.776488
1	0	3.022813	-0.210700	3.521281
1	0	3.689794	-1.751127	2.934564
6	0	1.517370	-1.665653	3.042756
6	0	-1.528600	2.081339	-0.004916
6	0	-1.560263	0.866345	-0.806173
6	0	-1.024099	-1.370772	-1.478161
1	0	-1.249015	-1.066129	-2.517616
6	0	0.253795	-2.234003	-1.485016
1	0	4.950251	1.937015	-4.005266
1	0	4.975310	-0.637728	1.307350
1	0	-2.291400	0.863771	-1.630371
6	0	-2.448154	3.120996	-0.338809
1	0	-3.107640	2.970177	-1.197753
6	0	-2.522173	4.302589	0.410302
1	0	-3.230092	5.085669	0.142112

6	0	-0.651697	2.249714	1.127227
6	0	-0.747075	3.458136	1.886613
6	0	-1.661407	4.461166	1.532965
1	0	-1.710682	5.374493	2.127673
1	0	-0.082228	3.571168	2.743851
1	0	-3.954627	-1.611457	-3.011520
6	0	-4.256540	-1.141397	-2.068380
6	0	-5.356932	-0.254916	-2.046576
6	0	-3.507185	-1.424437	-0.905027
6	0	-5.709060	0.354672	-0.813629
1	0	-5.922542	-0.046534	-2.955503
6	0	-3.866569	-0.831111	0.366453
6	0	-2.243770	-2.266625	-1.014442
6	0	-4.985420	0.074381	0.360792
1	0	-6.551019	1.050052	-0.772599
8	0	-3.184592	-1.099598	1.491306
1	0	-2.344081	-3.019954	-1.816322
8	0	-1.945882	-2.973820	0.207988
1	0	-5.255714	0.542112	1.311494
1	0	-2.262056	-2.359974	0.952696

Int3

Fe,0,-1.4091945464,-0.3104066942,-0.0289581772
O,0,-2.9517589898,0.5276068115,0.5230115591
O,0,-0.1620805778,-1.3455683663,-1.3020132047
O,0,0.7267203754,-3.4548620709,-1.2871401962
O,0,-0.3946073465,1.1396021762,-1.1046145078
O,0,-0.4228741406,-1.052150872,1.4602845333
O,0,1.0567167143,-2.512573289,2.4175815379
N,0,-2.5008386032,-2.0126161708,-0.4583228406
N,0,1.4319633574,0.6563226584,0.7186640372
C,0,-4.2721448755,0.2131466322,0.4972509202
C,0,-5.2197386114,1.1748141845,0.9277995553
H,0,-4.8562861556,2.1459239412,1.260738233
C,0,-6.5908295213,0.864271813,0.9177730445
C,0,-7.0476958599,-0.4082906691,0.4838102111
H,0,-8.1112028753,-0.6388005477,0.4818935165
C,0,-6.1158503656,-1.3650716548,0.0587725645
H,0,-6.448835577,-2.3485783273,-0.2772493864
C,0,-4.7183447508,-1.0802105779,0.0538775791
C,0,-3.8105785324,-2.1261910658,-0.3908689112
C,0,-1.679978744,-3.16786107,-0.8900650353
H,0,-2.0997459991,-3.6629560157,-1.7792749737

H,0,-1.6118228198,-3.916639003,-0.0866776007
C,0,-0.2623878131,-2.6829022715,-1.2005841505
C,0,0.4313923194,2.8508278101,0.43400246
C,0,1.1768692336,1.8520326087,1.1928883431
C,0,1.9713717509,-0.4226784514,1.5486767516
H,0,2.3919769332,-0.0663062332,2.5036118258
C,0,0.800162111,-1.423635485,1.8499983661
H,0,-7.3097038314,1.6129608342,1.2494381171
H,0,-4.277666674,-3.0780499357,-0.681825684
H,0,1.4889873676,2.1102200351,2.2145408703
C,0,0.401793991,4.2026947793,0.8736677769
H,0,1.0008288107,4.4897548342,1.738963114
C,0,-0.3845231273,5.1531736541,0.2031380114
H,0,-0.3942333789,6.1884670158,0.5382428176
C,0,-0.373710044,2.4675025566,-0.6869250002
C,0,-1.1840278857,3.415068425,-1.342700294
C,0,-1.178016974,4.7543656508,-0.9021166972
H,0,-1.7969652733,5.4885245459,-1.4166289067
H,0,-1.7996283978,3.0906051039,-2.1804295741
H,0,5.5007291315,-0.9667476821,1.8677063643
C,0,5.4170834673,-0.2364317323,1.0600673166
C,0,6.5022657147,0.6181694016,0.7695256937
C,0,4.2149664167,-0.1739126769,0.3213661994
C,0,6.3941282392,1.5478122905,-0.2900317765
H,0,7.4183515045,0.5519740851,1.3545685493
C,0,4.1104387783,0.7799380332,-0.7473166674
C,0,3.0768622112,-1.1154033372,0.692695798
C,0,5.2097465985,1.6242865237,-1.0468220712
H,0,7.2284062655,2.2069070316,-0.5286443031
O,0,2.9705886372,0.9231729929,-1.5083863598
H,0,3.4431754514,-2.0096603892,1.2134701207
O,0,2.4015426441,-1.5076829811,-0.5520121323
H,0,5.1027028516,2.3306252387,-1.8697762681
H,0,2.1230748712,-2.4515232258,-0.6939632439
Fe,0,1.3325225435,0.0897191279,-1.3129328246

Int4

Fe,0,-1.4234904644,-0.3374915902,-0.0745243505
O,0,-2.8920546535,0.6842545667,0.411368188
O,0,-0.223035725,-1.4113891617,-1.2888553745
O,0,0.469916741,-3.6220085826,-1.2432379261
O,0,-0.2491704041,1.0898533816,-1.0965430905
O,0,-0.6011110651,-1.1027785537,1.5203282959

O,0,0.6773030903,-2.7625296069,2.4497341159
N,0,-2.6621188971,-1.9243530037,-0.5837413613
N,0,1.4522879859,0.3509068681,0.7853443607
C,0,-4.2349881243,0.464958446,0.3857343107
C,0,-5.103729985,1.5156459108,0.7820729918
H,0,-4.6556130704,2.4661050452,1.0720111721
C,0,-6.4961672831,1.3244826428,0.7975815706
C,0,-7.0522053864,0.0714821854,0.4257745894
H,0,-8.130979844,-0.078015949,0.4416788974
C,0,-6.2016046714,-0.9743739744,0.0392119815
H,0,-6.61763634,-1.9425311398,-0.2478786231
C,0,-4.7831599487,-0.8107952187,-0.0015007522
C,0,-3.9787394965,-1.9540860836,-0.4078858371
C,0,-1.8737783225,-3.0337197391,-0.8906724068
H,0,-2.2736902054,-4.046862671,-0.8510450467
C,0,-0.5070198603,-2.7766378858,-1.1644498969
C,0,0.6977128704,2.6466849258,0.5327879644
C,0,1.3075575746,1.5531920258,1.2841752885
C,0,1.8498408969,-0.7958762394,1.6040934372
H,0,2.2931415548,-0.5009911843,2.5711343268
C,0,0.5598113969,-1.6428519337,1.8884204289
H,0,-7.1489076594,2.1432412295,1.1005472641
H,0,-4.5105387221,-2.902202478,-0.5717131825
H,0,1.6129548219,1.7523082044,2.3218065321
C,0,0.8003484784,3.9807326752,1.0153213205
H,0,1.3930592138,4.1729531764,1.9111003563
C,0,0.1540872544,5.0342037384,0.3495650566
H,0,0.2467199657,6.0540447217,0.7184011091
C,0,-0.0979828194,2.3844036426,-0.6306408256
C,0,-0.7681094004,3.4421195487,-1.2821445843
C,0,-0.6324006865,4.7586161108,-0.7981645641
H,0,-1.144552315,5.5720458585,-1.311559435
H,0,-1.3810469351,3.2132337667,-2.1531903645
H,0,5.2690022141,-1.6683902675,2.0504143525
C,0,5.2919969366,-0.9314929571,1.2440251455
C,0,6.4647032911,-0.1819979268,1.0099098409
C,0,4.1348708092,-0.7582701641,0.4516164946
C,0,6.4891501791,0.7543047653,-0.0491717041
H,0,7.3432501391,-0.3327599039,1.6359770943
C,0,4.1617676103,0.2047686536,-0.6144003771
C,0,2.8980788963,-1.5944545705,0.762914152
C,0,5.3506510224,0.9414417534,-0.8562478731
H,0,7.3904179219,1.3344911673,-0.2479525366
O,0,3.0762897199,0.4623963287,-1.4222375419

H,0,3.1611686623,-2.5201937173,1.2938625949
O,0,2.2645253383,-1.9109377376,-0.5137716961
H,0,5.3473685995,1.6578364509,-1.6781621697
H,0,1.7478104366,-2.7753292395,-0.6455442783
Fe,0,1.3350516631,-0.1841563108,-1.2490974342

Int4-Sal VW

Fe	0	-0.59515	0.31498	0.85105
O	0	-1.71982	1.76891	1.0306
O	0	0.09063	-1.39229	0.06817
O	0	0.29486	-3.59357	0.72813
O	0	0.49451	0.88275	-0.86886
O	0	0.47653	0.0175	2.44894
O	0	1.59503	-1.59313	3.63759
N	0	-2.18653	-0.98608	1.18349
N	0	2.47247	0.45179	0.79692
C	0	-3.05681	1.90706	1.24487
C	0	-3.61768	3.21118	1.23299
H	0	-2.95544	4.05083	1.02149
C	0	-4.987	3.40049	1.49151
C	0	-5.82168	2.28863	1.78109
H	0	-6.87972	2.43601	1.99401
C	0	-5.27423	0.99678	1.7893
H	0	-5.90924	0.13286	1.99888
C	0	-3.89459	0.76631	1.50735
C	0	-3.42699	-0.61153	1.47706
C	0	-1.74673	-2.31274	1.17235
H	0	-2.35287	-3.1178	1.5887
C	0	-0.43922	-2.5297	0.67093
C	0	2.11782	2.60339	-0.27179
C	0	2.70402	1.73949	0.75195
C	0	2.85945	-0.38886	1.92927
H	0	3.58196	0.10275	2.60487
C	0	1.5577	-0.70518	2.74793
H	0	-5.40412	4.40755	1.47624
H	0	-4.17217	-1.3902	1.6991
H	0	3.31829	2.21291	1.53193
C	0	2.58775	3.93527	-0.43691
H	0	3.43711	4.27229	0.15953
C	0	1.9699	4.80291	-1.35214
H	0	2.34306	5.81717	-1.48181
C	0	0.98911	2.16328	-1.03893
C	0	0.34824	3.04761	-1.93231

C	0	0.84599	4.35603	-2.09334
H	0	0.35544	5.03243	-2.79288
H	0	-0.52473	2.69231	-2.4794
H	0	6.08299	-1.91288	2.09673
C	0	6.02234	-1.53848	1.07213
C	0	7.2046	-1.26321	0.35255
C	0	4.74688	-1.35053	0.49471
C	0	7.11263	-0.80185	-0.98078
H	0	8.17689	-1.416	0.81947
C	0	4.65916	-0.86214	-0.85452
C	0	3.50847	-1.67626	1.32249
C	0	5.8527	-0.60762	-1.57924
H	0	8.01722	-0.59617	-1.55335
O	0	3.46102	-0.61819	-1.48809
H	0	3.73831	-2.38292	2.13215
O	0	2.53838	-2.26891	0.4033
H	0	5.75982	-0.25039	-2.60516
H	0	1.85751	-2.94139	0.73263
Fe	0	1.73318	-0.73747	-0.79277
C	0	-3.76977	-0.53214	-1.73167
C	0	-3.5734	-1.93883	-1.56138
C	0	-5.03498	0.04424	-1.48165
C	0	-4.65697	-2.73886	-1.10324
C	0	-6.0955	-0.77215	-1.05182
H	0	-5.15755	1.1196	-1.61286
C	0	-5.91234	-2.16701	-0.84707
H	0	-4.49081	-3.80943	-0.96236
H	0	-7.06857	-0.32071	-0.85726
H	0	-6.74087	-2.78434	-0.50406
O	0	-2.74718	0.30275	-2.13736
H	0	-1.92377	-0.23499	-2.31588
C	0	-2.28587	-2.56044	-1.87826
H	0	-2.19968	-3.64824	-1.68995
O	0	-1.30833	-1.92307	-2.3864

Ts3

26	0	-0.53309	0.48972	0.39482
8	0	-1.64368	1.93883	0.63473
8	0	0.19207	-1.21483	-0.41213
8	0	0.25638	-3.44648	0.1326
8	0	0.76234	1.11172	-1.09975
8	0	0.37688	0.05125	2.07229
8	0	1.28972	-1.66335	3.29123

7	0	-2.13874	-0.79666	0.63655
7	0	2.57106	0.51857	0.72405
6	0	-2.94275	2.08566	1.01663
6	0	-3.46632	3.39347	1.17505
1	0	-2.81134	4.23879	0.96599
6	0	-4.7961	3.57676	1.59467
6	0	-5.62525	2.45847	1.87028
1	0	-6.65244	2.60397	2.20112
6	0	-5.11185	1.16158	1.71327
1	0	-5.73998	0.29285	1.92158
6	0	-3.77211	0.94121	1.27791
6	0	-3.33138	-0.43626	1.08944
6	0	-1.80541	-2.15589	0.37653
1	0	-2.31849	-2.94087	0.93999
6	0	-0.40089	-2.35322	0.06532
6	0	2.32964	2.75373	-0.19567
6	0	2.79227	1.80571	0.81489
6	0	2.79732	-0.40315	1.83802
1	0	3.44332	0.02229	2.62524
6	0	1.39101	-0.72233	2.46418
1	0	-5.18814	4.58702	1.71181
1	0	-4.0547	-1.21983	1.35776
1	0	3.30424	2.21065	1.6998
6	0	2.82695	4.08582	-0.20053
1	0	3.60098	4.36166	0.51715
6	0	2.33307	5.02896	-1.11606
1	0	2.72707	6.04347	-1.12265
6	0	1.29467	2.39383	-1.11891
6	0	0.78014	3.34921	-2.01922
6	0	1.30782	4.65635	-2.02185
1	0	0.91528	5.38894	-2.72642
1	0	-0.01913	3.05328	-2.69747
1	0	5.94564	-2.07017	2.25931
6	0	6.00443	-1.63669	1.25841
6	0	7.26478	-1.36907	0.68117
6	0	4.80508	-1.36262	0.56471
6	0	7.33342	-0.82822	-0.62328
1	0	8.17545	-1.58901	1.23675
6	0	4.88315	-0.79904	-0.75448
6	0	3.46982	-1.67605	1.23082
6	0	6.15228	-0.5508	-1.33732
1	0	8.30084	-0.62684	-1.08305
8	0	3.76785	-0.47116	-1.49393
1	0	3.57569	-2.44411	2.00886

8	0	2.57647	-2.15751	0.17264
1	0	6.1798	-0.13352	-2.34387
1	0	1.88966	-2.86174	0.37175
26	0	1.9812	-0.53227	-1.00312
6	0	-4.48819	-0.92722	-1.6141
6	0	-3.97333	-2.21334	-1.26923
6	0	-5.83097	-0.5904	-1.31704
6	0	-4.82887	-3.14452	-0.6285
6	0	-6.66042	-1.5312	-0.68001
1	0	-6.19269	0.40181	-1.58845
6	0	-6.16514	-2.81685	-0.33383
1	0	-4.4288	-4.12714	-0.36323
1	0	-7.69321	-1.26756	-0.45046
1	0	-6.81539	-3.54257	0.1533
8	0	-3.69382	0.00835	-2.25415
1	0	-2.80705	-0.44899	-2.46017
6	0	-2.53968	-2.53665	-1.54643
1	0	-2.27481	-3.60998	-1.45867
8	0	-1.87198	-1.79344	-2.40769

Int5

Fe	-1.000878119087	0.300000309020	-0.136248937321
O	-2.144763583881	1.493717579253	0.759240667832
O	0.159502087767	-1.399946497390	-0.659338784421
O	0.392463786296	-3.582592752792	-0.008731413458
O	0.662858468193	1.000025092412	-1.250439485266
O	0.090971082069	0.069155044854	1.686242332122
O	0.904435574942	-1.594839655545	3.054687630586
N	-2.170865432968	-1.295959386704	0.536878295240
N	2.398904164261	0.681009091910	0.714491088823
C	-3.052817786653	1.310049494185	1.739843761519
C	-3.563329043753	2.449128907625	2.424769685887
H	-3.180407945865	3.428381636903	2.138262467917
C	-4.527094375964	2.305217904797	3.435457114782
C	-5.022770628061	1.021917163765	3.792558913916
H	-5.773080164352	0.917575322816	4.574438112334
C	-4.536833371708	-0.107452519420	3.121163450792
H	-4.911285004331	-1.101388389510	3.375439101334
C	-3.547821848897	0.002333110636	2.097510576908
C	-3.119397825488	-1.225504795351	1.439315808980
C	-1.863942626165	-2.565867641674	-0.148952692550
H	-2.194744667715	-3.433459598997	0.442190401596
C	-0.330064590028	-2.586446163846	-0.281808694058

C	1.922600082769	2.849061389258	-0.266805834445
C	2.416171731912	1.983510486568	0.803855398196
C	2.533445171282	-0.203964844928	1.871602858563
H	3.021691801362	0.276629974429	2.736189568386
C	1.051806836818	-0.622316103346	2.253031605931
H	-4.900039975048	3.191818362040	3.948826843377
H	-3.649326216983	-2.145015688121	1.733230911758
H	2.754496826474	2.462033454353	1.734450068448
C	2.218960298403	4.239450322802	-0.257402568223
H	2.889201671894	4.629262805176	0.510389120864
C	1.660390088289	5.097181793763	-1.219164686196
H	1.903177733266	6.158225897018	-1.212586340931
C	1.018150207614	2.337353114604	-1.254264774694
C	0.435382819996	3.206039532888	-2.202604899291
C	0.765636564219	4.575837410099	-2.187936324248
H	0.321454422473	5.241006666729	-2.927905759988
H	-0.263778762924	2.791979504700	-2.928636432720
H	5.756557115361	-1.615135008329	2.587743117070
C	5.862265234675	-1.233014749228	1.569761534436
C	7.142877810375	-0.920966551185	1.065628947398
C	4.700219085264	-1.071799938164	0.782601550190
C	7.270929466302	-0.451382178700	-0.261512032771
H	8.023201016913	-1.052833856944	1.693351529252
C	4.836421700227	-0.580136075470	-0.561600424456
C	3.347508165505	-1.438230537231	1.382766829970
C	6.128425258114	-0.287535444531	-1.068574014414
H	8.254692806552	-0.215882378681	-0.667551559656
O	3.760185509108	-0.366237340623	-1.400075784175
H	3.445920264308	-2.167810417976	2.196805647425
O	2.551518304229	-2.016689756628	0.291998294257
H	6.203834622618	0.074825933230	-2.093988721633
H	1.961538031006	-2.797679482433	0.469583794931
Fe	1.956861260520	-0.473119334266	-0.965380514414
C	-3.317835597713	-0.223154731329	-1.864060170829
C	-3.651283129902	-1.611131839052	-1.767506535658
C	-4.347869466724	0.739163982115	-1.998863299981
C	-5.005548189443	-2.003323644083	-1.806412764555
C	-5.698512000829	0.328018025347	-2.033517921306
H	-4.071155989957	1.792925265555	-2.061236695636
C	-6.034612613756	-1.042229630208	-1.937810857429
H	-5.253010499388	-3.065123744000	-1.731614705593
H	-6.485268631517	1.076783426237	-2.134519808919
H	-7.077432849120	-1.357424076219	-1.965259503143
O	-1.993011907467	0.154850796452	-1.810357631282

H	-1.283364386783	-1.536763646487	-2.697574618086
C	-2.533908283647	-2.629960721997	-1.603793262749
H	-2.932230836367	-3.646856078676	-1.718236161063
O	-1.532704718886	-2.492433601768	-2.649303415138

Ts4

26	0	-1.08455	0.28089	0.16819
8	0	-2.2878	0.83133	1.51574
8	0	0.11122	-0.86993	-1.16823
8	0	0.2606	-3.04741	-1.86781
8	0	0.95967	1.59891	-0.95446
8	0	-0.06352	-0.77409	1.5789
8	0	0.71128	-2.92056	1.83676
7	0	-2.28596	-1.35865	-0.21419
7	0	2.25694	0.18039	0.89751
6	0	-3.17151	0.11758	2.2421
6	0	-3.67355	0.66934	3.45566
1	0	-3.30147	1.6463	3.76328
6	0	-4.61624	-0.03076	4.22384
6	0	-5.10261	-1.29994	3.80492
1	0	-5.83809	-1.83366	4.40422
6	0	-4.62762	-1.8512	2.60889
1	0	-4.9945	-2.82107	2.26639
6	0	-3.65575	-1.17364	1.81126
6	0	-3.23462	-1.81173	0.57241
6	0	-1.96233	-2.015	-1.49661
1	0	-2.35214	-3.04346	-1.53061
6	0	-0.42344	-2.03959	-1.55143
6	0	2.06638	2.60494	0.97474
6	0	2.37248	1.30434	1.55849
6	0	2.36016	-1.13487	1.5317
1	0	2.83074	-1.09469	2.52944
6	0	0.89082	-1.67976	1.66622
1	0	-4.98216	0.40836	5.15227
1	0	-3.76469	-2.73519	0.29309
1	0	2.67899	1.28216	2.61465
6	0	2.39238	3.78947	1.69562
1	0	2.92667	3.69511	2.64291
6	0	2.03699	5.05301	1.20168
1	0	2.30042	5.95301	1.75451
6	0	1.34146	2.71443	-0.26259
6	0	0.96167	3.99357	-0.74029
6	0	1.31599	5.14767	-0.01875

1	0	1.02614	6.1266	-0.40064
1	0	0.39367	4.04904	-1.66864
1	0	5.51924	-2.8212	1.69935
6	0	5.69704	-1.99963	1.00138
6	0	7.00744	-1.51465	0.80488
6	0	4.59538	-1.45091	0.30714
6	0	7.22634	-0.46509	-0.11681
1	0	7.84051	-1.95368	1.3525
6	0	4.82223	-0.37733	-0.62107
6	0	3.20668	-2.02151	0.56813
6	0	6.14549	0.09397	-0.82565
1	0	8.23404	-0.08463	-0.28508
8	0	3.80779	0.23211	-1.32502
1	0	3.2562	-3.04667	0.95839
8	0	2.49965	-2.01602	-0.71992
1	0	6.2933	0.90363	-1.54075
1	0	1.87007	-2.75205	-0.9295
26	0	1.96618	-0.02193	-1.14923
6	0	-3.24513	0.98557	-1.63925
6	0	-3.61359	-0.19943	-2.34955
6	0	-4.23695	1.92537	-1.27317
6	0	-4.96921	-0.42266	-2.66855
6	0	-5.59003	1.68369	-1.59906
1	0	-3.93399	2.82169	-0.73014
6	0	-5.9635	0.51028	-2.29373
1	0	-5.24395	-1.32985	-3.2122
1	0	-6.3497	2.41067	-1.30939
1	0	-7.00807	0.32641	-2.54412
8	0	-1.91561	1.18378	-1.31455
1	0	-1.18181	0.26935	-2.94109
6	0	-2.52713	-1.18757	-2.74818
1	0	-2.93208	-1.92799	-3.45077
8	0	-1.4534	-0.52324	-3.47025

Int6

26	0	1.29265	-0.85152	-0.26095
8	0	2.69821	-1.79882	-1.13072
8	0	-0.04058	-0.49175	1.38118
8	0	-0.10211	-0.06281	3.63442
8	0	-1.43854	1.81841	0.59247
8	0	-0.13585	-1.48942	-1.35506
8	0	-1.10788	-3.33017	-2.31409
7	0	2.58106	-0.66279	1.36341

7	0	-2.40313	-0.16038	-1.07461
6	0	3.97836	-2.09752	-0.83749
6	0	4.77048	-2.78482	-1.80219
1	0	4.30568	-3.04686	-2.7523
6	0	6.1074	-3.10807	-1.52469
6	0	6.70482	-2.75886	-0.28071
1	0	7.7437	-3.01342	-0.07834
6	0	5.9394	-2.08471	0.67719
1	0	6.37571	-1.80513	1.63841
6	0	4.57487	-1.74609	0.42497
6	0	3.84407	-1.02993	1.45047
6	0	2.02165	0.1927	2.42447
1	0	2.52211	0.01278	3.3883
6	0	0.53484	-0.14607	2.5637
6	0	-2.3256	2.22952	-1.64247
6	0	-2.57343	0.82676	-1.92709
6	0	-2.56799	-1.5597	-1.50511
1	0	-3.19348	-1.65946	-2.4059
6	0	-1.16809	-2.19544	-1.7724
1	0	6.69604	-3.63496	-2.27607
1	0	4.41026	-0.76723	2.35749
1	0	-2.91233	0.58919	-2.94625
6	0	-2.60583	3.18415	-2.66669
1	0	-3.03931	2.83009	-3.60406
6	0	-2.32727	4.54439	-2.48432
1	0	-2.54751	5.26222	-3.27224
6	0	-1.74527	2.6808	-0.40646
6	0	-1.4487	4.06039	-0.23893
6	0	-1.74083	4.97594	-1.26326
1	0	-1.51087	6.03146	-1.11779
1	0	-0.99387	4.37649	0.70004
1	0	-5.5582	-3.44233	-0.98528
6	0	-5.71711	-2.55791	-0.36379
6	0	-7.02854	-2.1623	-0.02848
6	0	-4.58968	-1.83708	0.09479
6	0	-7.22041	-1.02987	0.79697
1	0	-7.88167	-2.73227	-0.39419
6	0	-4.79097	-0.68265	0.92051
6	0	-3.20819	-2.32749	-0.31034
6	0	-6.11333	-0.30082	1.27028
1	0	-8.22776	-0.71761	1.0731
8	0	-3.75452	0.08921	1.38657
1	0	-3.22705	-3.40144	-0.54307
8	0	-2.27748	-2.07749	0.80709

1	0	-6.23866	0.57575	1.90629
1	0	-1.70067	-2.82087	1.05974
26	0	-1.94846	0.01716	0.92194
6	0	2.64711	1.69294	-0.45818
6	0	3.02819	2.06982	0.866
6	0	3.46803	2.03297	-1.56065
6	0	4.24002	2.77449	1.04683
6	0	4.6714	2.74087	-1.35543
1	0	3.15159	1.72263	-2.55743
6	0	5.06485	3.11224	-0.04973
1	0	4.53434	3.06369	2.05861
1	0	5.29835	2.99606	-2.21031
1	0	5.99463	3.65653	0.11319
8	0	1.48664	0.9741	-0.66446
1	0	0.30208	2.11039	1.22263
6	0	2.15034	1.7614	2.07373
1	0	2.61665	2.22082	2.95655
8	0	0.85188	2.39733	1.99668

TS5

Fe,0,1.490070582,0.2876822938,0.4730529264
O,0,2.2055224528,2.0446186838,0.5302851349
O,0,0.0973393429,-0.2212522882,-1.1828121952
O,0,0.0294094849,-1.5402899961,-3.0660697703
O,0,-2.3658861858,-1.8677981334,-0.8584401616
O,0,-0.0062169633,0.4533405547,1.6686074893
O,0,-0.4246346638,2.272024052,3.0067483469
N,0,2.6470279873,-0.0297771084,-1.201593332
N,0,-2.5960097207,0.1232212115,1.0279712821
C,0,3.4166897051,2.4942469847,0.1249565546
C,0,3.9230897795,3.6995854561,0.6892144577
H,0,3.3160222478,4.204771322,1.4400194633
C,0,5.1680686834,4.2092046529,0.2883553035
C,0,5.9475450212,3.5433020354,-0.6971260939
H,0,6.9107174659,3.9473017938,-1.0040087309
C,0,5.4565846165,2.3649182825,-1.2733597383
H,0,6.0328519473,1.8433641411,-2.0405564981
C,0,4.2009711071,1.8146567272,-0.8776627986
C,0,3.7365301451,0.6091534083,-1.5487607062
C,0,2.1715689303,-1.2315039899,-1.8913956606
H,0,2.6804209332,-1.4066563306,-2.8512849351
C,0,0.6589737048,-1.0174247767,-2.1224219966
C,0,-3.7581266936,-2.0416784824,1.1304752444

C,0,-3.379919398,-0.7383692804,1.6430315677
C,0,-2.2570019399,1.4063621964,1.6672403514
H,0,-2.931347068,1.6574596327,2.5002989531
C,0,-0.787067953,1.3931340552,2.1819997971
H,0,5.5389091782,5.1303612905,0.7384411802
H,0,4.3386542964,0.2414185985,-2.3936453858
H,0,-3.7888670936,-0.4651541783,2.6268399705
C,0,-4.656994327,-2.8367408874,1.9049691119
H,0,-5.0363548256,-2.4292518813,2.8442791819
C,0,-5.0472248156,-4.1109673283,1.4769105657
H,0,-5.7348845867,-4.7067066347,2.0743579897
C,0,-3.2371685786,-2.5691186617,-0.1050322062
C,0,-3.6381481336,-3.8675551746,-0.5256855612
C,0,-4.5309348632,-4.6205275951,0.2529251742
H,0,-4.8297872127,-5.612430373,-0.0865232993
H,0,-3.2338386275,-4.251837677,-1.4614754694
H,0,-4.242450179,4.3094859844,1.1579017371
C,0,-4.5695122622,3.6627871605,0.3398156448
C,0,-5.8360494393,3.8594233275,-0.246093332
C,0,-3.6962544693,2.6440242586,-0.1105162817
C,0,-6.2348044632,3.0324996078,-1.3229545057
H,0,-6.4929907688,4.6471536291,0.1206123281
C,0,-4.1122783299,1.7983534396,-1.1925555589
C,0,-2.3427189005,2.5049534537,0.5713639846
C,0,-5.3808320889,2.0177981189,-1.7938264222
H,0,-7.2067195267,3.1790773052,-1.7948895435
O,0,-3.3382126224,0.7725875581,-1.6804217105
H,0,-2.0321999661,3.4633150545,1.0156260761
O,0,-1.3122846044,2.0500199935,-0.3783509169
H,0,-5.6703806117,1.3699023264,-2.6216102562
H,0,-1.1449546714,2.6831651374,-1.1035379103
Fe,0,-1.8627868057,-0.055835633,-0.8745010053
C,0,3.7296387264,-1.5972086364,1.0260690699
C,0,3.6170089571,-2.4508984037,-0.1225877708
C,0,4.9341479129,-1.6069789956,1.7791515348
C,0,4.713746004,-3.2674273603,-0.4839421409
C,0,6.0141273687,-2.4274776451,1.397754325
H,0,4.9961603829,-0.9542195727,2.6506375471
C,0,5.9123801424,-3.2613913883,0.2598637491
H,0,4.6176114029,-3.9165514803,-1.3577353555
H,0,6.9312922919,-2.4160270268,1.9874836726
H,0,6.7453727117,-3.8976094961,-0.0370519271
O,0,2.7132910775,-0.7716060592,1.4315693779
H,0,1.2597711275,-3.1646359052,0.6042682091

C,0,2.351790162,-2.4937466056,-0.9655098224
H,0,2.3723359325,-3.3779738539,-1.6251113115
O,0,1.1486695478,-2.5339288886,-0.1349939919

Int7

Fe,0,-1.7174853587,-0.1003446576,1.199246471
O,0,-2.3507426763,-1.8864781862,1.320254641
O,0,0.0240406658,0.1148454465,-2.2618944569
O,0,-0.7385428435,1.9510020635,-3.4023078464
O,0,1.97131394,1.8696004885,-1.1942617424
O,0,-0.1565410286,-0.3094299955,2.3023790879
O,0,0.590009323,-2.225859527,3.316859233
N,0,-2.3267463574,-0.0617415825,-0.7805029972
N,0,2.1639518252,0.0145281266,0.8715421752
C,0,-2.9208352717,-2.743534031,0.4525351845
C,0,-3.2495070792,-4.0602637627,0.8843712085
H,0,-3.0179695757,-4.333865485,1.9133163566
C,0,-3.8522346861,-4.968232738,0.0002621897
C,0,-4.1515882203,-4.5986094432,-1.3413445021
H,0,-4.6214007318,-5.3110970121,-2.0168217798
C,0,-3.8318188185,-3.3093314859,-1.7799413385
H,0,-4.0502724269,-3.0048480687,-2.8056226967
C,0,-3.2131499532,-2.3628675404,-0.9055649083
C,0,-2.9031909168,-1.0516899462,-1.437147349
C,0,-2.067103765,1.1944565077,-1.5241342514
H,0,-2.935594092,1.4885248407,-2.1349718101
C,0,-0.8432272312,1.0943636024,-2.4862382507
C,0,2.8546857118,2.3783322649,1.0172822327
C,0,2.670029245,1.0371051414,1.5341824265
C,0,1.9979661526,-1.2667510215,1.5947388465
H,0,2.8607529002,-1.483420161,2.24534155
C,0,0.7189882382,-1.2869116798,2.4882635438
H,0,-4.0950283931,-5.9720141719,0.349685683
H,0,-3.1880990929,-0.8853209404,-2.4875418572
H,0,2.984520556,0.88026164,2.5772026396
C,0,3.4131183223,3.3602799024,1.8932540602
H,0,3.6869726013,3.0583799295,2.9062301234
C,0,3.6072057266,4.6799056462,1.472030133
H,0,4.0326517993,5.4185813086,2.1487588069
C,0,2.4903434021,2.7567367074,-0.3246339414
C,0,2.6876082742,4.1054951387,-0.7372581088
C,0,3.2366939144,5.0465550073,0.1475893108
H,0,3.3813548434,6.0737065105,-0.1879487778

H,0,2.4009574327,4.3757682554,-1.7532252265
H,0,3.4587256701,-4.4785218138,1.0993133387
C,0,3.852673823,-3.9107717846,0.2525879824
C,0,5.0505244455,-4.3186096533,-0.3683178354
C,0,3.1349422952,-2.7764501938,-0.1977949674
C,0,5.5385344014,-3.5867070954,-1.4767066292
H,0,5.5867892958,-5.1933154807,-0.0025686838
C,0,3.638917506,-2.0368863519,-1.3160650735
C,0,1.8597616165,-2.4038181335,0.5465105407
C,0,4.8376879926,-2.4614044712,-1.9486702695
H,0,6.4590570538,-3.8940112042,-1.9735736881
O,0,3.0026122331,-0.9286905296,-1.8150754574
H,0,1.4526434312,-3.2913262768,1.0538310956
O,0,0.832908618,-1.8553718859,-0.3616851576
H,0,5.1948391803,-1.8858680718,-2.803055502
H,0,0.41056472,-2.5165814108,-0.9430832324
Fe,0,1.5581761078,0.0179379836,-1.1078325929
C,0,-3.5676678743,2.1704933664,1.3940896979
C,0,-3.0071286031,2.8373739071,0.2573760475
C,0,-4.7083936029,2.7253168213,2.0336422093
C,0,-3.616452891,4.0267698983,-0.2095391413
C,0,-5.3006596671,3.9056505972,1.5473318678
H,0,-5.1087601355,2.2035607389,2.9033209459
C,0,-4.7595306627,4.5628619439,0.4169270749
H,0,-3.180351185,4.5354884303,-1.0728782485
H,0,-6.1781870899,4.3131680857,2.0499209041
H,0,-5.2125066491,5.4786915804,0.0394398762
O,0,-3.0423823987,1.0095009427,1.9022178257
H,0,-0.36501749,2.3161060549,1.0153826289
C,0,-1.7864344383,2.323080956,-0.4942149612
H,0,-1.2938473419,3.1571406948,-1.0184394698
O,0,-0.8140387161,1.6883432643,0.4155278117

TS6

26	0	1.67641	-0.42936	-1.01969
8	0	2.1707	-2.23549	-1.27769
8	0	-0.28181	-0.19808	2.32236
8	0	0.84853	0.95098	3.94477
8	0	-1.70696	2.05997	1.24138
8	0	0.23327	-0.29987	-2.28031
8	0	-0.78837	-1.98548	-3.44811
7	0	2.20395	-0.60648	0.98005
7	0	-2.09795	0.4391	-1.01052

6	0	2.7186	-3.18317	-0.49112
6	0	3.03413	-4.45358	-1.04948
1	0	2.81419	-4.61833	-2.10378
6	0	3.61303	-5.45432	-0.2537
6	0	3.89451	-5.22629	1.12262
1	0	4.34448	-6.01004	1.72921
6	0	3.58606	-3.9831	1.68496
1	0	3.79464	-3.78681	2.73863
6	0	2.99866	-2.94237	0.9008
6	0	2.7227	-1.67825	1.55222
6	0	1.9947	0.59286	1.83314
1	0	2.87773	0.79986	2.45724
6	0	0.77956	0.44257	2.79558
6	0	-2.38185	2.89084	-0.95075
6	0	-2.4156	1.5842	-1.5837
6	0	-2.1379	-0.79668	-1.82525
1	0	-2.95402	-0.77418	-2.56525
6	0	-0.80564	-1.0608	-2.59459
1	0	3.84973	-6.42054	-0.69964
1	0	2.98891	-1.62542	2.61929
1	0	-2.72799	1.57441	-2.63873
6	0	-2.71048	4.02607	-1.75537
1	0	-2.98722	3.86073	-2.79852
6	0	-2.67597	5.32225	-1.2303
1	0	-2.92651	6.17765	-1.85485
6	0	-2.01778	3.09023	0.43105
6	0	-1.98492	4.41578	0.94988
6	0	-2.3061	5.50913	0.13094
1	0	-2.27294	6.51601	0.54744
1	0	-1.70411	4.54747	1.99449
1	0	-4.37235	-3.54984	-1.69518
6	0	-4.67564	-2.96717	-0.82168
6	0	-5.98014	-3.1037	-0.30615
6	0	-3.73508	-2.09055	-0.22938
6	0	-6.3516	-2.36007	0.8393
1	0	-6.68819	-3.78282	-0.77938
6	0	-4.12096	-1.33197	0.92249
6	0	-2.35654	-1.99694	-0.8659
6	0	-5.43117	-1.48802	1.44984
1	0	-7.35344	-2.46257	1.2572
8	0	-3.26893	-0.45992	1.54869
1	0	-2.13609	-2.92139	-1.42
8	0	-1.29759	-1.77435	0.1408
1	0	-5.69736	-0.90732	2.33348

1	0	-1.10972	-2.54903	0.70518
26	0	-1.60244	0.18101	0.98512
6	0	3.588	1.79782	-0.93174
6	0	2.99145	2.38113	0.23306
6	0	4.75438	2.38901	-1.48616
6	0	3.58756	3.53033	0.80698
6	0	5.33371	3.52572	-0.89272
1	0	5.18277	1.93177	-2.37834
6	0	4.7541	4.10287	0.26177
1	0	3.12341	3.97791	1.68921
1	0	6.23098	3.96275	-1.3314
1	0	5.1965	4.98577	0.72126
8	0	3.06762	0.69039	-1.55259
1	0	0.45653	1.9779	-0.69893
6	0	1.7489	1.81685	0.90811
1	0	1.25138	2.60859	1.492
8	0	0.78318	1.29086	-0.08144

Int8

Fe,0,1.8413284339,-0.6354395937,-1.0081611726
O,0,2.3781662097,-2.4122520008,-1.3226968228
O,0,-0.3620028469,0.112407872,2.4498352157
O,0,1.1555757384,-0.7490539562,3.9205860369
O,0,-1.4660002924,2.4346408172,0.8758206575
O,0,0.3932441992,-0.4174881941,-2.2613040707
O,0,-0.7002197338,-2.1287696782,-3.3221406997
N,0,2.3449551041,-0.8678838951,0.9932449148
N,0,-1.9763860181,0.5578594745,-1.1507817495
C,0,3.0272308414,-3.3393835522,-0.5864462345
C,0,3.4067967079,-4.5673501718,-1.1950794312
H,0,3.1571540598,-4.7182055258,-2.2447197688
C,0,4.0831647483,-5.547360541,-0.4513991904
C,0,4.4036368801,-5.3374952844,0.9187670355
H,0,4.9294518709,-6.1045950709,1.4842564186
C,0,4.0341160049,-4.1342704665,1.5297383026
H,0,4.2686411421,-3.9530471447,2.5805231236
C,0,3.3430991581,-3.1175382079,0.8004504681
C,0,2.9835072968,-1.9055923087,1.5089134283
C,0,2.0383750041,0.2760444457,1.9037936891
H,0,2.904513485,0.5013430454,2.5446895755
C,0,0.8715681401,-0.1528189971,2.8470489713
C,0,-2.6919372881,2.9218156984,-1.1777300729
C,0,-2.5705862452,1.5822726164,-1.7302717211

C,0,-2.0116842272,-0.7583500653,-1.8239208935
H,0,-2.8198504982,-0.8161987634,-2.571509446
C,0,-0.6834126616,-1.1415270876,-2.5412851297
H,0,4.366131616,-6.4828423732,-0.9342158532
H,0,3.2714278869,-1.864786425,2.5696424245
H,0,-3.0332686067,1.4323710217,-2.7175121385
C,0,-3.3866604576,3.8950350981,-1.9594995599
H,0,-3.7973476946,3.590407745,-2.9244132372
C,0,-3.5456380631,5.2107542007,-1.508418645
H,0,-4.0795745895,5.9410652199,-2.1137012666
C,0,-2.1427339385,3.3074074739,0.097405604
C,0,-2.3085163329,4.649016736,0.5413526404
C,0,-2.9986449181,5.5816266966,-0.2492909074
H,0,-3.1153448308,6.6041312807,0.1105120713
H,0,-1.8832075957,4.9230817821,1.5063818181
H,0,-4.3284023014,-3.4496272977,-1.3180222962
C,0,-4.6239878762,-2.7212918301,-0.558715977
C,0,-5.9381165374,-2.732054802,-0.0486578838
C,0,-3.663822143,-1.7845565141,-0.1065863223
C,0,-6.3002915808,-1.7935037378,0.9469338611
H,0,-6.6608180466,-3.461222555,-0.4128413498
C,0,-4.0382701748,-0.8313060191,0.8959197455
C,0,-2.2766393141,-1.8288431475,-0.7283936603
C,0,-5.3609046184,-0.8575368203,1.4170085141
H,0,-7.3103704621,-1.7948809504,1.3576554969
O,0,-3.1675522705,0.1013726841,1.3881250572
H,0,-2.0861858849,-2.8224224889,-1.1608613719
O,0,-1.2208728837,-1.5261058532,0.2637231899
H,0,-5.6198757948,-0.1289071889,2.1857539932
H,0,-1.078337683,-2.2378682688,0.9175143073
Fe,0,-1.4106596328,0.5314303475,0.8724739359
C,0,3.5769039784,1.7310840665,-0.739397075
C,0,2.9051688237,2.2184448241,0.4274045842
C,0,4.7060583488,2.4314435388,-1.238710141
C,0,3.3878650148,3.3920322232,1.0559993252
C,0,5.175119571,3.5882844467,-0.5889827343
H,0,5.1927677377,2.0430774138,-2.1334095074
C,0,4.5182088869,4.0755890147,0.5654507313
H,0,2.8657054303,3.767992373,1.9387537043
H,0,6.046039415,4.1109083647,-0.9847812939
H,0,4.8740726009,4.9743460059,1.0671641212
O,0,3.1538094432,0.615173425,-1.4154115055
H,0,0.5348245066,1.6924920265,-0.6400829645
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H,0,1.1417662283,2.2382194526,1.6711297851
O,0,0.7793610959,0.9994766565,0.0132067505

TS7

Fe,0,1.7524469169,0.1558114627,-1.0441369165
O,0,2.8965628816,-1.2884182142,-1.4593561929
O,0,-0.3686917198,-0.0198076843,2.5114173743
O,0,1.364181836,-0.0820802559,3.9959376081
O,0,-2.4218476607,1.6226799367,1.0754742777
O,0,0.3491233018,-0.1026118434,-2.323155036
O,0,-0.1973334379,-1.8889354777,-3.6440138022
N,0,2.3591542132,0.0604377143,0.9305501099
N,0,-2.1496262745,-0.2074064836,-1.0431390644
C,0,3.784936566,-2.0081907287,-0.7414819319
C,0,4.5294522228,-3.0328414452,-1.3886273907
H,0,4.3489147954,-3.2057047591,-2.4489643205
C,0,5.4660507349,-3.7912662545,-0.6689561622
C,0,5.6943552589,-3.5543805831,0.7153400384
H,0,6.4245015112,-4.1480887437,1.2621060559
C,0,4.9697114487,-2.5488546362,1.3639254929
H,0,5.1298093951,-2.3492991573,2.4252942175
C,0,4.0057333404,-1.7614193815,0.6604520414
C,0,3.2992133771,-0.7405395039,1.4071041534
C,0,1.7512400911,1.0462607074,1.8766456479
H,0,2.5356661944,1.5583897975,2.4538157387
C,0,0.8651585592,0.2665453995,2.8925093525
C,0,-3.6829965125,1.7292750186,-1.0119083561
C,0,-3.0798785406,0.5441516273,-1.5988464322
C,0,-1.6724266604,-1.3977564513,-1.7846667298
H,0,-2.4548979745,-1.8116387908,-2.4405537857
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H,0,6.0263760022,-4.5732960458,-1.1815623206
H,0,3.5839479757,-0.6365199781,2.4647010842
H,0,-3.4530149863,0.2679519029,-2.5967388301
C,0,-4.660597077,2.4221532457,-1.7898569278
H,0,-4.9137017631,2.0291645527,-2.7767194123
C,0,-5.2849140048,3.5792050222,-1.3096164185
H,0,-6.0274820347,4.0969824051,-1.9139418436
C,0,-3.3381087202,2.2334572075,0.2931889352
C,0,-3.9794385862,3.4112978527,0.7678226136
C,0,-4.9344442761,4.0709684688,-0.0221223378
H,0,-5.4130536664,4.972604965,0.3605937458
H,0,-3.7036942451,3.7795525681,1.755480909

H,0,-2.2810693061,-4.9144395424,-1.2802078424
C,0,-2.8424202144,-4.4364020355,-0.4736531564
C,0,-3.9372767618,-5.1051032482,0.1106148767
C,0,-2.44569746,-3.1496669818,-0.0365718608
C,0,-4.6456494948,-4.4808059406,1.164730296
H,0,-4.227235974,-6.0939947744,-0.2421833472
C,0,-3.1698130069,-2.5201309919,1.0268851406
C,0,-1.2779919466,-2.4856844975,-0.7477382013
C,0,-4.2637530148,-3.2058168096,1.6215471032
H,0,-5.4896601177,-4.9882084031,1.6328034258
O,0,-2.8372145208,-1.2843877465,1.5056485526
H,0,-0.6708936996,-3.2491287911,-1.2581466727
O,0,-0.4063994667,-1.7398802872,0.1938199196
H,0,-4.7936056947,-2.7105164244,2.4356870108
H,0,0.0743993505,-2.3275030427,0.8112897892
Fe,0,-1.5321722711,-0.0490247798,0.9591235453
C,0,2.5583585495,2.9820854772,-0.7664754152
C,0,1.7926042499,3.191004413,0.4245739408
C,0,3.3434655267,4.0433613359,-1.2877376722
C,0,1.8370095522,4.4578601277,1.0555671043
C,0,3.3826292177,5.2897699092,-0.6354527065
H,0,3.9103250276,3.8590330698,-2.2003245571
C,0,2.6289030246,5.5045325209,0.542501355
H,0,1.2425710692,4.6173544994,1.957921752
H,0,3.9943428265,6.0924599581,-1.0474745695
H,0,2.6516913209,6.4700115009,1.0458623315
O,0,2.5439410825,1.789881629,-1.4420316831
H,0,-0.2792962469,1.8754303646,-0.568309738
C,0,0.9543041986,2.1028420447,1.0759235752
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Com2

26	0	-1.51195	-0.26173	-0.99115
8	0	-2.82367	1.04981	-1.31767
8	0	0.35691	0.03256	2.52502
8	0	-1.20572	-0.49362	4.10422
8	0	2.8218	-1.04695	1.32015
8	0	-0.35601	-0.03836	-2.52426
8	0	1.20612	0.48686	-4.10415
7	0	-2.22085	-0.44968	0.97007
7	0	2.22003	0.44817	-0.96998
6	0	-3.91172	1.47052	-0.63595

6	0	-4.79687	2.39839	-1.25001
1	0	-4.56196	2.73941	-2.25769
6	0	-5.93572	2.85343	-0.5665
6	0	-6.23165	2.3975	0.7476
1	0	-7.11811	2.75505	1.2681
6	0	-5.36833	1.48342	1.36308
1	0	-5.57657	1.12215	2.37211
6	0	-4.19916	1.00502	0.69629
6	0	-3.35383	0.06718	1.41288
6	0	-1.50782	-1.4048	1.8662
1	0	-2.22318	-2.04684	2.40228
6	0	-0.74135	-0.57992	2.93735
6	0	4.19848	-1.0056	-0.69292
6	0	3.35301	-0.06974	-1.41168
6	0	1.50758	1.40208	-1.8678
1	0	2.22341	2.04271	-2.40493
6	0	0.74127	0.57525	-2.93764
1	0	-6.60205	3.56547	-1.05355
1	0	-3.70867	-0.22795	2.4123
1	0	3.70785	0.22335	-2.4117
6	0	5.36853	-1.48432	-1.35793
1	0	5.57689	-1.12544	-2.3678
6	0	6.23269	-2.39559	-0.73955
1	0	7.11986	-2.75346	-1.25863
6	0	3.91089	-1.46782	0.64042
6	0	4.79709	-2.39275	1.25751
6	0	5.93683	-2.84815	0.57576
1	0	6.60398	-3.55781	1.06515
1	0	4.56214	-2.73122	2.26604
1	0	0.54185	4.92839	-1.66095
6	0	1.16965	4.75024	-0.78499
6	0	1.84458	5.82564	-0.17363
6	0	1.28727	3.43056	-0.28616
6	0	2.64524	5.58049	0.96734
1	0	1.74366	6.8335	-0.57382
6	0	2.09652	3.18796	0.87154
6	0	0.57845	2.31492	-1.03251
6	0	2.76617	4.2787	1.4883
1	0	3.16876	6.40374	1.454
8	0	2.22777	1.94384	1.41881
1	0	-0.19603	2.73581	-1.69186
8	0	-0.11592	1.39589	-0.07185
1	0	3.37117	4.07268	2.37146
1	0	-0.66417	1.91446	0.55801

26	0	1.50892	0.26289	0.99039
6	0	-2.09737	-3.18725	-0.87402
6	0	-1.28541	-3.43062	0.28165
6	0	-2.76601	-4.27801	-1.49185
6	0	-1.16427	-4.75115	0.77737
6	0	-2.64138	-5.58071	-0.97402
1	0	-3.37309	-4.07123	-2.3734
6	0	-1.83807	-5.82664	0.16492
1	0	-0.53461	-4.92996	1.65188
1	0	-3.16412	-6.404	-1.46146
1	0	-1.73435	-6.83513	0.56279
8	0	-2.23235	-1.9422	-1.41825
1	0	0.66523	-1.9099	-0.55973
6	0	-0.57772	-2.31518	1.02938
1	0	0.19715	-2.73629	1.6881
8	0	0.1153	-1.39353	0.07048