Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Effect of Hydrogenation on the Structure and Magnetic Properties of an Iron Oxide Cluster

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Excerpts from Gaussian 09 outputs.

$Fe_8O_{12}H$

$$$$$$$$$$$$$ Fe8O12H NEUTRAL S = 8 head fe8o12h_8_GF.out

```
 ---------------------------------------------------------------------
 # UBPW91/6-311+G*
scf=(VSHIFT=5,NoIncFock,Maxcycle=90,Tight,NoVarAcc)  NOSYMM
 OPT=RFO IOP(5/13=1,5/36=1,8/11=1) INT=UltraFine GUESS=READ
GEOM=CHECKPOINT
 ---------------------------------------------------------------------
 Charge =  0 Multiplicity = 8
                    Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic          Coordinates (Angstroms)
 Number     Number       Type             X           Y           Z
 ---------------------------------------------------------------------
     1         26          0       -0.781701   -1.650570   -0.164941
     2         26          0       -1.063459    0.749540   -1.314632
     3         26          0       -1.307901    0.580124    1.221672
     4         26          0       -1.762919    2.960108    0.051213
     5         26          0        1.605653   -2.985155   -0.018517
```

6	26	0	1.309112	-0.513875	-1.199255
7	26	0	1.054720	-0.691318	1.411942
8	26	0	0.785253	1.650326	0.207444
9	8	0	-0.155785	-3.281523	-0.216879
10	8	0	0.760675	1.289862	-1.636939
11	8	0	-0.753455	-1.198935	1.679293
12	8	0	0.129347	3.490781	0.141727
13	8	0	-2.170971	-0.312434	-0.212559
14	8	0	-1.968685	2.235972	-1.571277
15	8	0	1.943570	-2.191066	1.560751
16	8	0	2.164450	0.350895	0.269207
17	8	0	-0.398468	-0.953865	-1.892967
18	8	0	-2.252302	2.032346	1.496251
19	8	0	2.232455	-1.989102	-1.380049
20	8	0	0.399402	1.039896	1.952178
21	1	0	0.441768	3.887988	-0.694094

Distance matrix (angstroms):

		1	2	3	4	5
1	Fe	0.000000				
2	Fe	2.676136	0.000000			
3	Fe	2.678727	2.553682	0.000000		
4	Fe	4.718883	2.690982	2.690973	0.000000	
5	Fe	2.738981	4.769908	4.768447	6.833615	0.000000
6	Fe	2.594875	2.690469	3.729139	4.803082	2.754869
7	Fe	2.603683	3.741251	2.689748	4.808698	2.758882
8	Fe	3.672864	2.558490	2.560329	2.869340	4.712940
9	O	1.747707	4.275325	4.278916	6.450791	1.797177
10	O	3.632057	1.929585	3.599221	3.465271	4.648553
11	O	1.898939	3.585560	1.918822	4.579006	3.411529
12	O	5.230443	3.325382	3.421094	1.967352	6.644013
13	O	1.929494	1.889163	1.896990	3.308416	4.630764
14	O	4.300223	1.759199	3.313463	1.788627	6.515146
15	O	3.270665	5.094823	4.285620	6.523140	1.799681
16	O	3.588056	3.617577	3.607902	4.720141	3.394741
17	O	1.902193	1.917883	3.589034	4.578291	3.414118
18	O	4.299546	3.310589	1.753920	1.785601	6.507969
19	O	3.267450	4.285731	5.089597	6.519678	1.799659
20	O	3.621575	3.591145	1.913090	3.460710	4.641090
21	H	5.696709	3.535623	4.203982	2.505412	7.003651

		6	7	8	9	10
6	Fe	0.000000				
7	Fe	2.629553	0.000000			
8	Fe	2.633818	2.647022	0.000000		
9	O	3.281899	3.290523	5.038724	0.000000	
10	O	1.935411	3.647905	1.879438	4.873811	0.000000

11	O	3.606871	1.897009	3.557000	2.879210	4.414079
12	O	4.384900	4.467629	1.954943	6.787783	2.899357
13	O	3.622861	3.631479	3.573247	3.588382	3.631909
14	O	4.294649	5.158450	3.330316	5.963536	2.889437
15	O	3.291373	1.749698	4.234316	2.959114	4.872507
16	O	1.906780	1.903563	1.895922	4.337537	2.546691
17	O	1.894902	3.619821	3.548906	2.878569	2.538400
18	O	5.141270	4.285073	3.321702	5.963841	4.409784
19	O	1.749727	3.296441	4.226106	2.954152	3.603295
20	O	3.629505	1.928315	1.888280	4.867002	3.615904
21	H	4.514850	5.077513	2.436777	7.210180	2.782250

		11	12	13	14	15
11	O	0.000000				
12	O	5.013669	0.000000			
13	O	2.524746	4.458859	0.000000		
14	O	4.882784	2.985074	2.895066	0.000000	
15	O	2.876164	6.130940	4.858327	6.686854	0.000000
16	O	3.592280	3.743899	4.412253	4.901398	2.859797
17	O	3.598209	4.916649	2.525266	3.569892	4.352468
18	O	3.566682	3.103872	2.902523	3.087334	5.953715
19	O	4.347367	6.063661	4.854319	5.961325	2.961849
20	O	2.532965	3.059003	3.622390	4.410576	3.602331
21	H	5.739190	0.976717	4.970093	3.051047	6.655421

		16	17	18	19	20
16	O	0.000000				
17	O	3.598047	0.000000			
18	O	4.882685	4.882720	0.000000		
19	O	2.863609	2.873422	6.675193	0.000000	
20	O	2.534266	4.404182	2.867815	4.861960	0.000000
21	H	4.050507	5.058343	3.936881	6.182012	3.887953

		21
21	H	0.000000

Alpha occ. eigenvalues -- -0.25181 -0.24978 -0.24763 -0.24704 -0.24267
Alpha occ. eigenvalues -- -0.24204 -0.22698 -0.22571 -0.22378 -0.21914
Alpha occ. eigenvalues -- -0.21881
Alpha virt. eigenvalues -- -0.20013 -0.19279 -0.18986 -0.18574 -0.18263
0.51 eV
Beta occ. eigenvalues -- -0.25021 -0.24532 -0.23446 -0.23313 -0.22416
Beta occ. eigenvalues -- -0.21472 -0.21430 -0.20665 -0.20517
Beta virt. eigenvalues -- -0.18474 -0.18358 -0.18060 -0.17973 -0.17417
0.56 eV
Mulliken atomic spin densities:

		1
1	Fe	2.297514
2	Fe	2.203989
3	Fe	2.184969

```
     4  Fe  -3.637474
     5  Fe  -3.481045
     6  Fe   2.338680
     7  Fe   2.356871
     8  Fe   2.418925
     9  O   -0.015421
    10  O    0.093381
    11  O    0.121771
    12  O   -0.058509
    13  O    0.066472
    14  O   -0.117017
    15  O   -0.011110
    16  O    0.144804
    17  O    0.116147
    18  O   -0.111940
    19  O   -0.011998
    20  O    0.107141
    21  H   -0.006150
 Sum of Mulliken atomic spin densities =   7.00000
Dipole moment (field-independent basis, Debye):
   X=              0.4699    Y=              2.8357    Z=             -0.7567  Tot=
2.9723


Isotropic polarizability for W=    0.000000      258.04 Bohr**3.   1.821   A**3
per atom

Frequencies --    93.1484              99.9655             115.0218
 Frequencies --   128.1522             142.3815             146.4085
 Frequencies --   148.6216             150.2412             158.3324
 Frequencies --   163.7093             167.5495             178.6008
 Frequencies --   201.7433             204.2942             212.0163
 Frequencies --   229.0824             237.0365             240.4329
 Frequencies --   244.4429             245.6118             247.7209
 Frequencies --   253.3962             257.2920             280.0586
 Frequencies --   364.5283             381.6489             386.1957
 Frequencies --   393.0248             424.0249             433.0703
 Frequencies --   449.2178             452.8174             460.2024
 Frequencies --   466.0948             468.8134             493.6195
 Frequencies --   495.8556             499.2499             507.1809
 Frequencies --   534.4398             536.8973             544.0443
 Frequencies --   549.4092             557.7618             581.5328
 Frequencies --   583.5931             584.9040             589.8289
 Frequencies --   591.4740             623.4505             630.1275
 Frequencies --   631.9533             640.9941             652.1496
```

```
Frequencies --   658.0980            851.8006           3639.1832
[headnode:~/feon] ggutsev% grep "Inten" fe8o12h_8.out
IR Inten    --     0.1971             1.3417            17.7552
IR Inten    --     3.4162            19.0251             3.5026
IR Inten    --     7.8987            29.3799             3.4853
IR Inten    --     2.0705             5.2820             3.6845
IR Inten    --     0.7858             0.7957             1.9422
IR Inten    --     1.0086             3.4501             8.8097
IR Inten    --     0.0832             5.0013             1.8072
IR Inten    --     2.3718             3.4251             0.0856
IR Inten    --     0.4729            12.6765             3.6273
IR Inten    --     1.7321             0.7559             0.8237
IR Inten    --     6.2398             4.8349            15.5193
IR Inten    --    34.5800            11.8560             4.4824
IR Inten    --    16.4575            21.4644             8.3696
IR Inten    --    20.0785            16.9959             7.5483
IR Inten    --    67.4509            47.5023             8.8971
IR Inten    --    31.6264            50.7627             3.4851
IR Inten    --    10.4753            93.4904            40.0151
IR Inten    --    39.6351            99.4734           136.0361
IR Inten    --    57.3001            48.7864            96.6934
Zero-point vibrational energy     150744.1 (Joules/Mol)
                                  36.02871 (Kcal/Mol)   1.562 eV

  Atom  No         Natural Electron Configuration
 ----------------------------------------------------------------------
    Fe    1     [core]4S( 0.26)3d( 6.51)4p( 0.51)4d( 0.03)5p( 0.01)
    Fe    2     [core]4S( 0.26)3d( 6.53)4p( 0.53)4d( 0.03)5p( 0.01)
    Fe    3     [core]4S( 0.26)3d( 6.53)4p( 0.53)4d( 0.03)5p( 0.01)
    Fe    4     [core]4S( 0.20)3d( 6.31)4p( 0.31)4d( 0.02)
    Fe    5     [core]4S( 0.19)3d( 6.32)4p( 0.33)4d( 0.02)
    Fe    6     [core]4S( 0.26)3d( 6.50)4p( 0.51)4d( 0.03)5p( 0.01)
    Fe    7     [core]4S( 0.26)3d( 6.50)4p( 0.50)4d( 0.03)5p( 0.01)
    Fe    8     [core]4S( 0.26)3d( 6.49)4p( 0.49)4d( 0.03)5p( 0.01)
     O    9    [core]2S( 1.78)2p( 4.77)3S( 0.01)3p( 0.01)
     O   10     [core]2S( 1.73)2p( 4.82)3S( 0.01)3p( 0.01)
     O   11     [core]2S( 1.73)2p( 4.78)3S( 0.01)3p( 0.01)
     O   12     [core]2S( 1.73)2p( 5.09)3p( 0.01)
     O   13     [core]2S( 1.72)2p( 4.77)3S( 0.01)3p( 0.01)
     O   14     [core]2S( 1.78)2p( 4.78)3S( 0.01)3p( 0.01)
     O   15     [core]2S( 1.78)2p( 4.77)3S( 0.01)3p( 0.01)
     O   16     [core]2S( 1.73)2p( 4.78)3S( 0.01)3p( 0.01)
     O   17     [core]2S( 1.72)2p( 4.78)3S( 0.01)3p( 0.01)
     O   18     [core]2S( 1.77)2p( 4.77)3S( 0.01)3p( 0.01)
     O   19     [core]2S( 1.78)2p( 4.77)3S( 0.01)3p( 0.01)
     O   20     [core]2S( 1.73)2p( 4.80)3S( 0.01)3p( 0.01)
```

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    H   21          1S( 0.51)


************************************************
*******        Alpha spin orbitals        *******
************************************************
  Atom  No         Natural Electron Configuration
--------------------------------------------------------------------------------
    Fe    1     [core]3d( 4.31)4p( 0.17)4d( 0.01)5p( 0.10)6S( 0.14)5d( 0.01)
2.17  close to the Mulliken value of  2.2
    Fe    2     [core]3d( 4.27)4p( 0.17)4d( 0.02)5p( 0.11)6S( 0.15)5d( 0.01)
    Fe    3     [core]3d( 4.27)4p( 0.17)4d( 0.01)5p( 0.11)6S( 0.15)5d( 0.01)
    Fe    4     [core]4S( 0.07)3d( 1.49)4p( 0.15)4d( 0.01)
    Fe    5     [core]4S( 0.07)3d( 1.57)4p( 0.15)4d( 0.01)
    Fe    6     [core]3d( 4.32)4p( 0.16)4d( 0.02)5p( 0.11)6S( 0.15)5d( 0.01)
    Fe    7     [core]3d( 4.33)4p( 0.16)4d( 0.02)5p( 0.11)6S( 0.15)5d( 0.01)
    Fe    8     [core]3d( 4.36)4p( 0.17)5S( 0.15)4d( 0.01)5p( 0.09)5d( 0.01)
     O    9    [core]2S( 0.89)2p( 2.37)
     O   10     [core]2S( 0.87)2p( 2.49)4p( 0.01)
     O   11     [core]2S( 0.87)2p( 2.48)4p( 0.01)
     O   12     [core]2S( 0.86)2p( 2.51)
     O   13     [core]2S( 0.87)2p( 2.44)4p( 0.01)
     O   14     [core]2S( 0.89)2p( 2.33)
     O   15     [core]2S( 0.89)2p( 2.37)
     O   16     [core]2S( 0.87)2p( 2.49)4p( 0.01)
     O   17     [core]2S( 0.87)2p( 2.47)4p( 0.01)
     O   18     [core]2S( 0.89)2p( 2.33)
     O   19     [core]2S( 0.89)2p( 2.37)
     O   20     [core]2S( 0.87)2p( 2.48)4p( 0.01)
     H   21          1S( 0.25)


************************************************
*******        Beta  spin orbitals        *******
************************************************
  Atom  No         Natural Electron Configuration
--------------------------------------------------------------------------------
    Fe    1     [core]3d( 2.20)4p( 0.16)4d( 0.01)5p( 0.08)6S( 0.11)5d( 0.01)
    Fe    2     [core]3d( 2.26)4p( 0.16)4d( 0.01)5p( 0.10)6S( 0.12)
    Fe    3     [core]3d( 2.26)4p( 0.16)4d( 0.01)5p( 0.10)6S( 0.12)
    Fe    4     [core]4S( 0.13)3d( 4.83)4p( 0.17)4d( 0.01)
    Fe    5     [core]4S( 0.12)3d( 4.75)4p( 0.17)4d( 0.01)
    Fe    6     [core]3d( 2.18)4p( 0.15)4d( 0.01)5p( 0.09)6S( 0.11)
    Fe    7     [core]3d( 2.17)4p( 0.15)4d( 0.01)5p( 0.09)6S( 0.11)
    Fe    8     [core]3d( 2.12)4p( 0.15)5S( 0.11)4d( 0.01)5p( 0.08)5d( 0.01)
     O    9    [core]2S( 0.89)2p( 2.40)
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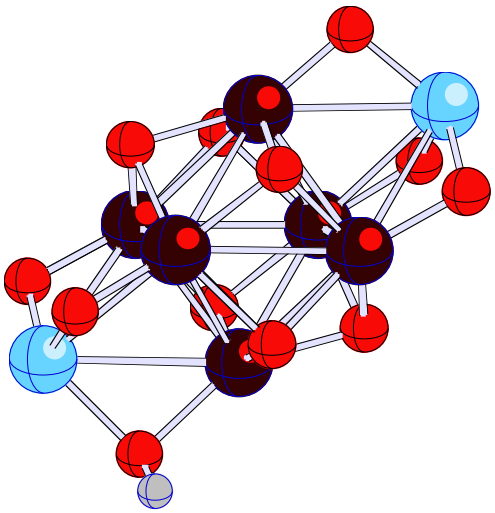
```
O   10      [core]2S( 0.86)2p( 2.33)
O   11      [core]2S( 0.86)2p( 2.30)
O   12      [core]2S( 0.87)2p( 2.58)
O   13      [core]2S( 0.86)2p( 2.32)
O   14      [core]2S( 0.89)2p( 2.45)4p( 0.01)
O   15      [core]2S( 0.89)2p( 2.40)
O   16      [core]2S( 0.86)2p( 2.29)
O   17      [core]2S( 0.86)2p( 2.30)
O   18      [core]2S( 0.89)2p( 2.45)4p( 0.01)
O   19      [core]2S( 0.89)2p( 2.40)4p( 0.01)
O   20      [core]2S( 0.86)2p( 2.31)
H   21          1S( 0.25)
```

HF= -11014.7496907\S2=23.405116\S2-1=0.\S2A=42.15209

```
TITLE
Fe      -0.781700763,-1.650569687,-0.1649408538
 Fe      -1.0634593765,0.74953994,-1.314631873
 Fe      -1.3079011596,0.5801239991,1.2216721117
 Ga      -1.7629186944,2.9601076402,0.0512129663
 Ga      1.6056528942,-2.9851552047,-0.0185172646
 Fe      1.3091116576,-0.5138751555,-1.1992545453
 Fe      1.0547195216,-0.6913180724,1.4119419707
 Fe      0.7852527623,1.6503263501,0.2074443412
 O      -0.1557849319,-3.2815234613,-0.2168786013
 O      0.760675229,1.2898618748,-1.6369391179
 O      -0.7534546122,-1.1989348814,1.6792925958
 O      0.1293466732,3.490780754,0.1417265005
 O      -2.1709712614,-0.3124342433,-0.2125594794
 O      -1.9686852906,2.2359720837,-1.571277458
 O      1.9435703938,-2.1910662304,1.5607508945
 O      2.1644496393,0.3508948702,0.2692073675
 O      -0.3984677525,-0.9538652172,-1.8929666451
 O      -2.2523024385,2.0323457152,1.496250608
 O      2.2324553974,-1.9891018379,-1.3800494339
 O      0.3994022635,1.0398961556,1.9521783373
 H      0.4417678484,3.8879876084,-0.6940944211
END
```



$Fe_8O_{12}H_2$

$$$$$$$$$$$$$ Fe8O12H2 NEUTRAL S = 9 head fe8o12h2_9_GF.out

BPW91/6-311+G* scf=(VSHIFT=5,Tight,NoVarAcc) OPT IOP(5/13=1,5/36=1 ,8/11=1) INT=UltraFine GUESS=READ GEOM=CHECKPOINT

Charge = 0 Multiplicity = 9

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	-0.750621	-1.624819	-0.274563
2	26	0	-1.043058	0.762745	-1.350587
3	26	0	-1.343263	0.470266	1.207348
4	26	0	-1.717930	2.841868	0.136234
5	26	0	1.718028	-2.842180	-0.136843
6	26	0	1.343435	-0.470425	-1.207521
7	26	0	1.042703	-0.762929	1.349421
8	26	0	0.750189	1.624422	0.273967
9	8	0	-0.140957	-3.483731	-0.314590
10	8	0	0.778437	1.332719	-1.582705
11	8	0	-0.778365	-1.333084	1.582337
12	8	0	0.140616	3.483346	0.316722

13	8	0	-2.172256	-0.347888	-0.305156
14	8	0	-1.971354	2.247854	-1.533106
15	8	0	1.971304	-2.247965	1.532255
16	8	0	2.172295	0.347587	0.304516
17	8	0	-0.343800	-0.920294	-1.978585
18	8	0	-2.342779	1.883556	1.512152
19	8	0	2.342625	-1.883837	-1.512677
20	8	0	0.343818	0.919878	1.978161
21	1	0	0.468408	3.974120	-0.460070
22	1	0	-0.467456	-3.971217	0.464852

Distance matrix (angstroms):

		1	2	3	4	5
1	Fe	0.000000				
2	Fe	2.635111	0.000000			
3	Fe	2.633755	2.592045	0.000000		
4	Fe	4.588653	2.643642	2.629098	0.000000	
5	Fe	2.755931	4.700239	4.706447	6.647464	0.000000
6	Fe	2.566731	2.690079	3.732940	4.706264	2.629048
7	Fe	2.568304	3.737395	2.689570	4.699731	2.643544
8	Fe	3.620895	2.568540	2.566285	2.755496	4.588682
9	O	1.956744	4.463142	4.404080	6.534775	1.974590
10	O	3.577189	1.922653	3.609686	3.385872	4.516982
11	O	1.879881	3.614499	1.926603	4.517103	3.385989
12	O	5.218934	3.403333	3.474732	1.974403	6.535000
13	O	1.911161	1.897767	1.908998	3.252042	4.624298
14	O	4.251084	1.760851	3.326320	1.789908	6.439684
15	O	3.325925	5.144077	4.298918	6.439388	1.789729
16	O	3.573395	3.640084	3.631708	4.624241	3.252040
17	O	1.888266	1.927683	3.617008	4.529300	3.367015
18	O	4.246883	3.337780	1.757649	1.789399	6.445302
19	O	3.341883	4.300409	5.150350	6.445099	1.789263
20	O	3.570440	3.609526	1.908546	3.367127	4.529323
21	H	5.733111	3.659301	4.282455	2.533307	6.937432
22	H	2.476388	5.102698	4.587495	6.934681	2.532410

		6	7	8	9	10
6	Fe	0.000000				
7	Fe	2.591129	0.000000			
8	Fe	2.633463	2.634693	0.000000		
9	O	3.475739	3.401874	5.218598	0.000000	
10	O	1.926477	3.613715	1.879659	5.064740	0.000000
11	O	3.609643	1.922398	3.577031	2.937669	4.421270
12	O	4.404815	4.462183	1.956785	7.001286	2.939360
13	O	3.631716	3.639484	3.572965	3.736278	3.628107
14	O	4.299171	5.143764	3.325805	6.138909	2.898497
15	O	3.325694	1.760983	4.250857	3.065877	4.893588

16	O	1.908509	1.897643	1.911446	4.518121	2.544588
17	O	1.908843	3.608708	3.570207	3.062880	2.547980
18	O	5.150342	4.300215	3.341662	6.082169	4.429848
19	O	1.757622	3.337340	4.246861	3.187985	3.577404
20	O	3.616731	1.927587	1.888332	4.988335	3.610969
21	H	4.591115	5.103303	2.477759	7.484118	2.886768
22	H	4.281554	3.654607	5.729770	0.975589	5.820350

		11	12	13	14	15
11	O	0.000000				
12	O	5.064021	0.000000			
13	O	2.544833	4.518237	0.000000		
14	O	4.894111	3.067365	2.878558	0.000000	
15	O	2.898309	6.138148	4.914821	6.719626	0.000000
16	O	3.628205	3.736423	4.441903	4.915048	2.878303
17	O	3.611012	4.989503	2.543868	3.589505	4.410036
18	O	3.577582	3.186790	2.882886	3.089380	5.973373
19	O	4.429787	6.082944	4.919491	5.973416	3.089026
20	O	2.547903	3.061542	3.626486	4.410503	3.589257
21	H	5.821708	0.975557	5.067234	3.175507	6.703909
22	H	2.881871	7.480789	4.077716	6.703013	3.171198

		16	17	18	19	20
16	O	0.000000				
17	O	3.626403	0.000000			
18	O	4.919703	4.903340	0.000000		
19	O	2.882786	2.891775	6.730220	0.000000	
20	O	2.543999	4.417566	2.891997	4.903264	0.000000
21	H	4.079162	5.188531	4.020309	6.239898	3.910100
22	H	5.064193	3.910730	6.236349	4.020489	5.183732

		21	22
21	H	0.000000	
22	H	8.053552	0.000000

Alpha occ. eigenvalues -- -0.25505 -0.25227 -0.24967 -0.24752 -0.24336
Alpha occ. eigenvalues -- -0.24284 -0.23913 -0.22604 -0.22375 -0.22317
Alpha occ. eigenvalues -- -0.22158 -0.20397
Alpha virt. eigenvalues -- -0.19371 -0.17962 -0.17818 -0.17767 -0.17323
0.28 eV
Beta occ. eigenvalues -- -0.24346 -0.23867 -0.23545 -0.23085 -0.22017
Beta occ. eigenvalues -- -0.21381 -0.21333 -0.21050 -0.20518
Beta virt. eigenvalues -- -0.18878 -0.18273 -0.18246 -0.17855 -0.17485
0.45 eV

Mulliken atomic spin densities:

		1
1	Fe	2.489950
2	Fe	2.347515
3	Fe	2.307912

```
     4  Fe  -3.465390
     5  Fe  -3.465543
     6  Fe   2.307278
     7  Fe   2.346589
     8  Fe   2.490028
     9  O   -0.015141
    10  O    0.100484
    11  O    0.100296
    12  O   -0.015064
    13  O    0.137081
    14  O   -0.019290
    15  O   -0.019784
    16  O    0.137053
    17  O    0.120280
    18  O    0.003200
    19  O    0.003047
    20  O    0.120210
    21  H   -0.005346
    22  H   -0.005364
 Sum of Mulliken atomic spin densities =   8.00000
Dipole moment (field-independent basis, Debye):
    X=              0.0030    Y=              0.0038    Z=             -0.0001  Tot=
0.0049

Isotropic polarizability for W=    0.000000      282.42 Bohr**3.   1.902 A**3


Frequencies --    83.6453           92.2312          117.5856
 Frequencies --   117.6427          132.4232          134.3090
 Frequencies --   140.5775          141.4005          145.4617
 Frequencies --   156.9254          158.7199          164.1041
 Frequencies --   200.8877          201.2293          208.3707
 Frequencies --   213.5690          217.8889          224.0812
 Frequencies --   229.3854          234.4210          238.5889
 Frequencies --   248.3687          251.4463          283.2033
 Frequencies --   359.1924          365.5048          373.5966
 Frequencies --   379.4776          388.5348          423.5425
 Frequencies --   428.7151          436.0820          443.8301
 Frequencies --   449.5379          452.0474          462.7417
 Frequencies --   471.2083          478.7800          493.7247
 Frequencies --   496.9455          511.7470          538.0356
 Frequencies --   543.0684          543.6137          557.5234
 Frequencies --   561.9950          569.3069          583.3043
 Frequencies --   585.0334          589.2209          609.7233
 Frequencies --   613.9865          638.9038          645.5274
 Frequencies --   648.0188          658.0585          806.3396
```

```
Frequencies --   809.4510          3653.8347          3654.4845
[headnode:~/feon] ggutsev% grep "Inten" fe8o12h2_9_GF.out
IR Inten    --    12.3385            0.3720            0.1668
IR Inten    --     5.8010            0.0002           41.8575
IR Inten    --    42.2623            0.0256            0.0003
IR Inten    --     0.0001            7.8491            0.0000
IR Inten    --     7.6891            0.0001            0.0001
IR Inten    --     0.0000            0.0000            0.0572
IR Inten    --     3.6437            0.0000            1.9315
IR Inten    --     0.4996            1.4955            0.0000
IR Inten    --     0.0004           10.4922            0.0005
IR Inten    --     1.7132            4.6564            0.0001
IR Inten    --     0.0003           91.1833            4.3401
IR Inten    --    28.2276            0.0041            0.0002
IR Inten    --     0.0807            0.0003            0.0004
IR Inten    --   109.1627            2.6168            0.0015
IR Inten    --    70.9053            0.3411            0.0300
IR Inten    --    65.3588           74.6734           58.8359
IR Inten    --     0.0040            0.0020            1.1519
IR Inten    --   133.4266            0.0029          213.4572
IR Inten    --   132.0598            0.0271           53.4250
IR Inten    --     0.5247          187.3762           26.0864
Zero-point vibrational energy     176814.7 (Joules/Mol)
                                  42.25972 (Kcal/Mol)   1.833 eV

  Atom  No        Natural Electron Configuration
 ----------------------------------------------------------------------------
    Fe    1     [core]4S( 0.26)3d( 6.49)4p( 0.50)4d( 0.03)5p( 0.01)
    Fe    2     [core]4S( 0.26)3d( 6.52)4p( 0.53)4d( 0.03)5p( 0.01)
    Fe    3     [core]4S( 0.26)3d( 6.53)4p( 0.54)4d( 0.03)5p( 0.01)
    Fe    4     [core]4S( 0.21)3d( 6.36)4p( 0.32)4d( 0.02)
    Fe    5     [core]4S( 0.21)3d( 6.36)4p( 0.32)4d( 0.02)
    Fe    6     [core]4S( 0.26)3d( 6.53)4p( 0.54)4d( 0.03)5p( 0.01)
    Fe    7     [core]4S( 0.26)3d( 6.52)4p( 0.53)4d( 0.03)5p( 0.01)
    Fe    8     [core]4S( 0.26)3d( 6.49)4p( 0.50)4d( 0.03)5p( 0.01)
     O    9    [core]2S( 1.73)2p( 5.10)3S( 0.01)3p( 0.01)
     O   10     [core]2S( 1.72)2p( 4.80)3S( 0.01)3p( 0.01)
     O   11     [core]2S( 1.72)2p( 4.80)3S( 0.01)3p( 0.01)
     O   12     [core]2S( 1.73)2p( 5.10)3S( 0.01)3p( 0.01)
     O   13     [core]2S( 1.72)2p( 4.77)3S( 0.01)3p( 0.01)
     O   14     [core]2S( 1.77)2p( 4.78)3S( 0.01)3p( 0.01)
     O   15     [core]2S( 1.77)2p( 4.78)3S( 0.01)3p( 0.01)
     O   16     [core]2S( 1.72)2p( 4.77)3S( 0.01)3p( 0.01)
     O   17     [core]2S( 1.72)2p( 4.79)3S( 0.01)3p( 0.01)
     O   18     [core]2S( 1.77)2p( 4.77)3S( 0.01)3p( 0.01)
     O   19     [core]2S( 1.77)2p( 4.77)3S( 0.01)3p( 0.01)
```

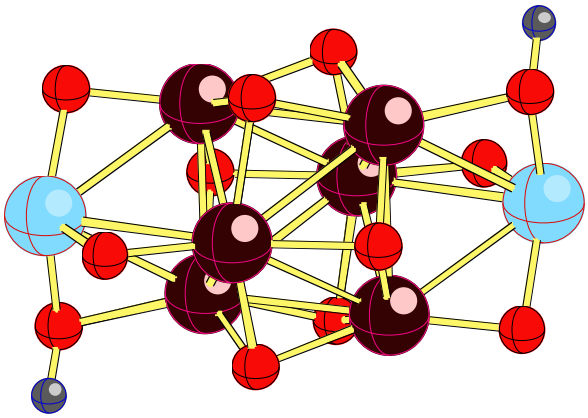
```
   O   20      [core]2S( 1.72)2p( 4.79)3S( 0.01)3p( 0.01)
   H   21           1S( 0.51)
   H   22           1S( 0.51)


***************************************************
*******        Alpha spin orbitals        *******
***************************************************
  Atom  No         Natural Electron Configuration
-----------------------------------------------------------------------------
   Fe    1      [core]3d( 4.39)4p( 0.18)5S( 0.14)4d( 0.01)5p( 0.09)5d( 0.01)
   Fe    2      [core]3d( 4.33)4p( 0.17)5S( 0.15)4d( 0.02)5p( 0.11)
   Fe    3      [core]3d( 4.32)4p( 0.17)4d( 0.01)5p( 0.11)6S( 0.15)5d( 0.01)
   Fe    4      [core]3d( 1.58)4p( 0.16)5S( 0.08)4d( 0.01)
   Fe    5      [core]3d( 1.58)4p( 0.16)5S( 0.08)4d( 0.01)
   Fe    6      [core]3d( 4.32)4p( 0.17)4d( 0.01)5p( 0.11)6S( 0.15)5d( 0.01)
   Fe    7      [core]3d( 4.33)4p( 0.17)5S( 0.15)4d( 0.02)5p( 0.11)
   Fe    8      [core]3d( 4.39)4p( 0.18)5S( 0.14)4d( 0.01)5p( 0.09)5d( 0.01)
    O    9     [core]2S( 0.86)2p( 2.54)
    O   10      [core]2S( 0.87)2p( 2.49)4p( 0.01)
    O   11      [core]2S( 0.87)2p( 2.49)4p( 0.01)
    O   12      [core]2S( 0.86)2p( 2.54)
    O   13      [core]2S( 0.87)2p( 2.47)4p( 0.01)
    O   14      [core]2S( 0.89)2p( 2.38)
    O   15      [core]2S( 0.89)2p( 2.38)
    O   16      [core]2S( 0.87)2p( 2.47)4p( 0.01)
    O   17      [core]2S( 0.87)2p( 2.48)4p( 0.01)
    O   18      [core]2S( 0.89)2p( 2.39)3p( 0.01)
    O   19      [core]2S( 0.89)2p( 2.39)3p( 0.01)
    O   20      [core]2S( 0.87)2p( 2.48)4p( 0.01)
    H   21           1S( 0.25)
    H   22           1S( 0.25)


***************************************************
*******        Beta  spin orbitals        *******
***************************************************
  Atom  No         Natural Electron Configuration
-----------------------------------------------------------------------------
   Fe    1      [core]3d( 2.10)4p( 0.16)5S( 0.11)4d( 0.01)5p( 0.08)5d( 0.01)
   Fe    2      [core]3d( 2.20)4p( 0.16)5S( 0.12)4d( 0.01)5p( 0.10)
   Fe    3      [core]3d( 2.21)4p( 0.16)4d( 0.01)5p( 0.10)6S( 0.12)5d( 0.01)
   Fe    4      [core]3d( 4.78)4p( 0.17)5S( 0.13)4d( 0.01)
   Fe    5      [core]3d( 4.78)4p( 0.17)5S( 0.13)4d( 0.01)
   Fe    6      [core]3d( 2.21)4p( 0.16)4d( 0.01)5p( 0.10)6S( 0.12)5d( 0.01)
   Fe    7      [core]3d( 2.20)4p( 0.16)5S( 0.12)4d( 0.01)5p( 0.10)
```

Fe	8	[core]3d(2.10)4p(0.16)5S(0.11)4d(0.01)5p(0.08)5d(0.01)
O	9	[core]2S(0.87)2p(2.56)
O	10	[core]2S(0.86)2p(2.32)
O	11	[core]2S(0.86)2p(2.32)
O	12	[core]2S(0.87)2p(2.56)
O	13	[core]2S(0.86)2p(2.29)
O	14	[core]2S(0.89)2p(2.40)
O	15	[core]2S(0.89)2p(2.40)
O	16	[core]2S(0.86)2p(2.29)
O	17	[core]2S(0.86)2p(2.30)
O	18	[core]2S(0.89)2p(2.39)
O	19	[core]2S(0.89)2p(2.39)
O	20	[core]2S(0.86)2p(2.30)
H	21	1S(0.25)
H	22	1S(0.25)

HF= -11015.3599511\S2=27.116483\S2-1=0.\S2A=41.932629



TITLE

Fe	-0.7506206431,-1.6248191436,-0.2745626017
Fe	-1.0430579403,0.7627445554,-1.3505874308
Fe	-1.3432628157,0.4702657745,1.2073477978
Ga	-1.7179301923,2.8418678469,0.1362337009
Ga	1.718027613,-2.8421799746,-0.136842555
Fe	1.3434351542,-0.470424843,-1.2075213956
Fe	1.0427026246,-0.7629288018,1.3494205328
Fe	0.7501892838,1.6244216782,0.2739665489
O	-0.1409566416,-3.4837309689,-0.3145898777
O	0.7784371449,1.3327186575,-1.5827051047
O	-0.7783647979,-1.333084321,1.5823368174
O	0.1406161976,3.483346293,0.3167218801
O	-2.1722560018,-0.3478881217,-0.3051562763

```
 O       -1.9713542652,2.24785368,-1.5331062182
 O       1.9713042762,-2.247964542,1.5322553662
 O       2.1722946814,0.3475865811,0.3045155155
 O       -0.3437996576,-0.920294246,-1.9785848095
 O       -2.3427790925,1.8835563951,1.5121521376
 O       2.3426245475,-1.8838372544,-1.5126774494
 O       0.343818457,0.9198779844,1.9781605578
 H       0.4684078968,3.9741197872,-0.4600695998
 H       -0.4674558291,-3.9712170164,0.4648524639
END
```

$Fe_8O_{12}H_3$

```
$$$$$$$$$$$$$  Fe8O12H3    NEUTRAL    S = 10    head
fe8o12h3_10_GF.out
-----------------------------------------------------------------------
 # UBPW91/6-311+G*
scf=(VSHIFT=5,NoIncFock,Maxcycle=90,Tight,NoVarAcc)  NOSYMM
 OPT=RFO IOP(5/13=1,5/36=1,8/11=1) INT=UltraFine GUESS=READ
GEOM=CHECKPOINT
 -----------------------------------------------------------------------
 Charge =  0 Multiplicity = 10
                    Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic           Coordinates (Angstroms)
 Number     Number       Type             X           Y           Z
 ---------------------------------------------------------------------
     1         26          0        0.977949   -0.861629   -1.218459
     2         26          0       -0.888258    0.902380   -1.329977
     3         26          0       -1.330178   -1.242518   -0.077162
     4         26          0       -3.246228    0.539224   -0.278397
     5         26          0        3.359456   -0.498055    0.153217
     6         26          0        1.585806    1.578692   -0.023113
     7         26          0        0.950264   -0.849997    1.304262
     8         26          0       -0.933519    0.988056    1.181248
     9          8          0        2.833841   -1.501300   -1.439190
    10          8          0       -0.411223    2.463396   -0.076830
    11          8          0        0.365434   -2.154755    0.012960
    12          8          0       -2.816862    1.473520    1.401243
```

13	8	0	-0.824920	-0.895040	-1.877644
14	8	0	-2.539608	1.382182	-1.694999
15	8	0	2.636526	-1.287655	1.585655
16	8	0	0.863116	0.981863	1.729507
17	8	0	0.954740	0.923672	-1.785118
18	8	0	-3.097145	-1.233933	-0.134869
19	8	0	3.338224	1.277328	0.038017
20	8	0	-0.927096	-0.791408	1.740017
21	1	0	-3.185068	1.078789	2.212786
22	1	0	2.864632	-2.470792	-1.339317
23	1	0	-0.908073	3.297989	-0.145937

Distance matrix (angstroms):

		1	2	3	4	5
1	Fe	0.000000				
2	Fe	2.570388	0.000000			
3	Fe	2.602900	2.522980	0.000000		
4	Fe	4.548602	2.607245	2.624185	0.000000	
5	Fe	2.772229	4.712129	4.753942	6.700544	0.000000
6	Fe	2.784512	2.878591	4.057722	4.949163	2.736750
7	Fe	2.522900	3.659263	2.694962	4.695241	2.693134
8	Fe	3.582407	2.513094	2.591601	2.771396	4.657789
9	O	1.975407	4.432113	4.388751	6.517546	1.954107
10	O	3.780068	2.057842	3.818151	3.432247	4.800118
11	O	1.887788	3.566693	1.927536	4.515142	3.424689
12	O	5.168786	3.391943	3.431148	1.969379	6.602391
13	O	1.919890	1.880072	1.902041	3.236886	4.668082
14	O	4.199403	1.757955	3.311973	1.793502	6.461435
15	O	3.285640	5.071614	4.301365	6.435757	1.788288
16	O	3.478814	3.526198	3.608665	4.595031	3.302507
17	O	1.873216	1.898486	3.581946	4.479524	3.400162
18	O	4.233104	3.297165	1.767930	1.785192	6.504783
19	O	3.424144	4.458155	5.306304	6.633243	1.779242
20	O	3.519476	3.506465	1.915233	3.350067	4.580231
21	H	5.733182	4.225829	3.751393	2.549679	7.039819
22	H	2.482656	5.046044	4.549518	6.894081	2.522737
23	H	4.691461	2.672319	4.560604	3.618742	5.719374

		6	7	8	9	10
6	Fe	0.000000				
7	Fe	2.839783	0.000000			
8	Fe	2.854178	2.634807	0.000000		
9	O	3.612370	3.390957	5.220784	0.000000	
10	O	2.184883	3.839223	2.008029	5.301442	0.000000
11	O	3.928007	1.926625	3.595753	2.937478	4.683864
12	O	4.628535	4.427118	1.957308	6.989138	2.991931
13	O	3.920489	3.643876	3.593697	3.734478	3.833167

14	O	4.455655	5.114430	3.317778	6.103594	2.884011
15	O	3.450811	1.764712	4.252955	3.038793	5.111068
16	O	1.987501	1.882588	1.878436	4.482242	2.661153
17	O	1.982916	3.562329	3.516958	3.087260	2.674856
18	O	5.463825	4.312775	3.369076	6.078596	4.570316
19	O	1.779192	3.439657	4.431528	3.187054	3.934247
20	O	3.878231	1.928158	1.865142	4.975535	3.763085
21	H	5.292484	4.652591	2.478261	7.498070	3.854049
22	H	4.445909	3.644214	5.722135	0.975109	6.055684
23	H	3.031584	4.770983	2.664181	6.221543	0.973746

		11	12	13	14	15
11	O	0.000000				
12	O	5.021824	0.000000			
13	O	2.564801	4.508770	0.000000		
14	O	4.885316	3.109972	2.856440	0.000000	
15	O	2.895358	6.115353	4.912249	6.684541	0.000000
16	O	3.610069	3.727160	4.402699	4.844174	2.883815
17	O	3.613458	4.967918	2.546265	3.525453	4.368121
18	O	3.585975	3.125460	2.883594	3.096596	5.986491
19	O	4.540628	6.307294	5.071558	6.128886	3.076800
20	O	2.551877	2.969155	3.620587	4.373102	3.601318
21	H	5.282150	0.974675	5.118390	3.972335	6.315403
22	H	2.859112	7.439599	4.047911	6.646632	3.163433
23	H	5.601740	3.060380	4.537313	2.954965	6.049027

		16	17	18	19	20
16	O	0.000000				
17	O	3.516300	0.000000			
18	O	4.906049	4.878150	0.000000		
19	O	3.012407	3.021570	6.910158	0.000000	
20	O	2.519813	4.348492	2.901748	5.036807	0.000000
21	H	4.078082	5.757196	3.296650	6.879126	2.969779
22	H	5.034339	3.920307	6.206714	4.021161	5.165252
23	H	3.466820	3.434293	5.032939	4.706161	4.503371

		21	22	23
21	H	0.000000		
22	H	7.862305	0.000000	
23	H	3.958930	6.995448	0.000000

Alpha occ. eigenvalues -- -0.24728 -0.24454 -0.24074 -0.23910 -0.23682
Alpha occ. eigenvalues -- -0.22890 -0.22593 -0.22442 -0.21485 -0.21314
Alpha occ. eigenvalues -- -0.20654 -0.20359 -0.19082
Alpha virt. eigenvalues -- -0.18089 -0.16775 -0.16728 -0.16290 -0.16251
0.27 eV
Beta occ. eigenvalues -- -0.22960 -0.22498 -0.22290 -0.21814 -0.21103
Beta occ. eigenvalues -- -0.20112 -0.19956 -0.19727 -0.19288
Beta virt. eigenvalues -- -0.17823 -0.17207 -0.16788 -0.16371 -0.16281
0.40 eV

Mulliken atomic spin densities:

		1
1	Fe	2.454574
2	Fe	2.178613
3	Fe	2.260904
4	Fe	-3.479556
5	Fe	-3.365360
6	Fe	3.576933
7	Fe	2.472372
8	Fe	2.258021
9	O	-0.017246
10	O	0.005592
11	O	0.091689
12	O	-0.035844
13	O	0.082654
14	O	0.007299
15	O	0.025353
16	O	0.189037
17	O	0.190012
18	O	-0.038863
19	O	0.078430
20	O	0.073174
21	H	-0.006323
22	H	-0.006074
23	H	0.004608

Sum of Mulliken atomic spin densities = 9.00000

Dipole moment (field-independent basis, Debye):

X= -1.0659 Y= 1.9874 Z= 1.2828 Tot= 2.5946

Isotropic polarizability for W= 0.000000 296.11 Bohr**3. 1.908 A**3

Frequencies --	73.5110	83.3629	91.6953
Frequencies --	105.7870	110.2389	118.5577
Frequencies --	128.3516	140.4268	141.7906
Frequencies --	148.9572	152.7958	161.6913
Frequencies --	173.9255	179.1284	180.7913
Frequencies --	194.0705	205.5707	212.1919
Frequencies --	224.8919	226.5318	236.6870
Frequencies --	237.4739	249.6173	268.6874
Frequencies --	272.6508	285.7208	363.7011
Frequencies --	373.8898	378.7751	390.2749
Frequencies --	406.9986	413.1623	427.0227
Frequencies --	427.9364	440.6748	444.1240
Frequencies --	449.1895	454.9405	468.8699

```
Frequencies --   483.5888            487.7945            522.9677
Frequencies --   531.0715            537.7200            551.3147
Frequencies --   555.1573            566.2364            579.6002
Frequencies --   584.4294            591.9524            603.7875
Frequencies --   611.8903            617.9967            629.4569
Frequencies --   636.7921            647.6029            664.0748
Frequencies --   695.5786            798.3599            816.6747
Frequencies --  3659.2061           3659.8399           3661.0264
[headnode:~/feon] ggutsev% grep "Inten" fe8o12h3_10_GF.out
IR Inten    --    10.5493             0.4916              2.0612
IR Inten    --     3.0473             1.4638              2.7504
IR Inten    --     3.9411            14.2998             34.7041
IR Inten    --    15.0008             0.8022              3.1808
IR Inten    --     9.1774             2.7490              4.7481
IR Inten    --     0.9603             2.2399              3.5053
IR Inten    --     0.4584             3.2360              0.8081
IR Inten    --     0.6931             0.8748              2.6297
IR Inten    --     1.3281             4.6097             20.8099
IR Inten    --    15.6644             3.9670              0.6482
IR Inten    --     0.7391             0.7225             17.3342
IR Inten    --     1.3070             4.3594              0.6783
IR Inten    --    36.6789            44.6440              9.2986
IR Inten    --    23.8525            89.0421             12.7450
IR Inten    --    17.4111            24.0041              6.6755
IR Inten    --    45.9939            91.7777             44.7317
IR Inten    --    21.4948            16.3049             16.4458
IR Inten    --   190.4766            38.6257             29.0428
IR Inten    --    67.1921           144.6358             62.8582
IR Inten    --    60.9853            22.7205             24.7141
IR Inten    --   119.6870            26.3849             89.1196
Zero-point vibrational energy     201802.7 (Joules/Mol)
                                  48.23201 (Kcal/Mol)    2.091 eV

  Atom  No         Natural Electron Configuration
 ----------------------------------------------------------------------
    Fe    1      [core]4S( 0.25)3d( 6.50)4p( 0.51)4d( 0.04)5p( 0.01)
    Fe    2      [core]4S( 0.26)3d( 6.59)4p( 0.55)4d( 0.03)5p( 0.01)
    Fe    3      [core]4S( 0.26)3d( 6.55)4p( 0.53)4d( 0.03)5p( 0.01)
    Fe    4      [core]4S( 0.21)3d( 6.37)4p( 0.33)4d( 0.02)
    Fe    5      [core]4S( 0.23)3d( 6.38)4p( 0.32)4d( 0.02)
    Fe    6      [core]4S( 0.23)3d( 6.34)4p( 0.39)4d( 0.03)5p( 0.01)
    Fe    7      [core]4S( 0.26)3d( 6.49)4p( 0.52)4d( 0.04)5p( 0.01)
    Fe    8      [core]4S( 0.25)3d( 6.56)4p( 0.48)4d( 0.03)5p( 0.01)
     O    9     [core]2S( 1.73)2p( 5.11)3S( 0.01)3p( 0.01)
     O   10      [core]2S( 1.68)2p( 5.14)3S( 0.01)3p( 0.01)
     O   11      [core]2S( 1.73)2p( 4.81)3S( 0.01)3p( 0.01)
```

O	12	[core]2S(1.72)2p(5.12)3p(0.01)
O	13	[core]2S(1.72)2p(4.75)3S(0.01)3p(0.01)
O	14	[core]2S(1.77)2p(4.78)3S(0.01)3p(0.01)
O	15	[core]2S(1.77)2p(4.79)3S(0.01)3p(0.02)
O	16	[core]2S(1.74)2p(4.87)3S(0.01)3p(0.02)
O	17	[core]2S(1.73)2p(4.88)3S(0.01)3p(0.01)
O	18	[core]2S(1.77)2p(4.79)3S(0.01)3p(0.01)
O	19	[core]2S(1.79)2p(4.87)3S(0.01)3p(0.02)
O	20	[core]2S(1.72)2p(4.81)3S(0.01)3p(0.01)
H	21	1S(0.51)
H	22	1S(0.51)
H	23	1S(0.49)

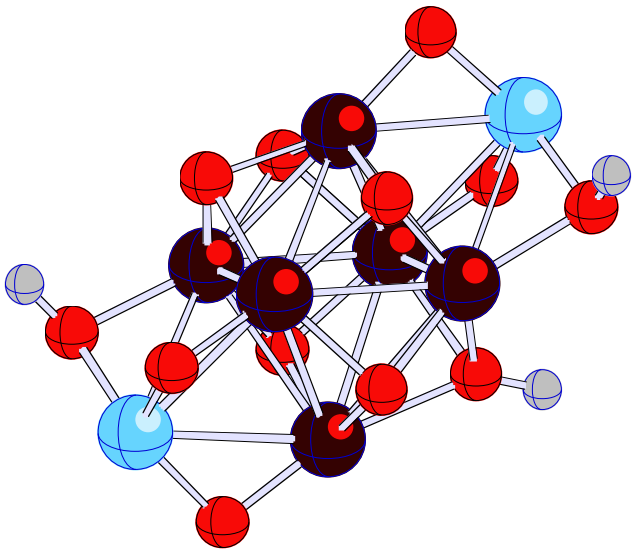
****
******* Alpha spin orbitals *******
****

Atom	No	Natural Electron Configuration
Fe	1	[core]3d(4.39)4p(0.17)5S(0.14)4d(0.01)5p(0.11)5d(0.01)
Fe	2	[core]3d(4.28)4p(0.17)4d(0.01)5p(0.12)6S(0.14)5d(0.01)
Fe	3	[core]3d(4.30)4p(0.17)5S(0.15)4d(0.01)5p(0.11)5d(0.01)
Fe	4	[core]3d(1.59)4p(0.16)5S(0.08)4d(0.01)
Fe	5	[core]4S(0.10)3d(1.63)4p(0.16)4d(0.01)
Fe	6	[core]3d(4.81)4p(0.13)5S(0.14)4d(0.02)5p(0.08)
Fe	7	[core]3d(4.37)4p(0.16)5S(0.15)4d(0.01)5p(0.11)5d(0.01)
Fe	8	[core]3d(4.32)4p(0.15)5S(0.14)4d(0.01)5p(0.10)5d(0.01)
O	9	[core]2S(0.86)2p(2.54)4p(0.01)
O	10	[core]2S(0.85)2p(2.59)4p(0.01)
O	11	[core]2S(0.87)2p(2.49)4p(0.01)
O	12	[core]2S(0.86)2p(2.53)
O	13	[core]2S(0.86)2p(2.43)4p(0.01)
O	14	[core]2S(0.89)2p(2.39)
O	15	[core]2S(0.89)2p(2.41)
O	16	[core]2S(0.88)2p(2.58)4S(0.01)4p(0.01)
O	17	[core]2S(0.88)2p(2.58)4S(0.01)4p(0.01)
O	18	[core]2S(0.89)2p(2.37)
O	19	[core]2S(0.90)2p(2.46)
O	20	[core]2S(0.86)2p(2.47)4p(0.01)
H	21	1S(0.26)
H	22	1S(0.26)
H	23	1S(0.25)

****
******* Beta spin orbitals *******
****

Atom	No	Natural Electron Configuration
Fe	1	[core]3d(2.11)4p(0.15)5S(0.11)4d(0.01)5p(0.09)5d(0.01)
Fe	2	[core]3d(2.31)4p(0.16)4d(0.01)5p(0.10)6S(0.12)5d(0.01)
Fe	3	[core]3d(2.25)4p(0.16)5S(0.12)4d(0.01)5p(0.10)
Fe	4	[core]3d(4.78)4p(0.18)5S(0.13)4d(0.01)
Fe	5	[core]4S(0.13)3d(4.74)4p(0.17)4d(0.01)
Fe	6	[core]3d(1.53)4p(0.12)4d(0.01)5p(0.07)6S(0.10)
Fe	7	[core]3d(2.13)4p(0.15)5S(0.11)4d(0.01)5p(0.10)5d(0.01)
Fe	8	[core]3d(2.24)4p(0.14)5S(0.11)4d(0.01)5p(0.09)5d(0.01)
O	9	[core]2S(0.87)2p(2.57)4p(0.01)
O	10	[core]2S(0.83)2p(2.55)
O	11	[core]2S(0.86)2p(2.33)
O	12	[core]2S(0.86)2p(2.58)
O	13	[core]2S(0.86)2p(2.32)
O	14	[core]2S(0.88)2p(2.39)
O	15	[core]2S(0.89)2p(2.38)4p(0.01)
O	16	[core]2S(0.86)2p(2.30)
O	17	[core]2S(0.86)2p(2.30)
O	18	[core]2S(0.89)2p(2.42)
O	19	[core]2S(0.90)2p(2.40)
O	20	[core]2S(0.85)2p(2.33)
H	21	1S(0.26)
H	22	1S(0.26)
H	23	1S(0.24)

HF=-11015.960135\S2=31.762528\S2-1=0.\S2A=44.550825



TITLE
Fe 0.9779494087,-0.8616289984,-1.2184589438
Fe -0.8882582085,0.9023803488,-1.3299774785

```
 Fe     -1.3301778528,-1.2425181214,-0.0771623223
 Ga      -3.2462276818,0.5392240139,-0.2783966284
 Ga     3.3594556229,-0.4980545058,0.1532172636
 Fe     1.585806027,1.5786921865,-0.0231131296
 Fe     0.9502640034,-0.8499967005,1.3042621066
 Fe     -0.9335187549,0.9880558478,1.181247997
 O     2.8338406403,-1.5013000232,-1.43919023
 O     -0.4112232917,2.4633963202,-0.0768298157
 O     0.3654335663,-2.1547553472,0.0129595884
 O     -2.8168615918,1.4735202207,1.4012430281
 O     -0.8249200959,-0.8950397798,-1.8776435686
 O     -2.5396080048,1.3821815712,-1.6949986267
 O     2.6365263367,-1.2876551886,1.5856547981
 O     0.8631162182,0.9818630914,1.7295065274
 O     0.9547401379,0.9236716867,-1.7851177202
 O     -3.0971450846,-1.2339325961,-0.1348693041
 O     3.3382237655,1.2773275142,0.0380165624
 O     -0.9270957142,-0.7914078957,1.7400174826
 H     -3.1850679319,1.0787894334,2.2127863284
 H     2.8646315336,-2.4707920923,-1.3393172599
 H     -0.9080730477,3.2979890143,-0.1459366547
END
```

$Fe_8O_{12}H_4$

```
$$$$$$$$$$$$$  Fe8O12H4       NEUTRAL    S = 9   QB
fe8o12h4_A1_s_9_GF.out
-----------------------------------------------------------------
 # BPW91/6-311+G* scf=(VSHIFT=5,Tight,NoVarAcc) OPT
IOP(5/13=1,5/36=1
 ,8/11=1) INT=UltraFine GUESS=READ GEOM=CHECKPOINT
 ----------------------------------------------------------------
Charge =  0 Multiplicity = 9
                    Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic          Coordinates (Angstroms)
 Number     Number       Type             X         Y         Z
 ---------------------------------------------------------------------
     1         26          0        0.952566  -0.107544   1.712793
     2         26          0        0.152104  -1.763098  -0.029602
     3         26          0       -1.720056   0.228492   1.101377
     4         26          0       -2.687196  -1.366171  -0.838734
     5         26          0        2.550630   1.480230   0.347195
```

6	26	0	1.374434	0.006554	-1.645458
7	26	0	0.058556	1.856205	0.048702
8	26	0	-1.909601	0.799108	-1.733087
9	8	0	2.579872	0.856614	2.207988
10	8	0	1.240932	-1.942769	-1.676582
11	8	0	-0.341495	1.259888	1.906528
12	8	0	-3.189871	-0.432469	-2.516339
13	8	0	-0.609130	-1.199272	1.601935
14	8	0	-1.271919	-2.453584	-0.777959
15	8	0	1.513124	3.156888	0.312090
16	8	0	-0.040553	1.165331	-1.833333
17	8	0	1.707977	-1.511702	0.953984
18	8	0	-3.149564	-0.722535	0.768048
19	8	0	2.975867	0.612895	-1.131859
20	8	0	-2.011900	1.638476	-0.056669
21	1	0	-3.115345	-0.842089	-3.393058
22	1	0	3.278458	0.251405	2.509425
23	1	0	2.103916	-2.329383	-1.436223
24	1	0	1.484052	3.772270	1.063177

Distance matrix (angstroms):

		1	2	3	4	5
1	Fe	0.000000				
2	Fe	2.533286	0.000000			
3	Fe	2.762184	2.958129	0.000000		
4	Fe	4.619772	2.978904	2.691160	0.000000	
5	Fe	2.634329	4.051429	4.513801	6.078096	0.000000
6	Fe	3.386567	2.690120	4.143698	4.362569	2.743324
7	Fe	2.724841	3.621358	2.630786	4.325552	2.537891
8	Fe	4.570351	3.703699	2.897537	2.468391	4.968417
9	O	1.955235	4.214707	4.484251	6.478063	1.962728
10	O	3.865109	1.982516	4.604225	4.057665	4.186634
11	O	1.892617	3.623629	1.900652	4.464859	3.293092
12	O	5.928821	4.373012	3.960442	1.984652	6.694147
13	O	1.908679	1.886609	1.877026	3.209841	4.328763
14	O	4.081186	1.750614	3.305490	1.785824	5.599353
15	O	3.596207	5.116188	4.433050	6.278945	1.972012
16	O	3.896345	3.444743	3.508692	3.795055	3.401190
17	O	1.765813	1.857790	3.847260	4.748953	3.167004
18	O	4.254201	3.552468	1.749015	1.791591	6.125480
19	O	3.564382	3.851486	5.214097	6.006073	1.766550
19	O	3.564382	3.851486	5.214097	6.006073	1.766550
20	O	3.868803	4.031668	1.847782	3.177350	4.583102
21	H	6.569412	4.778841	4.826275	2.642451	7.175370
22	H	2.484601	4.503218	5.193098	7.029634	2.591329
23	H	4.022247	2.471605	5.254037	4.923365	4.230046

24	H	3.969563	5.797288	4.777670	6.886229	2.627483
		6	7	8	9	10
6	Fe	0.000000				
7	Fe	2.832477	0.000000			
8	Fe	3.379454	2.857598	0.000000		
9	O	4.126104	3.466805	5.974174	0.000000	
10	O	1.954137	4.336683	4.176954	4.971840	0.000000
11	O	4.139065	1.991770	3.989746	2.964438	5.059621
12	O	4.667339	4.729666	1.941483	7.567757	4.755862
13	O	3.991755	3.492030	4.099649	3.842357	3.837212
14	O	3.715914	4.585609	3.449480	5.891484	2.717145
15	O	3.711581	1.968990	4.632162	3.166013	5.480457
16	O	1.838545	2.007283	1.907225	4.826408	3.365570
17	O	3.028771	3.857839	5.064293	2.818093	2.706257
18	O	5.179106	4.178443	3.179400	6.115029	5.171233
19	O	1.787743	3.383822	4.925846	3.372060	3.136581
20	O	4.081014	2.084537	1.877600	5.179223	5.101995
21	H	4.892077	5.403716	2.627327	8.166567	4.809880
22	H	4.576933	4.358705	6.724199	0.972195	5.146705
23	H	2.456119	4.889544	5.097441	4.863885	0.975697
24	H	4.639972	2.594707	5.308075	3.318504	6.342480
		11	12	13	14	15
11	O	0.000000				
12	O	5.526217	0.000000			
13	O	2.492364	4.920203	0.000000		
14	O	4.675685	3.284115	2.770647	0.000000	
15	O	3.095230	6.557566	5.014359	6.357835	0.000000
16	O	3.753140	3.596897	4.209002	3.965680	3.314069
17	O	3.576225	6.098919	2.426198	3.573031	4.716537
18	O	3.620966	3.297417	2.715962	2.985334	6.082638
19	O	4.544808	6.405147	4.858990	5.250926	3.270551
20	O	2.605326	3.424385	3.573730	4.220520	3.855821
21	H	6.340202	0.970556	5.599880	3.582441	7.151410
22	H	3.805861	8.219810	4.247511	6.231356	4.048026
23	H	5.480591	5.726179	4.227077	3.441657	5.788333
24	H	3.218061	7.234523	5.421061	7.053114	0.971428
		16	17	18	19	20
16	O	0.000000				
17	O	4.241815	0.000000			
18	O	4.471819	4.924740	0.000000		
19	O	3.145798	3.236078	6.550872	0.000000	
20	O	2.695665	4.978205	2.747510	5.204390	0.000000
21	H	3.989589	6.527603	4.162964	6.658293	4.301429
22	H	5.541719	2.827429	6.730559	3.671674	6.041249
23	H	4.119401	2.557041	5.919445	3.083818	5.881073
24	H	4.184534	5.289842	6.462257	4.126178	4.246034

```
             21        22        23        24
   21  H    0.000000
   22  H    8.770163   0.000000
   23  H    5.769050   4.858822   0.000000
   24  H    7.893338   4.208089   6.622794   0.000000
Alpha  occ. eigenvalues --   -0.21934 -0.21455 -0.21322 -0.20990 -0.20919
 Alpha  occ. eigenvalues --   -0.20238 -0.20031 -0.18819
 Alpha virt. eigenvalues --   -0.16515 -0.16132 -0.15372 -0.15079 -0.14842
  Beta  occ. eigenvalues --   -0.23774 -0.23237 -0.22703 -0.22436 -0.21924
  Beta  occ. eigenvalues --   -0.21385 -0.21060 -0.19257 -0.18297 -0.17560
  Beta virt. eigenvalues --   -0.16136 -0.15890 -0.15465 -0.15159 -0.15088
Mulliken charges and spin densities:
              1         2
    1  Fe   0.495047   2.595012
    2  Fe   1.051416  -2.548686
    3  Fe   0.523380  -2.597844
    4  Fe   0.014810   3.268871
    5  Fe   0.153607   3.345942
    6  Fe   0.052345  -3.533066
    7  Fe   0.710239   3.589426
    8  Fe   0.243244   3.450688
    9  O   -0.667322   0.088450
   10  O   -0.608820  -0.090558
   11  O   -0.346936   0.096441
   12  O   -0.652290   0.126438
   13  O   -0.091861  -0.090021
   14  O   -0.312353  -0.050054
   15  O   -0.715475   0.176302
   16  O   -0.171598   0.032784
   17  O   -0.433203   0.143281
   18  O   -0.216933  -0.081583
   19  O   -0.303234  -0.076383
   20  O   -0.277326   0.136377
   21  H    0.411184   0.009008
   22  H    0.379286   0.005840
   23  H    0.362836  -0.008854
   24  H    0.399956   0.012190
 Sum of Mulliken charges =   0.00000   8.00000

Dipole moment (field-independent basis, Debye):
   X=              1.5710    Y=              1.0282    Z=             -2.6332  Tot=
3.234

Isotropic polarizability for W=    0.000000      277.87 Bohr**3.    1.716 A**3

Frequencies --     58.6690              71.1747              77.2209
```

Frequencies --	92.2706	96.2232	107.6939
Frequencies --	108.9759	115.5718	122.9756
Frequencies --	129.7012	134.2274	151.1661
Frequencies --	152.7736	159.7367	169.5918
Frequencies --	171.2192	179.8525	188.2464
Frequencies --	194.4533	199.5119	201.0176
Frequencies --	218.9148	220.9201	233.0731
Frequencies --	264.4794	273.1047	291.7805
Frequencies --	322.8727	344.0877	357.3018
Frequencies --	363.9136	381.0989	388.0290
Frequencies --	398.6212	409.7175	421.5563
Frequencies --	437.1180	442.2318	463.2018
Frequencies --	477.5898	482.9684	494.3786
Frequencies --	507.1817	525.5432	528.9202
Frequencies --	533.7028	542.8796	551.1561
Frequencies --	560.1526	576.5700	586.5327
Frequencies --	597.4813	619.4848	625.1742
Frequencies --	635.1207	651.1359	660.8095
Frequencies --	696.2569	729.4361	730.7878
Frequencies --	795.4866	830.7533	3651.5697
Frequencies --	3698.2192	3704.6921	3709.5503

Zero-point vibrational energy 226200.9 (Joules/Mol)
54.06330 (Kcal/Mol) 2.344 eV

Atom	No	Natural Electron Configuration
Fe	1	[core]4S(0.27)3d(6.51)4p(0.49)4d(0.03)5p(0.01)
Fe	2	[core]4S(0.26)3d(6.50)4p(0.48)4d(0.03)
Fe	3	[core]4S(0.26)3d(6.47)4p(0.49)4d(0.04)5p(0.01)
Fe	4	[core]4S(0.25)3d(6.44)4p(0.34)4d(0.02)
Fe	5	[core]4S(0.24)3d(6.45)4p(0.33)4d(0.02)
Fe	6	[core]4S(0.24)3d(6.35)4p(0.37)4d(0.03)
Fe	7	[core]4S(0.25)3d(6.42)4p(0.48)4d(0.04)5p(0.01)
Fe	8	[core]4S(0.25)3d(6.43)4p(0.29)4d(0.02)
O	9	[core]2S(1.72)2p(5.13)3p(0.01)
O	10	[core]2S(1.73)2p(5.09)3p(0.01)
O	11	[core]2S(1.74)2p(4.89)3S(0.01)3p(0.01)
O	12	[core]2S(1.73)2p(5.21)3S(0.01)3p(0.01)
O	13	[core]2S(1.73)2p(4.80)3S(0.01)3p(0.01)
O	14	[core]2S(1.77)2p(4.82)3S(0.01)3p(0.02)
O	15	[core]2S(1.72)2p(5.17)3S(0.01)3p(0.01)
O	16	[core]2S(1.76)2p(5.08)3S(0.01)3p(0.02)
O	17	[core]2S(1.76)2p(4.77)3p(0.01)
O	18	[core]2S(1.77)2p(4.77)3S(0.01)3p(0.01)
O	19	[core]2S(1.79)2p(4.90)3S(0.01)3p(0.01)
O	20	[core]2S(1.76)2p(4.95)3S(0.01)3p(0.01)

```
    H   21          1S( 0.51)
    H   22          1S( 0.51)
    H   23          1S( 0.51)
    H   24          1S( 0.51)

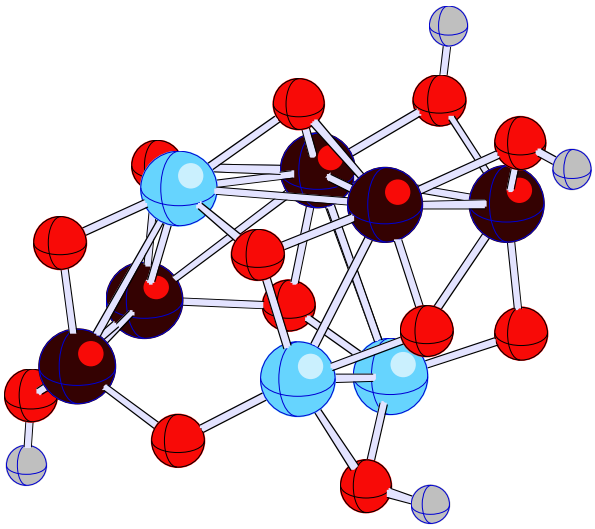

************************************************
*******        Alpha spin orbitals        *******
************************************************
  Atom  No         Natural Electron Configuration
--------------------------------------------------------------------------------
   Fe    1      [core]3d( 4.38)4p( 0.25)5S( 0.14)4d( 0.01)
   Fe    2      [core]3d( 2.11)4p( 0.24)5S( 0.12)4d( 0.02)
   Fe    3      [core]3d( 2.12)4p( 0.25)5S( 0.12)4d( 0.02)
   Fe    4      [core]4S( 0.13)3d( 4.73)4p( 0.18)4d( 0.01)
   Fe    5      [core]3d( 4.81)4p( 0.18)5S( 0.14)4d( 0.01)
   Fe    6      [core]3d( 1.55)4p( 0.18)5S( 0.10)4d( 0.01)
   Fe    7      [core]3d( 4.82)4p( 0.15)5S( 0.13)4d( 0.02)5p( 0.09)
   Fe    8      [core]3d( 4.84)4p( 0.16)5S( 0.14)4d( 0.01)
    O    9     [core]2S( 0.87)2p( 2.63)3p( 0.01)
    O   10      [core]2S( 0.86)2p( 2.48)
    O   11      [core]2S( 0.88)2p( 2.53)4p( 0.01)
    O   12      [core]2S( 0.88)2p( 2.69)
    O   13      [core]2S( 0.86)2p( 2.34)4p( 0.01)
    O   14      [core]2S( 0.89)2p( 2.39)4p( 0.01)
    O   15      [core]2S( 0.87)2p( 2.69)3p( 0.01)4S( 0.01)
    O   16      [core]2S( 0.89)2p( 2.57)4S( 0.01)4p( 0.01)
    O   17      [core]2S( 0.88)2p( 2.45)
    O   18      [core]2S( 0.89)2p( 2.35)
    O   19      [core]2S( 0.90)2p( 2.42)4p( 0.01)
    O   20      [core]2S( 0.89)2p( 2.55)4S( 0.01)4p( 0.01)
    H   21          1S( 0.26)
    H   22          1S( 0.26)
    H   23          1S( 0.25)
    H   24          1S( 0.26)


NBO analysis skipped by request.


************************************************
*******        Beta  spin orbitals        *******
************************************************
  Atom  No         Natural Electron Configuration
--------------------------------------------------------------------------------
   Fe    1      [core]3d( 2.13)4p( 0.25)5S( 0.13)4d( 0.01)
```

Fe 2 [core]3d(4.39)4p(0.24)5S(0.14)4d(0.02)
Fe 3 [core]3d(4.35)4p(0.24)5S(0.13)4d(0.01)
Fe 4 [core]3d(1.71)4p(0.17)5S(0.12)4d(0.01)
Fe 5 [core]3d(1.64)4p(0.16)5S(0.10)4d(0.01)
Fe 6 [core]3d(4.80)4p(0.19)5S(0.13)4d(0.01)
Fe 7 [core]3d(1.60)4p(0.14)5S(0.11)4d(0.01)5p(0.10)
Fe 8 [core]3d(1.59)4p(0.13)5S(0.11)4d(0.01)
O 9 [core]2S(0.85)2p(2.50)
O 10 [core]2S(0.87)2p(2.61)4p(0.01)
O 11 [core]2S(0.87)2p(2.37)
O 12 [core]2S(0.86)2p(2.53)
O 13 [core]2S(0.86)2p(2.47)4p(0.01)
O 14 [core]2S(0.88)2p(2.43)4p(0.01)
O 15 [core]2S(0.84)2p(2.48)
O 16 [core]2S(0.88)2p(2.51)4S(0.01)4p(0.01)
O 17 [core]2S(0.88)2p(2.32)
O 18 [core]2S(0.89)2p(2.42)4p(0.01)
O 19 [core]2S(0.90)2p(2.48)4p(0.01)
O 20 [core]2S(0.87)2p(2.40)
H 21 1S(0.25)
H 22 1S(0.25)
H 23 1S(0.26)
H 24 1S(0.25)

HF= -11016.5791312\S2=28.985015\S2-1=0.\S2A=51.996086



TITLE
Fe 0.9525662146,-0.1075437759,1.7127926114

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 Ga       0.1521043172,-1.7630975115,-0.0296024574
 Ga       -1.7200561389,0.2284920409,1.1013773416
 Fe       -2.6871956346,-1.3661712185,-0.8387338724
 Fe       2.5506301909,1.4802303599,0.347195252
 Ga       1.3744338242,0.006553532,-1.6454580003
 Fe       0.0585556481,1.8562045946,0.0487022782
 Fe       -1.9096011409,0.7991080347,-1.7330874022
 O       2.5798724284,0.8566138138,2.2079880859
 O       1.2409324178,-1.942769029,-1.6765819927
 O       -0.341494536,1.2598884941,1.9065275213
 O       -3.1898714171,-0.4324691594,-2.5163394354
 O       -0.6091300401,-1.1992721769,1.6019354123
 O       -1.2719188966,-2.4535840213,-0.7779587572
 O       1.5131243284,3.1568877132,0.3120904704
 O       -0.0405531367,1.1653306612,-1.8333328468
 O       1.7079767983,-1.5117020208,0.9539844039
 O       -3.1495640843,-0.722534812,0.7680477477
 O       2.975867423,0.6128950241,-1.131858954
 O       -2.0118996597,1.6384759845,-0.0566689812
 H       -3.1153451592,-0.8420889482,-3.3930582704
 H       3.2784581606,0.2514053366,2.5094254585
 H       2.1039164986,-2.3293827928,-1.4362227156
 H       1.484051594,3.7722698767,1.0631771025
END
```

$Fe_8O_{12}H_5$

```
$$$$$$$$$$$$$  Fe8O12H5   NEUTRAL   S = 14  head
fe8o12h5_14_GF.out
---------------------------------------------------------------------
 # UBPW91/6-311+G*
scf=(VSHIFT=5,NoIncFock,Maxcycle=90,Tight,NoVarAcc)  NOSYMM
 OPT=RFO IOP(5/13=1,5/36=1,8/11=1) INT=UltraFine GUESS=READ
GEOM=CHECKPOINT
 ---------------------------------------------------------------------
 Charge =  0 Multiplicity = 14
                    Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic           Coordinates (Angstroms)
 Number     Number       Type             X           Y           Z
 ---------------------------------------------------------------------
     1         26          0       1.496681   -0.352493   -1.073235
     2         26          0       0.499404    1.921344    0.071960
```

3	26	0	-1.565753	0.234279	-1.703871
4	26	0	-1.939381	2.519690	-0.158499
5	26	0	2.147159	-2.678532	0.085422
6	26	0	1.622186	-0.362447	1.517433
7	26	0	-0.649724	-1.791223	-0.073355
8	26	0	-1.212236	0.534050	1.321464
9	8	0	2.684343	-1.819796	-1.630082
10	8	0	0.340908	1.376538	2.176236
11	8	0	-1.280823	-1.792062	-1.915266
12	8	0	-2.560695	1.916827	1.615696
13	8	0	0.216429	0.852528	-1.672966
14	8	0	-0.384017	3.701866	0.068226
15	8	0	0.413980	-3.165880	-0.088456
16	8	0	-0.224835	-1.059632	1.592157
17	8	0	2.206306	0.932805	0.186230
18	8	0	-2.531009	1.732282	-1.642006
19	8	0	2.692802	-1.822902	1.531447
20	8	0	-2.052527	-0.527146	0.082188
21	1	0	-3.459424	1.544434	1.646676
22	1	0	3.626437	-1.618400	-1.763134
23	1	0	0.245191	2.099956	2.819773
24	1	0	-0.734067	-2.275170	-2.556991
25	1	0	-0.144943	4.399084	-0.562308

Distance matrix (angstroms):

		1	2	3	4	5
1	Fe	0.000000				
2	Fe	2.734294	0.000000			
3	Fe	3.181274	3.203847	0.000000		
4	Fe	4.570853	2.521667	2.784040	0.000000	
5	Fe	2.678818	4.886117	5.046955	6.616707	0.000000
6	Fe	2.593725	2.926727	4.571197	4.878547	2.773175
7	Fe	2.770696	3.889057	2.756874	4.500493	2.938550
8	Fe	3.722736	2.532894	3.060636	2.581045	4.809783
9	O	1.968146	4.654786	4.721015	6.509648	1.992222
10	O	3.858033	2.179429	4.471616	3.457962	4.906897
11	O	3.239738	4.572489	2.057166	4.702248	4.066895
12	O	5.370518	3.427440	3.852325	1.974144	6.754476
13	O	1.857632	2.065723	1.886626	3.117781	4.391814
14	O	4.612785	1.987638	4.069519	1.966749	6.864155
15	O	3.171305	5.090469	4.253232	6.153772	1.808770
16	O	3.250842	3.423703	3.786301	4.337743	3.243060
17	O	1.934376	1.975799	4.276546	4.452388	3.613228
18	O	4.570784	3.486664	1.783132	1.780681	6.657668
19	O	3.221362	4.578261	5.730145	6.570475	1.766584
20	O	3.736626	3.536602	2.001681	3.058421	4.718668

21	H	5.963155	4.277162	4.065546	2.553490	7.190600
22	H	2.571837	5.067119	5.513145	7.118776	2.594089
23	H	4.768253	2.765322	5.217626	3.717343	5.824783
24	H	3.297644	5.103290	2.777922	5.495110	3.930205
25	H	5.053064	2.637551	4.546148	2.629675	7.467659

		6	7	8	9	10
6	Fe	0.000000				
7	Fe	3.119869	0.000000			
8	Fe	2.979272	2.769266	0.000000		
9	O	3.627518	3.679703	5.425453	0.000000	
10	O	2.258266	4.009579	1.962824	5.495115	0.000000
11	O	4.717487	1.947030	3.986467	3.975505	5.423138
12	O	4.764582	4.500482	1.953711	7.211647	3.004233
13	O	3.692013	3.209111	3.333034	3.637822	3.886700
14	O	4.758539	5.501334	3.505939	6.541241	3.221237
15	O	3.449330	1.738210	4.280413	3.056648	5.076193
16	O	1.975636	1.868070	1.894217	4.407265	2.568295
17	O	1.947042	3.955328	3.624112	3.332314	2.763464
18	O	5.623075	4.291269	3.457900	6.310094	4.790974
19	O	1.810895	3.707947	4.566030	3.161542	4.022881
20	O	3.948489	1.894714	1.835219	5.200072	3.706424
21	H	5.429150	4.688233	2.485255	7.733114	3.840722
22	H	4.044324	4.601170	6.128665	0.972524	5.939949
23	H	3.107352	4.930754	2.611720	6.412107	0.972951
24	H	5.080489	2.531753	4.812772	3.571002	6.074042
25	H	5.488191	6.230070	4.430146	6.915161	4.107488

		11	12	13	14	15
11	O	0.000000				
12	O	5.278411	0.000000			
13	O	3.048660	4.434010	0.000000		
14	O	5.909462	3.212313	3.392789	0.000000	
15	O	2.845516	6.130802	4.324037	6.915727	0.000000
16	O	3.735449	3.783663	3.809475	5.001957	2.769264
17	O	4.899107	5.073063	2.724456	3.793599	4.481864
18	O	3.749485	3.263060	2.885020	3.378421	5.922707
19	O	5.260273	6.449178	4.853721	6.490831	3.101727
20	O	2.487039	2.929656	3.183115	4.546280	3.616032
21	H	5.344712	0.973319	5.001065	4.074818	6.340426
22	H	4.912687	7.886376	4.212098	6.909620	3.939431
23	H	6.316416	3.058812	4.662790	3.245463	6.017916
24	H	0.971672	6.190374	3.386360	6.537527	2.864444
25	H	6.438245	4.091596	3.733927	0.969971	7.600368

		16	17	18	19	20
16	O	0.000000				
17	O	3.443383	0.000000			
18	O	4.855207	5.140404	0.000000		

19	O	3.016433	3.104868	7.070950	0.000000	
20	O	2.429816	4.503325	2.882153	5.128106	0.000000
21	H	4.152915	5.882813	3.422378	7.014422	2.952698
22	H	5.138335	3.510760	7.011125	3.430417	6.070146
23	H	3.422128	3.484790	5.267821	4.799937	4.435712
24	H	4.353422	5.144138	4.486187	5.353812	3.429168
25	H	5.869045	4.254852	3.737765	7.151902	5.321840

		21	22	23	24	25
21	H	0.000000				
22	H	8.475833	0.000000			
23	H	3.925421	6.801620	0.000000		
24	H	6.299823	4.480575	7.000733	0.000000	
25	H	4.900451	7.202458	4.108123	6.990815	0.000000

Alpha occ. eigenvalues -- -0.22405 -0.22266 -0.21833 -0.21324 -0.20858
Alpha occ. eigenvalues -- -0.19970 -0.19527 -0.19284 -0.18914 -0.18359
Alpha occ. eigenvalues -- -0.16841
Alpha virt. eigenvalues -- -0.16255 -0.14475 -0.14114 -0.13558 -0.12962
0.16 eV
Beta occ. eigenvalues -- -0.20721 -0.20209 -0.20008 -0.19817 -0.18888
Beta occ. eigenvalues -- -0.18377 -0.17792 -0.16979
Beta virt. eigenvalues -- -0.15193 -0.14760 -0.14519 -0.14378 -0.14078
0.49 eV
Mulliken atomic spin densities:

		1
1	Fe	3.429901
2	Fe	3.531605
3	Fe	-3.644108
4	Fe	3.310005
5	Fe	-3.067482
6	Fe	3.625163
7	Fe	2.559078
8	Fe	2.338906
9	O	0.027819
10	O	0.047646
11	O	0.017759
12	O	0.084778
13	O	0.054228
14	O	0.134669
15	O	0.158127
16	O	0.082516
17	O	0.425224
18	O	-0.107408
19	O	0.030647
20	O	-0.059938
21	H	0.005184
22	H	-0.001934

```
   23  H    0.013050
   24  H   -0.003486
   25  H    0.008050
 Sum of Mulliken atomic spin densities =  13.00000
Dipole moment (field-independent basis, Debye):
   X=              0.4814    Y=              2.9853    Z=             -1.5212  Tot=
3.3850


Isotropic polarizability for W=    0.000000      290.01 Bohr**3.    1.719 A**3


Frequencies --    64.5537              82.0704              83.0318
 Frequencies --    92.8250             101.9917             106.8827
 Frequencies --   111.5209             114.8129             123.3515
 Frequencies --   130.3812             131.1775             139.2632
 Frequencies --   146.0621             153.2986             161.7379
 Frequencies --   164.7592             174.9698             178.6736
 Frequencies --   186.7819             189.6134             199.4657
 Frequencies --   205.8531             219.9572             224.0337
 Frequencies --   228.3042             241.2230             256.0203
 Frequencies --   285.0071             300.6891             340.1600
 Frequencies --   346.0294             363.6231             380.6628
 Frequencies --   385.3392             403.3356             410.8690
 Frequencies --   422.6121             424.3901             439.8487
 Frequencies --   455.7705             459.4431             481.7941
 Frequencies --   486.8200             497.2058             504.4043
 Frequencies --   511.0546             519.7266             520.3181
 Frequencies --   537.8183             540.4220             550.3610
 Frequencies --   564.4679             580.6659             585.6172
 Frequencies --   595.9490             623.0479             625.6460
 Frequencies --   633.8740             679.9129             687.0726
 Frequencies --   723.1460             728.3324             772.5555
 Frequencies --   802.1085            3676.4107            3677.4163
 Frequencies --  3690.7105            3706.1454            3723.6313
 1\1\GINC-
NODE06\Freq\UBPW91\Gen\Fe8H5O12(14)\_MDNSRESPONDER\13-Oct-201
[headnode:~/feon] ggutsev% grep "Inten" fe8o12h5_14_GF.out
 IR Inten    --     0.7953               1.4873               0.3473
 IR Inten    --     2.2180               3.0841               4.3272
 IR Inten    --     6.0209               1.3423               3.9407
 IR Inten    --     2.2190               3.6152               7.5293
 IR Inten    --     6.6931               4.6686               1.8372
 IR Inten    --     4.2966              11.7308               2.8646
 IR Inten    --     4.8445               4.6283               0.9530
 IR Inten    --     8.7121              15.2459               5.7365
```

IR Inten	--	0.1113	9.2210	1.5797
IR Inten	--	12.1355	1.4422	7.8612
IR Inten	--	2.5991	0.8533	1.8839
IR Inten	--	8.3238	53.1280	75.3934
IR Inten	--	63.3946	58.9944	80.6787
IR Inten	--	52.1707	67.2849	104.2761
IR Inten	--	32.4058	42.0930	7.8499
IR Inten	--	27.4664	58.1026	23.8925
IR Inten	--	38.2283	33.8327	79.9903
IR Inten	--	47.6939	28.4384	11.0155
IR Inten	--	21.9254	36.9487	119.7726
IR Inten	--	32.8321	62.9157	54.4111
IR Inten	--	63.9257	48.1359	47.9570
IR Inten	--	63.3028	68.3432	54.2281
IR Inten	--	63.1067	47.7872	75.6157

Zero-point vibrational energy 250360.6 (Joules/Mol)
59.83763 (Kcal/Mol) 2.595 eV

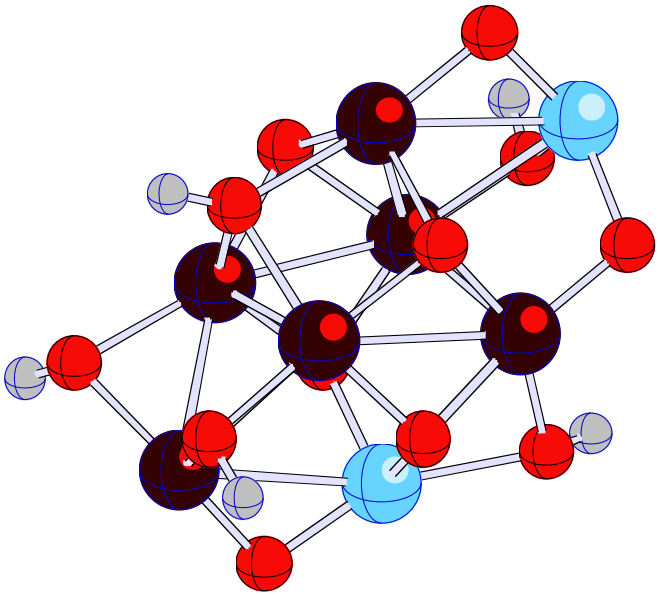
Atom	No	Natural Electron Configuration
Fe	1	[core]4S(0.26)3d(6.42)4p(0.40)4d(0.03)5p(0.01)
Fe	2	[core]4S(0.24)3d(6.42)4p(0.42)4d(0.03)5p(0.01)
Fe	3	[core]4S(0.21)3d(6.26)4p(0.40)4d(0.03)
Fe	4	[core]4S(0.25)3d(6.47)4p(0.33)4d(0.02)
Fe	5	[core]4S(0.27)3d(6.45)4p(0.31)4d(0.02)
Fe	6	[core]4S(0.23)3d(6.34)4p(0.39)4d(0.03)5p(0.01)
Fe	7	[core]4S(0.28)3d(6.45)4p(0.46)4d(0.04)
Fe	8	[core]4S(0.27)3d(6.56)4p(0.47)4d(0.03)
O	9	[core]2S(1.73)2p(5.20)3S(0.01)3p(0.01)
O	10	[core]2S(1.70)2p(5.18)3S(0.01)3p(0.01)
O	11	[core]2S(1.72)2p(5.13)3p(0.01)
O	12	[core]2S(1.72)2p(5.13)3S(0.01)3p(0.01)
O	13	[core]2S(1.77)2p(5.02)3S(0.01)3p(0.02)
O	14	[core]2S(1.72)2p(5.21)3S(0.01)3p(0.01)
O	15	[core]2S(1.77)2p(4.83)3S(0.01)3p(0.02)
O	16	[core]2S(1.74)2p(4.93)3S(0.01)3p(0.02)
O	17	[core]2S(1.77)2p(5.06)3S(0.01)3p(0.02)
O	18	[core]2S(1.79)2p(4.90)3S(0.01)3p(0.02)
O	19	[core]2S(1.80)2p(4.91)3S(0.01)3p(0.02)
O	20	[core]2S(1.74)2p(4.89)3S(0.01)3p(0.02)
H	21	1S(0.52)
H	22	1S(0.51)
H	23	1S(0.50)
H	24	1S(0.51)
H	25	1S(0.51)

```
************************************************
*******        Alpha spin orbitals        *******
************************************************
  Atom  No        Natural Electron Configuration
------------------------------------------------------------------------
   Fe    1     [core]3d( 4.83)4p( 0.22)5S( 0.14)4d( 0.02)
   Fe    2     [core]3d( 4.86)4p( 0.07)5S( 0.13)4d( 0.02)5p( 0.16)5d( 0.01)
   Fe    3     [core]3d( 1.44)4p( 0.12)5S( 0.10)4d( 0.02)5p( 0.08)
   Fe    4     [core]3d( 4.81)4p( 0.17)5S( 0.14)4d( 0.01)
   Fe    5     [core]3d( 1.78)4p( 0.15)5S( 0.15)4d( 0.01)
   Fe    6     [core]3d( 4.84)4p( 0.13)5S( 0.13)4d( 0.02)5p( 0.08)
   Fe    7     [core]3d( 4.39)4p( 0.23)5S( 0.15)4d( 0.02)
   Fe    8     [core]3d( 4.35)4p( 0.24)5S( 0.15)4d( 0.02)
    O    9    [core]2S( 0.87)2p( 2.61)
    O   10     [core]2S( 0.87)2p( 2.63)4S( 0.01)4p( 0.01)
    O   11     [core]2S( 0.86)2p( 2.57)
    O   12     [core]2S( 0.87)2p( 2.63)3p( 0.01)
    O   13     [core]2S( 0.89)2p( 2.53)4S( 0.01)4p( 0.01)
    O   14     [core]2S( 0.87)2p( 2.69)3p( 0.01)4S( 0.01)
    O   15     [core]2S( 0.88)2p( 2.49)4p( 0.01)
    O   16     [core]2S( 0.88)2p( 2.57)4S( 0.01)4p( 0.01)
    O   17     [core]2S( 0.90)2p( 2.78)4S( 0.01)4p( 0.01)
    O   18     [core]2S( 0.89)2p( 2.40)
    O   19     [core]2S( 0.90)2p( 2.47)4p( 0.01)
    O   20     [core]2S( 0.86)2p( 2.42)4p( 0.01)
    H   21          1S( 0.26)
    H   22          1S( 0.26)
    H   23          1S( 0.25)
    H   24          1S( 0.26)
    H   25          1S( 0.26)


************************************************
*******        Beta  spin orbitals        *******
************************************************
  Atom  No        Natural Electron Configuration
------------------------------------------------------------------------
   Fe    1     [core]3d( 1.59)4p( 0.19)5S( 0.12)4d( 0.01)
   Fe    2     [core]3d( 1.56)4p( 0.06)5S( 0.11)4d( 0.01)5p( 0.15)
   Fe    3     [core]3d( 4.82)4p( 0.13)5S( 0.12)4d( 0.01)5p( 0.08)
   Fe    4     [core]3d( 1.66)4p( 0.16)5S( 0.11)4d( 0.01)
   Fe    5     [core]3d( 4.67)4p( 0.15)5S( 0.12)4d( 0.01)
   Fe    6     [core]3d( 1.50)4p( 0.06)5S( 0.10)4d( 0.01)5p( 0.13)
   Fe    7     [core]3d( 2.06)4p( 0.23)5S( 0.13)4d( 0.02)
```

Fe	8	[core]3d(2.21)4p(0.23)5S(0.12)4d(0.01)
O	9	[core]2S(0.87)2p(2.59)
O	10	[core]2S(0.83)2p(2.54)
O	11	[core]2S(0.86)2p(2.56)
O	12	[core]2S(0.85)2p(2.50)
O	13	[core]2S(0.88)2p(2.49)4S(0.01)4p(0.01)
O	14	[core]2S(0.85)2p(2.52)
O	15	[core]2S(0.89)2p(2.34)4p(0.01)
O	16	[core]2S(0.86)2p(2.36)
O	17	[core]2S(0.87)2p(2.27)
O	18	[core]2S(0.90)2p(2.50)4p(0.01)
O	19	[core]2S(0.90)2p(2.44)
O	20	[core]2S(0.87)2p(2.47)4p(0.01)
H	21	1S(0.26)
H	22	1S(0.26)
H	23	1S(0.25)
H	24	1S(0.26)
H	25	1S(0.25)

HF=-11017.1821807\S2=56.009475\S2-1=0.\S2A=63.992152



TITLE

Fe	1.4966805162,-0.3524928618,-1.0732345648
Fe	0.4994040297,1.9213439502,0.0719602164
Ga	-1.5657527634,0.2342791616,-1.7038714997
Fe	-1.9393814122,2.5196896655,-0.1584988693
Ga	2.1471585037,-2.6785319967,0.0854219564
Fe	1.6221863879,-0.3624468188,1.5174326241
Fe	-0.6497236214,-1.7912230899,-0.0733545333

```
 Fe     -1.2122358271,0.5340501139,1.3214636593
 O      2.6843428679,-1.8197955288,-1.6300818713
 O      0.3409079015,1.3765381499,2.1762360841
 O      -1.2808226553,-1.7920619213,-1.9152660372
 O      -2.5606950792,1.91682687,1.6156963793
 O      0.2164287075,0.8525276534,-1.6729657414
 O      -0.3840171984,3.701865954,0.0682263209
 O      0.4139798328,-3.1658795943,-0.0884564795
 O      -0.2248350088,-1.0596323883,1.5921570871
 O      2.2063057754,0.9328050624,0.18622961
 O      -2.5310088216,1.7322822022,-1.6420058456
 O      2.6928016338,-1.8229015544,1.5314474292
 O      -2.0525265088,-0.5271456546,0.0821881164
 H      -3.4594242211,1.5444340851,1.646676211
 H      3.6264365121,-1.6184004735,-1.7631335848
 H      0.2451906556,2.0999555115,2.8197732526
 H      -0.7340670542,-2.275170158,-2.5569914275
 H      -0.1449431525,4.3990836609,-0.5623084925
END
```

$Fe_8O_{12}H_6$

```
$$$$$$$$$$$$$  Fe8O12H6      NEUTRAL    S = 15   head
fe8o12h6_15_GF.out
 ---------------------------------------------------------------------
 # UBPW91/6-311+G*
 scf=(VSHIFT=5,NoIncFock,Maxcycle=90,Tight,NoVarAcc)
  NOSYMM OPT=RFO IOP(5/13=1,5/36=1,8/11=1) INT=UltraFine
 GUESS=READ GEOM=CHECKPOINT
  ---------------------------------------------------------------------
 Charge =  0 Multiplicity = 15
                     Input orientation:
  ---------------------------------------------------------------------
  Center     Atomic      Atomic           Coordinates (Angstroms)
  Number     Number       Type             X           Y           Z
  ---------------------------------------------------------------------
       1         26           0        1.329621   -0.491600   -1.294265
       2         26           0        0.443035    1.874798   -0.046538
       3         26           0       -1.549688    0.423981   -1.674236
       4         26           0       -2.054860    2.610115   -0.094908
       5         26           0        2.030754   -2.592353    0.075994
       6         26           0        1.527634   -0.405707    1.658549
```

7	26	0	-0.467229	-1.856930	0.027518
8	26	0	-1.353770	0.509454	1.275325
9	8	0	2.610461	-1.974864	-1.719610
10	8	0	0.372280	1.472911	2.029901
11	8	0	-0.398922	-1.452030	-2.048696
12	8	0	-2.637118	1.991822	1.699645
13	8	0	0.200636	1.122967	-1.751915
14	8	0	-0.398683	3.693359	0.059553
15	8	0	0.374282	-3.674688	-0.080649
16	8	0	-0.223030	-1.102969	1.732849
17	8	0	1.981354	0.573020	0.111720
18	8	0	-2.613865	1.877824	-1.614867
19	8	0	2.590451	-1.861344	1.595532
20	8	0	-2.007061	-0.555374	-0.128267
21	1	0	-3.565495	1.811739	1.915493
22	1	0	3.538251	-1.798761	-1.941003
23	1	0	0.280467	2.206612	2.661806
24	1	0	-0.308886	-2.184555	-2.682209
25	1	0	-0.171664	4.394556	-0.571068
26	1	0	0.146247	-4.379937	0.545000

Distance matrix (angstroms):

		1	2	3	4	5
1	Fe	0.000000				
2	Fe	2.818279	0.000000			
3	Fe	3.045174	2.953847	0.000000		
4	Fe	4.744871	2.604325	2.743840	0.000000	
5	Fe	2.604296	4.742500	4.998113	6.617184	0.000000
6	Fe	2.960692	3.047029	4.611480	5.000406	2.745729
7	Fe	2.615321	3.841856	3.044706	4.742367	2.604442
8	Fe	3.847790	2.615339	2.957296	2.604197	4.744956
9	O	2.005378	4.724066	4.802431	6.739948	1.985332
10	O	3.978176	2.116157	4.302888	3.420388	4.805690
11	O	2.116472	3.973074	2.232465	4.802129	3.423152
12	O	5.555709	3.542624	3.876042	1.985378	6.740915
13	O	2.022592	1.879446	1.886332	3.169313	4.527051
14	O	4.725859	2.006716	3.875522	1.984994	6.738888
15	O	3.538020	5.550017	4.800027	6.737928	1.984915
16	O	3.456575	3.532274	3.962300	4.525847	3.169065
17	O	1.880150	2.021410	3.959811	4.525867	3.165960
18	O	4.611728	3.435738	1.802681	1.777360	6.664381
19	O	3.437560	4.611567	5.749334	6.665617	1.776691
20	O	3.535119	3.451867	1.886358	3.166025	4.527136
21	H	6.290475	4.463390	4.344596	2.638396	7.355120
22	H	2.646694	5.163758	5.558675	7.357251	2.640191
23	H	4.902200	2.733433	5.032743	3.635387	5.725381

24	H	2.734445	4.898009	3.059421	5.721137	3.639766
25	H	5.162499	2.646161	4.345274	2.637687	7.354334
26	H	4.461215	6.289651	5.556872	7.356302	2.639468

		6	7	8	9	10
6	Fe	0.000000				
7	Fe	2.957328	0.000000			
8	Fe	3.047437	2.818288	0.000000		
9	O	3.879011	3.540980	5.554871	0.000000	
10	O	2.236505	3.975192	2.115865	5.563761	0.000000
11	O	4.306980	2.116430	3.975962	3.072139	5.077892
12	O	4.805726	4.724121	2.006102	7.413702	3.071614
13	O	3.965985	3.534432	3.457855	3.924902	3.801849
14	O	4.803107	5.550805	3.539427	6.659514	3.067090
15	O	3.878307	2.006012	4.725661	3.252091	5.563470
16	O	1.885873	1.880490	2.021833	4.550641	2.660412
17	O	1.885855	3.450696	3.532856	3.200196	2.660515
18	O	5.751676	4.610191	3.437075	6.492130	4.729201
19	O	1.803449	3.436291	4.613035	3.317145	4.028178
20	O	3.963481	2.022226	1.879020	5.086141	3.799064
21	H	5.560850	5.159732	2.645277	8.105231	3.953980
22	H	4.352006	4.463444	6.293210	0.969960	6.041133
23	H	3.063684	4.900091	2.733753	6.489253	0.972651
24	H	5.037786	2.734050	4.900157	3.081096	6.003750
25	H	5.558897	6.287030	4.461005	7.044777	3.949294
26	H	4.352324	2.647585	5.166195	4.121309	6.042504

		11	12	13	14	15
11	O	0.000000				
12	O	5.560549	0.000000			
13	O	2.660481	4.552035	0.000000		
14	O	5.560553	3.255106	3.201175	0.000000	
15	O	3.067778	6.659378	5.083383	7.409808	0.000000
16	O	3.801692	3.925132	4.156665	5.082867	3.203013
17	O	3.799202	5.085743	2.635628	3.924769	4.545625
18	O	4.022699	3.316553	2.917191	3.317662	6.489471
19	O	4.731204	6.495014	5.081607	6.492217	3.318012
20	O	2.660480	3.197881	3.213563	4.546855	3.924689
21	H	6.032759	0.970002	5.301701	4.124767	7.043245
22	H	3.953878	8.109132	4.439811	7.047344	4.121980
23	H	6.003004	3.079641	4.545503	3.073009	6.489957
24	H	0.972644	6.485633	3.473436	6.486540	3.074952
25	H	6.034700	4.124043	3.498043	0.969999	8.102547
26	H	3.949317	7.048379	5.963282	8.106215	0.969955

		16	17	18	19	20
16	O	0.000000				
17	O	3.208785	0.000000			
18	O	5.080199	5.079335	0.000000		

19	O	2.917132	2.915274	7.167492	0.000000	
20	O	2.635598	4.151905	2.915243	5.080763	0.000000
21	H	4.438576	5.962848	3.656967	7.175624	3.494123
22	H	5.303635	3.501849	7.174411	3.661874	5.965107
23	H	3.474161	3.473410	5.174475	4.798044	4.543771
24	H	4.546419	4.544827	4.791145	5.177807	3.472844
25	H	5.960994	4.439124	3.658935	7.173543	5.297789
26	H	3.505120	5.299729	7.172365	3.663477	4.440417

		21	22	23	24	25
21	H	0.000000				
22	H	8.852767	0.000000			
23	H	3.937554	6.916792	0.000000		
24	H	6.907585	3.936837	6.941770	0.000000	
25	H	4.936802	7.348290	3.929758	6.910894	0.000000
26	H	7.347934	4.934407	6.919646	3.929596	8.850899

		26
26	H	0.000000

Alpha occ. eigenvalues -- -0.21195 -0.21077 -0.21075 -0.21021 -0.19618
Alpha occ. eigenvalues -- -0.19262 -0.19160 -0.18292 -0.18155 -0.17492
Alpha occ. eigenvalues -- -0.17024 -0.16611
Alpha virt. eigenvalues -- -0.14515 -0.14281 -0.13039 -0.12978 -0.12826
0.57 eV
Beta occ. eigenvalues -- -0.24092 -0.24057 -0.23767 -0.21043 -0.20991
Beta occ. eigenvalues -- -0.20798 -0.19686 -0.19161 -0.18453 -0.17667
Beta occ. eigenvalues -- -0.16703 -0.16144 -0.15654
Beta virt. eigenvalues -- -0.14578 -0.13567 -0.13007 -0.12547 -0.12537
0.29 eV
Mulliken atomic spin densities:

		1
1	Fe	3.426120
2	Fe	3.420792
3	Fe	-3.622692
4	Fe	3.358190
5	Fe	3.356748
6	Fe	-3.625199
7	Fe	3.424303
8	Fe	3.422579
9	O	0.130959
10	O	0.108961
11	O	0.108804
12	O	0.130747
13	O	0.042353
14	O	0.130606
15	O	0.130832
16	O	0.041113
17	O	0.042070

```
   18  O   -0.062707
   19  O   -0.061857
   20  O    0.043293
   21  H    0.009288
   22  H    0.009288
   23  H    0.008423
   24  H    0.008278
   25  H    0.009351
   26  H    0.009354
 Sum of Mulliken atomic spin densities =  14.00000
Dipole moment (field-independent basis, Debye):
   X=              0.0154    Y=             -0.0261    Z=             -0.0071  Tot=
0.0312


Isotropic polarizability for W=    0.000000      284.14 Bohr**3.   1.619 A**3


Frequencies --    58.6825              78.3359             82.1076
 Frequencies --    86.4323              89.8525             91.6616
 Frequencies --   100.1627             112.6894            117.6494
 Frequencies --   122.1625             122.4066            131.3438
 Frequencies --   139.3829             141.9387            146.4895
 Frequencies --   153.1076             158.7065            159.6228
 Frequencies --   162.3952             167.4743            178.1327
 Frequencies --   180.5621             193.3909            205.5590
 Frequencies --   207.8230             213.7101            216.2982
 Frequencies --   218.8752             315.5394            318.2074
 Frequencies --   321.8318             327.0012            337.8342
 Frequencies --   343.0173             350.5023            350.8274
 Frequencies --   362.7326             377.9094            384.5002
 Frequencies --   395.7542             420.5698            426.2561
 Frequencies --   439.9127             467.1864            470.5386
 Frequencies --   471.6593             476.9161            490.9790
 Frequencies --   502.6697             507.1207            507.5223
 Frequencies --   508.5847             536.5550            541.1155
 Frequencies --   555.1887             559.4185            579.4219
 Frequencies --   582.0931             597.5041            600.2767
 Frequencies --   677.7182             680.0260            692.9575
 Frequencies --   694.0776             704.2975            704.8232
 Frequencies --  3682.1282            3682.6158           3722.0343
 Frequencies --  3722.2498            3722.6328           3722.7487
[headnode:~/feon] ggutsev% grep "Inten" fe8o12h6_15_GF.out
 IR Inten    --     7.0346               0.0002              3.5907
 IR Inten    --    25.9316               0.0087              3.0183
 IR Inten    --     0.0007               0.0070              0.0080
```

IR Inten	--	0.0033	10.8058	0.0026
IR Inten	--	13.8686	6.7944	0.0021
IR Inten	--	2.9219	0.0006	0.1341
IR Inten	--	0.0003	23.6301	0.0003
IR Inten	--	2.8544	57.7637	3.0989
IR Inten	--	0.0007	0.0023	0.0026
IR Inten	--	2.7818	0.0050	0.0223
IR Inten	--	13.9832	22.6428	0.0064
IR Inten	--	32.2160	30.7881	0.0615
IR Inten	--	0.0709	490.4164	37.2326
IR Inten	--	2.1384	0.0125	83.6153
IR Inten	--	0.0150	0.6077	78.9024
IR Inten	--	0.1276	80.6043	18.0260
IR Inten	--	0.1022	25.8330	52.2611
IR Inten	--	0.0905	73.5332	0.0074
IR Inten	--	0.0041	97.8160	152.5646
IR Inten	--	7.2680	80.3377	3.0160
IR Inten	--	84.6728	0.0002	2.6638
IR Inten	--	48.7408	87.7200	96.5959
IR Inten	--	49.5008	0.0012	73.1746
IR Inten	--	59.7734	25.1053	66.8036
IR Inten	--	7.0346	0.0002	3.5907
IR Inten	--	25.9315	0.0087	3.0183
IR Inten	--	0.0007	0.0070	0.0080
IR Inten	--	0.0032	10.8058	0.0026
IR Inten	--	13.8685	6.7945	0.0021
IR Inten	--	2.9219	0.0006	0.1341
IR Inten	--	0.0003	23.6301	0.0003
IR Inten	--	2.8545	57.7638	3.0989
IR Inten	--	0.0007	0.0023	0.0026
IR Inten	--	2.7818	0.0050	0.0223
IR Inten	--	13.9832	22.6427	0.0064
IR Inten	--	32.2158	30.7879	0.0616
IR Inten	--	0.0709	490.4159	37.2330
IR Inten	--	2.1387	0.0125	83.6152
IR Inten	--	0.0150	0.6082	78.9024
IR Inten	--	0.1273	80.6042	18.0260
IR Inten	--	0.1023	25.8298	52.2648
IR Inten	--	0.0898	73.5359	0.0072
IR Inten	--	0.0041	97.8136	152.5659
IR Inten	--	7.2667	80.3376	3.0161
IR Inten	--	84.6732	0.0002	2.6613
IR Inten	--	48.7433	87.7185	96.5969
IR Inten	--	49.5008	0.0011	73.1704
IR Inten	--	59.7740	25.1275	66.7854

Zero-point vibrational energy 268396.7 (Joules/Mol)

64.14834 (Kcal/Mol) 2.782 eV

Atom	No	Natural Electron Configuration
Fe	1	[core]4S(0.25)3d(6.42)4p(0.43)4d(0.03)5p(0.01)
Fe	2	[core]4S(0.25)3d(6.42)4p(0.43)4d(0.03)5p(0.01)
Fe	3	[core]4S(0.21)3d(6.30)4p(0.39)4d(0.03)
Fe	4	[core]4S(0.23)3d(6.48)4p(0.32)4d(0.02)
Fe	5	[core]4S(0.23)3d(6.48)4p(0.32)4d(0.02)
Fe	6	[core]4S(0.21)3d(6.30)4p(0.39)4d(0.03)
Fe	7	[core]4S(0.25)3d(6.42)4p(0.43)4d(0.03)5p(0.01)
Fe	8	[core]4S(0.25)3d(6.42)4p(0.43)4d(0.03)5p(0.01)
O	9	[core]2S(1.72)2p(5.21)3S(0.01)3p(0.01)
O	10	[core]2S(1.72)2p(5.23)3S(0.01)3p(0.01)
O	11	[core]2S(1.72)2p(5.23)3S(0.01)3p(0.01)
O	12	[core]2S(1.72)2p(5.21)3S(0.01)3p(0.01)
O	13	[core]2S(1.76)2p(5.01)3S(0.01)3p(0.02)
O	14	[core]2S(1.72)2p(5.21)3S(0.01)3p(0.01)
O	15	[core]2S(1.72)2p(5.21)3S(0.01)3p(0.01)
O	16	[core]2S(1.76)2p(5.01)3S(0.01)3p(0.02)
O	17	[core]2S(1.76)2p(5.01)3S(0.01)3p(0.02)
O	18	[core]2S(1.79)2p(4.92)3S(0.01)3p(0.01)
O	19	[core]2S(1.79)2p(4.92)3S(0.01)3p(0.01)
O	20	[core]2S(1.76)2p(5.01)3S(0.01)3p(0.02)
H	21	1S(0.52)
H	22	1S(0.52)
H	23	1S(0.50)
H	24	1S(0.50)
H	25	1S(0.52)
H	26	1S(0.52)

****
******* Alpha spin orbitals *******
****

Atom	No	Natural Electron Configuration
Fe	1	[core]3d(4.80)4p(0.22)5S(0.13)4d(0.02)
Fe	2	[core]3d(4.80)4p(0.22)5S(0.13)4d(0.02)5d(0.01)
Fe	3	[core]3d(1.50)4p(0.19)5S(0.09)4d(0.02)
Fe	4	[core]3d(4.82)4p(0.17)5S(0.14)4d(0.01)
Fe	5	[core]3d(4.82)4p(0.17)5S(0.14)4d(0.01)
Fe	6	[core]3d(1.50)4p(0.19)5S(0.09)4d(0.02)
Fe	7	[core]3d(4.80)4p(0.22)5S(0.13)4d(0.02)5d(0.01)
Fe	8	[core]3d(4.80)4p(0.22)5S(0.13)4d(0.02)
O	9	[core]2S(0.87)2p(2.69)3p(0.01)4S(0.01)

O	10	[core]2S(0.87)2p(2.67)4S(0.01)4p(0.01)
O	11	[core]2S(0.87)2p(2.67)4S(0.01)4p(0.01)
O	12	[core]2S(0.87)2p(2.69)3p(0.01)4S(0.01)
O	13	[core]2S(0.88)2p(2.53)4S(0.01)4p(0.01)
O	14	[core]2S(0.87)2p(2.69)3p(0.01)4S(0.01)
O	15	[core]2S(0.87)2p(2.69)3p(0.01)4S(0.01)
O	16	[core]2S(0.88)2p(2.53)4S(0.01)4p(0.01)
O	17	[core]2S(0.88)2p(2.53)4S(0.01)4p(0.01)
O	18	[core]2S(0.90)2p(2.43)4p(0.01)
O	19	[core]2S(0.90)2p(2.43)4p(0.01)
O	20	[core]2S(0.88)2p(2.53)4S(0.01)4p(0.01)
H	21	1S(0.26)
H	22	1S(0.26)
H	23	1S(0.25)
H	24	1S(0.25)
H	25	1S(0.26)
H	26	1S(0.26)

****

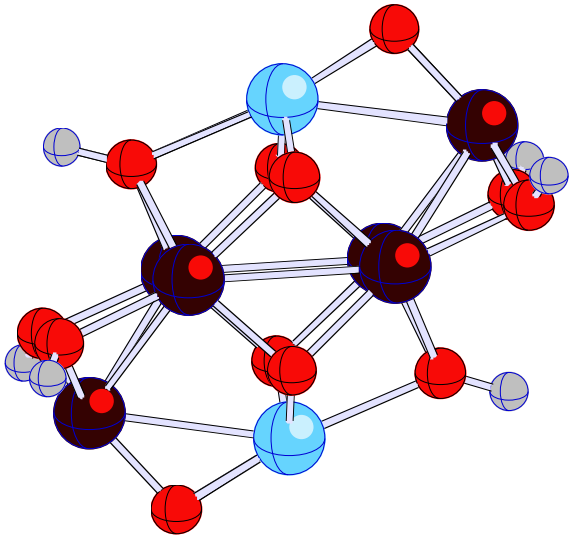
******* Beta spin orbitals *******

****

Atom	No	Natural Electron Configuration
Fe	1	[core]3d(1.61)4p(0.21)5S(0.11)4d(0.01)
Fe	2	[core]3d(1.62)4p(0.21)5S(0.11)4d(0.01)
Fe	3	[core]3d(4.80)4p(0.20)5S(0.11)4d(0.01)
Fe	4	[core]3d(1.65)4p(0.15)5S(0.10)4d(0.01)
Fe	5	[core]3d(1.65)4p(0.15)5S(0.10)4d(0.01)
Fe	6	[core]3d(4.81)4p(0.20)5S(0.11)4d(0.01)
Fe	7	[core]3d(1.61)4p(0.21)5S(0.11)4d(0.01)
Fe	8	[core]3d(1.61)4p(0.21)5S(0.11)4d(0.01)
O	9	[core]2S(0.85)2p(2.52)
O	10	[core]2S(0.85)2p(2.56)
O	11	[core]2S(0.85)2p(2.56)
O	12	[core]2S(0.85)2p(2.52)
O	13	[core]2S(0.88)2p(2.48)4S(0.01)4p(0.01)
O	14	[core]2S(0.85)2p(2.52)
O	15	[core]2S(0.85)2p(2.52)
O	16	[core]2S(0.88)2p(2.48)4S(0.01)4p(0.01)
O	17	[core]2S(0.88)2p(2.48)4S(0.01)
O	18	[core]2S(0.90)2p(2.48)
O	19	[core]2S(0.90)2p(2.48)
O	20	[core]2S(0.88)2p(2.48)4S(0.01)
H	21	1S(0.26)
H	22	1S(0.26)
H	23	1S(0.25)

H	24	1S(0.25)
H	25	1S(0.26)
H	26	1S(0.26)

HF= -11017.7884311\S2=63.864572\S2-1=0.\S2A=73.07947



TITLE

Fe	1.3296210386,-0.491599906,-1.294265009
Fe	0.4430345731,1.8747982213,-0.0465383292
Ga	-1.5496875105,0.4239805013,-1.6742362666
Fe	-2.0548604767,2.6101145791,-0.0949078983
Fe	2.0307544185,-2.5923529126,0.0759937429
Ga	1.5276343339,-0.4057074594,1.658549201
Fe	-0.4672291206,-1.8569298303,0.0275179474
Fe	-1.3537704664,0.5094536624,1.2753248732
O	2.6104608642,-1.9748636713,-1.7196098158
O	0.3722795627,1.4729109137,2.0299006538
O	-0.3989217786,-1.452030407,-2.048696444
O	-2.6371177679,1.9918224206,1.6996445948
O	0.2006356262,1.1229668339,-1.7519154203
O	-0.3986833094,3.6933591625,0.0595532878
O	0.3742816922,-3.6746880647,-0.0806487706
O	-0.2230295221,-1.1029690025,1.7328485504
O	1.9813536599,0.5730198432,0.1117198396
O	-2.6138645272,1.8778239198,-1.6148668413
O	2.5904509298,-1.8613437579,1.595531982
O	-2.0070607276,-0.5553738558,-0.128266692
H	-3.5654949194,1.8117392157,1.9154932051
H	3.5382509854,-1.7987611155,-1.9410031497
H	0.2804671778,2.2066115855,2.6618058796

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 H       -0.3088857737,-2.1845550712,-2.6822085973
 H       -0.1716638228,4.3945563311,-0.5710676339
 H       0.1462468604,-4.3799371357,0.5450001103
END
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$Fe_8O_{12}H_7$

```
$$$$$$$$$$$$$  Fe8O12H7    NEUTRAL    S = 14    head_2017_Jan
fe8o12h7_14_GF.out
-----------------------------------------------------------------------
 # UBPW91/6-311+G*
scf=(VSHIFT=5,NoIncFock,Maxcycle=90,Tight,NoVarAcc)  NOSYMM
 OPT=RFO IOP(5/13=1,5/36=1,8/11=1) INT=UltraFine GUESS=READ
GEOM=CHECKPOINT
 -----------------------------------------------------------------------
 Charge =  0 Multiplicity = 14
                    Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic          Coordinates (Angstroms)
 Number     Number       Type             X           Y           Z
 ---------------------------------------------------------------------
     1         26          0        0.833322    1.095109   -1.304994
     2         26          0       -1.938656    0.703213    0.511934
     3         26          0       -0.798361   -1.147578   -1.696948
     4         26          0       -3.085391   -1.538805   -0.104041
     5         26          0        3.075829    0.977828    0.159270
     6         26          0        0.791054    1.352451    1.553545
     7         26          0        1.527487   -0.982541    0.351381
     8         26          0       -0.992675   -1.456925    1.302752
     9          8          0        2.660138    1.665706   -1.646350
    10          8          0       -1.130841    1.738910    1.973500
    11          8          0        0.725507   -0.218390   -2.727113
    12          8          0       -2.671139   -2.413137    1.609841
    13          8          0       -0.951048    0.694987   -1.082845
    14          8          0       -3.851146    0.254608    0.314893
    15          8          0        3.490965   -0.972166    0.134443
    16          8          0        0.573069   -0.500417    1.920697
    17          8          0        0.579148    2.583703   -0.160070
    18          8          0       -2.493154   -1.757096   -1.761580
    19          8          0        2.555778    1.776362    1.656689
    20          8          0        0.084139   -2.030697   -0.293740
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21	1	0	-3.215374	-2.278542	2.402310
22	1	0	3.086351	1.383035	-2.471882
23	1	0	-1.362208	2.684039	1.955684
24	1	0	1.538041	-0.673756	-3.004033
25	1	0	-4.419796	0.731307	-0.311188
26	1	0	4.089356	-1.420991	0.752358
27	1	0	1.375476	3.149792	-0.164774

Distance matrix (angstroms):

		1	2	3	4	5
1	Fe	0.000000				
2	Fe	3.337464	0.000000			
3	Fe	2.801012	3.099170	0.000000		
4	Fe	4.871972	2.592503	2.814413	0.000000	
5	Fe	2.680795	5.034366	4.792937	6.660586	0.000000
6	Fe	2.870410	2.992955	4.397965	5.112121	2.702691
7	Fe	2.746284	3.857679	3.103620	4.668563	2.505458
8	Fe	4.080133	2.487261	3.021862	2.522941	4.877325
9	O	1.944058	5.170443	4.458514	6.757123	1.976420
10	O	3.875685	1.965046	4.681297	4.345096	4.644002
11	O	1.938899	4.294012	2.060778	4.811128	3.909751
12	O	5.751982	3.384312	4.005469	1.968108	6.828648
13	O	1.842124	1.875835	1.948200	3.240881	4.223575
14	O	5.027397	1.974257	3.915754	1.994547	6.966365
15	O	3.661785	5.694749	4.667235	6.605030	1.993848
16	O	3.608118	3.121234	3.922626	4.308381	3.398770
17	O	1.895091	3.213591	4.264035	5.516073	2.985671
18	O	4.405564	3.395505	1.802224	1.773649	6.494848
19	O	3.493212	4.760467	5.571944	6.775935	1.774929
20	O	3.369654	3.495006	1.878216	3.213078	4.266925
21	H	6.443413	3.754251	4.891313	2.616467	7.430640
22	H	2.553560	5.883536	4.700587	7.227325	2.662191
23	H	4.239938	2.518011	5.323621	5.004422	5.082758
24	H	2.551910	5.132785	2.718778	5.525793	3.885744
25	H	5.358661	2.614264	4.308750	2.641393	7.514419
26	H	4.600567	6.395856	5.473905	7.226639	2.670829
27	H	2.411588	4.174584	5.053763	6.471937	2.777343

		6	7	8	9	10
6	Fe	0.000000				
7	Fe	2.727585	0.000000			
8	Fe	3.337242	2.735208	0.000000		
9	O	3.718995	3.505288	5.638357	0.000000	
10	O	2.004843	4.135731	3.268388	5.242155	0.000000
11	O	4.560249	3.271731	4.552574	2.908722	5.419669
12	O	5.115624	4.610725	1.955987	7.460714	4.443451
13	O	3.227651	3.318771	3.213026	3.781599	3.234709

14	O	4.928442	5.519199	3.475063	6.945105	3.514852
15	O	3.834998	1.975453	4.658644	3.289356	5.665082
16	O	1.901431	1.898975	1.936058	4.666023	2.814372
17	O	2.120698	3.725457	4.575714	2.717033	2.861792
18	O	5.607616	4.607613	3.425152	6.187509	5.294221
19	O	1.817853	3.220677	4.813620	3.306540	3.700396
20	O	3.918913	1.896856	2.009361	4.704117	4.563605
21	H	5.473206	5.327350	2.612369	8.152937	4.546326
22	H	4.633938	3.999603	6.241129	0.971114	6.137815
23	H	2.563471	4.936389	4.208380	5.494626	0.973199
24	H	5.043314	3.369609	5.056310	2.928393	6.141638
25	H	5.569202	6.224664	4.374736	7.265069	4.129441
26	H	4.383227	2.629866	5.111875	4.162231	6.223072
27	H	2.554330	4.167218	5.383644	2.459255	3.583912

		11	12	13	14	15
11	O	0.000000				
12	O	5.929864	0.000000			
13	O	2.519665	4.457545	0.000000		
14	O	5.515731	3.191578	3.249335	0.000000	
15	O	4.050239	6.498055	4.898231	7.446081	0.000000
16	O	4.658853	3.778891	3.573960	4.766797	3.453601
17	O	3.803007	6.218148	2.600050	5.027701	4.605391
18	O	3.695897	3.439265	2.975145	3.194188	6.326192
19	O	5.152344	6.698862	4.579546	6.720478	3.278142
20	O	3.101147	3.370673	3.020538	4.591244	3.593089
21	H	6.788649	0.970729	5.110319	3.343406	7.198946
22	H	2.864138	8.013742	4.324745	7.560974	3.536045
23	H	5.891625	5.273909	3.654865	3.845665	6.343346
24	H	0.971727	6.483091	3.429283	6.396911	3.708503
25	H	5.763052	4.078686	3.553729	0.970867	8.104353
26	H	4.986828	6.886503	5.766369	8.127151	0.970225
27	H	4.281670	7.104261	3.504516	5.994143	4.642775

		16	17	18	19	20
16	O	0.000000				
17	O	3.720407	0.000000			
18	O	4.953800	5.553955	0.000000		
19	O	3.030603	2.803476	7.047099	0.000000	
20	O	2.735789	4.642800	2.978566	4.940331	0.000000
21	H	4.212598	6.678744	4.258108	7.092559	4.268127
22	H	5.399882	3.615543	6.441726	4.181066	5.040946
23	H	3.726565	2.873211	5.900913	4.032851	5.420384
24	H	5.021372	4.429294	4.355210	5.362947	3.361667
25	H	5.605993	5.333259	3.465218	7.322794	5.283408
26	H	3.817950	5.402932	7.054240	3.659610	4.184236
27	H	4.279845	0.977045	6.449313	2.568492	5.340566

		21	22	23	24	25

```
   21  H    0.000000
   22  H    8.767932   0.000000
   23  H    5.316100   6.409807   0.000000
   24  H    7.375557   2.628847   6.654700   0.000000
   25  H    4.227635   7.838086   4.277934   6.687409   0.000000
   26  H    7.537693   4.389113   6.929562   4.601961   8.841334
   27  H    7.558614   3.372132   3.494021   4.765222   6.281376
              26         27
   26  H    0.000000
   27  H    5.394288   0.000000
Alpha  occ. eigenvalues --   -0.19687  -0.19473  -0.18989  -0.18497  -0.18326
 Alpha  occ. eigenvalues --   -0.18097  -0.15022
 Alpha virt. eigenvalues --   -0.14040  -0.13265  -0.11998  -0.11791  -0.11318
gap = 0.27 eV
  Beta  occ. eigenvalues --   -0.20556  -0.20009  -0.19521  -0.18064  -0.17693
  Beta  occ. eigenvalues --   -0.16830  -0.16611  -0.15992  -0.15633
  Beta virt. eigenvalues --   -0.14316  -0.14006  -0.13434  -0.12943  -0.12681
gap = 0.36 eV
Mulliken atomic spin densities:
             1
    1  Fe   2.340659
    2  Fe   3.392074
    3  Fe  -3.666094
    4  Fe   3.305334
    5  Fe   3.440376
    6  Fe  -3.156299
    7  Fe   3.389531
    8  Fe   3.272791
    9  O    0.066847
   10  O    0.007881
   11  O   -0.042658
   12  O    0.110975
   13  O   -0.044675
   14  O    0.153352
   15  O    0.143761
   16  O    0.229521
   17  O    0.017311
   18  O   -0.075127
   19  O    0.056814
   20  O    0.042055
   21  H    0.012277
   22  H    0.003960
   23  H    0.003646
   24  H   -0.007512
   25  H    0.006701
   26  H    0.004954
```

27 H -0.008457
Sum of Mulliken atomic spin densities = 13.00000
Dipole moment (field-independent basis, Debye):
X= 0.7746 Y= 0.0555 Z= -0.7187 Tot= 1.0581

Isotropic polarizability for W= 0.000000 301.59 Bohr**3. 1.655 A**3

Frequencies --	55.4348	70.7402	80.2762
Frequencies --	86.4887	94.3019	102.2439
Frequencies --	104.5455	105.8402	108.2553
Frequencies --	118.3376	123.1025	125.7394
Frequencies --	133.5873	137.1243	140.8813
Frequencies --	147.0533	153.1628	163.1560
Frequencies --	173.3449	181.6703	187.2915
Frequencies --	187.9150	191.6213	197.8557
Frequencies --	218.7636	228.3519	267.6546
Frequencies --	287.8058	306.6345	323.7627
Frequencies --	331.7649	338.8490	344.7381
Frequencies --	357.3097	369.6773	375.2404
Frequencies --	401.5500	406.1847	411.4524
Frequencies --	418.8513	424.0449	440.2970
Frequencies --	446.5697	450.4002	457.1652
Frequencies --	473.9833	484.0159	493.0819
Frequencies --	510.4443	517.1248	519.7300
Frequencies --	521.6724	542.4773	545.6034
Frequencies --	556.4949	568.6929	581.1967
Frequencies --	588.1928	622.2199	623.0823
Frequencies --	697.5928	714.4448	720.9881
Frequencies --	742.0491	765.0081	813.2216
Frequencies --	850.8249	890.1197	3621.1014
Frequencies --	3680.5280	3690.4126	3693.5785
Frequencies --	3705.0025	3706.3160	3714.3859

Zero-point vibrational energy 304632.8 (Joules/Mol)
72.80898 (Kcal/Mol) 3.157 eV

Atom	No	Natural Electron Configuration
Fe	1	[core]4S(0.27)3d(6.55)4p(0.47)4d(0.03)
Fe	2	[core]4S(0.27)3d(6.50)4p(0.37)4d(0.03)
Fe	3	[core]4S(0.21)3d(6.27)4p(0.42)4d(0.03)
Fe	4	[core]4S(0.25)3d(6.50)4p(0.33)4d(0.02)
Fe	5	[core]4S(0.24)3d(6.48)4p(0.34)4d(0.02)
Fe	6	[core]4S(0.25)3d(6.44)4p(0.43)4d(0.03)

Fe	7	[core]4S(0.26)3d(6.45)4p(0.40)4d(0.03)5p(0.01)
Fe	8	[core]4S(0.28)3d(6.52)4p(0.35)4d(0.03)
O	9	[core]2S(1.70)2p(5.17)3S(0.01)3p(0.01)
O	10	[core]2S(1.73)2p(5.18)3S(0.01)3p(0.01)
O	11	[core]2S(1.71)2p(5.14)3p(0.01)
O	12	[core]2S(1.72)2p(5.21)3S(0.01)3p(0.01)
O	13	[core]2S(1.73)2p(4.97)3S(0.01)3p(0.03)
O	14	[core]2S(1.73)2p(5.21)3S(0.01)3p(0.01)
O	15	[core]2S(1.72)2p(5.22)3S(0.01)3p(0.01)
O	16	[core]2S(1.75)2p(5.05)3S(0.01)3p(0.02)
O	17	[core]2S(1.73)2p(5.05)3S(0.01)3p(0.01)
O	18	[core]2S(1.79)2p(4.92)3S(0.01)3p(0.02)
O	19	[core]2S(1.79)2p(4.92)3S(0.01)3p(0.02)
O	20	[core]2S(1.77)2p(5.05)3S(0.01)3p(0.02)
H	21	1S(0.51)
H	22	1S(0.52)
H	23	1S(0.52)
H	24	1S(0.53)
H	25	1S(0.52)
H	26	1S(0.52)
H	27	1S(0.52)

****
******* Alpha spin orbitals *******
****

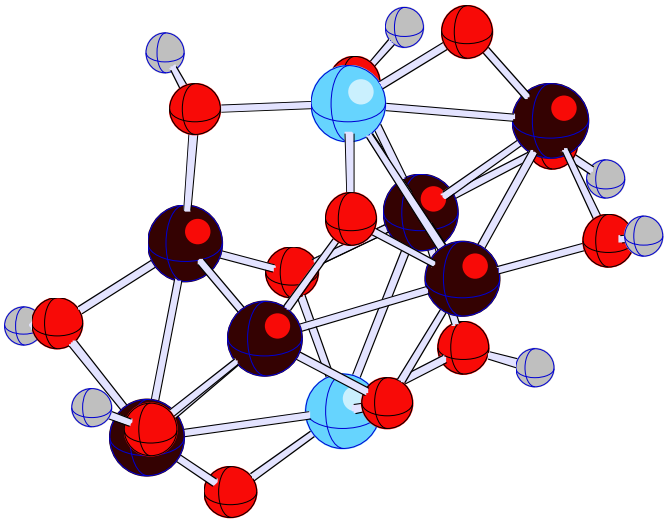
Atom	No	Natural Electron Configuration
Fe	1	[core]3d(4.30)4p(0.23)5S(0.14)4d(0.02)
Fe	2	[core]3d(4.83)4p(0.19)5S(0.14)4d(0.02)
Fe	3	[core]3d(1.44)4p(0.21)5S(0.10)4d(0.02)
Fe	4	[core]3d(4.81)4p(0.17)5S(0.14)4d(0.01)
Fe	5	[core]3d(4.85)4p(0.18)5S(0.15)4d(0.01)
Fe	6	[core]3d(1.81)4p(0.21)5S(0.13)4d(0.02)
Fe	7	[core]3d(4.84)4p(0.13)5S(0.14)4d(0.02)5p(0.08)
Fe	8	[core]3d(4.84)4p(0.10)5S(0.15)4d(0.02)5p(0.07)
O	9	[core]2S(0.86)2p(2.64)4p(0.01)
O	10	[core]2S(0.86)2p(2.60)
O	11	[core]2S(0.85)2p(2.55)
O	12	[core]2S(0.87)2p(2.68)3p(0.01)
O	13	[core]2S(0.87)2p(2.49)4S(0.01)4p(0.02)
O	14	[core]2S(0.88)2p(2.70)3p(0.01)
O	15	[core]2S(0.87)2p(2.70)3p(0.01)
O	16	[core]2S(0.88)2p(2.64)4S(0.01)4p(0.01)
O	17	[core]2S(0.86)2p(2.54)
O	18	[core]2S(0.89)2p(2.43)

```
    O   19      [core]2S( 0.89)2p( 2.49)4p( 0.01)
    O   20      [core]2S( 0.89)2p( 2.54)4S( 0.01)4p( 0.01)
    H   21           1S( 0.26)
    H   22           1S( 0.26)
    H   23           1S( 0.26)
    H   24           1S( 0.26)
    H   25           1S( 0.26)
    H   26           1S( 0.26)
    H   27           1S( 0.26)


NBO analysis skipped by request.


***********************************************
*******        Beta  spin orbitals        *******
****    Atom  No         Natural Electron Configuration
-----------------------------------------------------------------------
   Fe    1     [core]3d( 2.26)4p( 0.23)5S( 0.13)4d( 0.02)
   Fe    2     [core]3d( 1.68)4p( 0.18)5S( 0.14)4d( 0.01)
   Fe    3     [core]3d( 4.82)4p( 0.22)5S( 0.11)4d( 0.01)
   Fe    4     [core]3d( 1.69)4p( 0.16)5S( 0.11)4d( 0.01)
   Fe    5     [core]3d( 1.64)4p( 0.16)5S( 0.10)4d( 0.01)
   Fe    6     [core]3d( 4.62)4p( 0.22)5S( 0.12)4d( 0.01)
   Fe    7     [core]3d( 1.61)4p( 0.13)5S( 0.12)4d( 0.01)5p( 0.07)
   Fe    8     [core]3d( 1.68)4p( 0.10)5S( 0.13)4d( 0.01)5p( 0.07)
    O    9    [core]2S( 0.85)2p( 2.53)
    O   10     [core]2S( 0.86)2p( 2.58)
    O   11     [core]2S( 0.86)2p( 2.59)4p( 0.01)
    O   12     [core]2S( 0.85)2p( 2.53)
    O   13     [core]2S( 0.86)2p( 2.48)4p( 0.01)
    O   14     [core]2S( 0.85)2p( 2.51)
    O   15     [core]2S( 0.85)2p( 2.52)
    O   16     [core]2S( 0.87)2p( 2.41)
    O   17     [core]2S( 0.87)2p( 2.51)
    O   18     [core]2S( 0.90)2p( 2.50)
    O   19     [core]2S( 0.89)2p( 2.43)
    O   20     [core]2S( 0.88)2p( 2.51)4S( 0.01)
    H   21          1S( 0.25)
    H   22          1S( 0.26)
    H   23          1S( 0.26)
    H   24          1S( 0.26)
    H   25          1S( 0.26)
    H   26          1S( 0.26)
    H   27          1S( 0.26)
***********************************************
```

HF= -11018.3947119\S2=56.066517\S2-1=0.\S2A=64.264611



TITLE

Fe	0.8333220009,1.0951092973,-1.3049939711
Fe	-1.9386555083,0.7032129559,0.5119336256
Ga	-0.7983613676,-1.1475784116,-1.6969479293
Fe	-3.0853913144,-1.5388053675,-0.104040651
Fe	3.0758288365,0.9778282152,0.1592697291
Ga	0.7910544595,1.3524510218,1.5535446837
Fe	1.5274868455,-0.9825411033,0.3513812791
Fe	-0.992675377,-1.4569253296,1.3027517057
O	2.6601377405,1.6657059679,-1.6463500817
O	-1.1308414555,1.7389102059,1.9734996195
O	0.7255070495,-0.2183900118,-2.7271131673
O	-2.6711388773,-2.4131370875,1.6098406372
O	-0.9510475938,0.694987285,-1.0828452069
O	-3.8511458748,0.2546081058,0.3148934741
O	3.4909648494,-0.9721656799,0.134443265
O	0.5730694934,-0.5004171187,1.920696815
O	0.5791477183,2.5837034399,-0.1600695184
O	-2.4931544569,-1.7570957759,-1.761579773
O	2.5557777976,1.7763619686,1.6566892791
O	0.0841393011,-2.0306965313,-0.2937402269
H	-3.2153740597,-2.2785424515,2.40231022
H	3.0863507886,1.383035095,-2.471881774
H	-1.3622081809,2.6840393779,1.955684077
H	1.5380409931,-0.6737562401,-3.0040328311
H	-4.4197960761,0.7313070045,-0.3111880653
H	4.0893563806,-1.420991221,0.7523584484

H 1.3754758877,3.1497923891,-0.1647736626
END

$Fe_8O_{12}H_8$

$$$$$$$$$$$$$ Fe8O12H8 NEUTRAL S = 1 head fe8o12h8_Oh_s_GF.out NOSYMM

UBPW91/6-311+G* scf=(VSHIFT=5,NoIncFock,Maxcycle=90,Tight,NoVarAcc) NOSYMM OPT=RFO IOP(5/13=1,5/36=1,8/11=1) INT=UltraFine GUESS=READ GEOM =CHECKPOINT

Charge = 0 Multiplicity = 1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	-0.092964	2.315265	-1.030820
2	26	0	-0.192669	1.571833	1.462393
3	26	0	-1.852728	0.416464	-1.009112
4	26	0	-2.049059	-0.274574	1.486310
5	26	0	2.035435	0.156142	-1.638626
6	26	0	1.911494	-0.613648	0.905764
7	26	0	0.200034	-1.565986	-1.438600
8	26	0	-0.070347	-2.389303	0.965508
9	8	0	1.453738	1.817775	-1.721867
10	8	0	1.315199	0.750557	1.849012
11	8	0	-1.135913	-0.681642	-2.175051
12	8	0	-1.326025	-1.783645	2.041461
13	8	0	-1.952901	2.303074	-1.715039
14	8	0	-1.829767	1.381330	2.582888
15	8	0	1.882710	-1.558999	-2.552053
16	8	0	1.791881	-2.408329	1.718519
17	8	0	-0.294988	3.361003	0.638884
18	8	0	-3.398169	0.334210	0.203036
19	8	0	3.450523	-0.281692	-0.288970
20	8	0	0.277779	-3.403299	-0.655999
21	1	0	-2.118143	2.403712	-2.667324
22	1	0	-1.734893	1.299812	3.546364
23	1	0	-1.102522	3.888507	0.751973
24	1	0	-3.913468	1.136185	0.387243

25	1	0	2.601888	-2.201096	-2.434736
26	1	0	1.887946	-2.471541	2.683514
27	1	0	4.076491	0.414203	-0.028110
28	1	0	1.079077	-3.952063	-0.669604

Distance matrix (angstroms):

		1	2	3	4	5
1	Fe	0.000000				
2	Fe	2.603602	0.000000			
3	Fe	2.588955	3.193589	0.000000		
4	Fe	4.107252	2.618392	2.596769	0.000000	
5	Fe	3.092139	4.072462	3.947387	5.160798	0.000000
6	Fe	4.043111	3.084423	4.347096	4.017211	2.661176
7	Fe	3.913597	4.291373	2.885897	3.909126	2.524764
8	Fe	5.110656	3.994052	3.866307	2.942553	4.206557
9	O	1.765596	3.593140	3.661203	5.190367	1.762477
10	O	3.567165	1.760010	4.279749	3.535630	3.610497
11	O	3.373197	4.381650	1.754729	3.795406	3.323715
12	O	5.268816	3.588740	3.797880	1.763028	5.348386
13	O	1.981834	3.705294	2.016846	4.111222	4.530119
14	O	4.116747	1.992960	3.719403	1.998146	5.853380
15	O	4.607317	5.497735	4.498513	5.780738	1.949201
16	O	5.781337	4.454855	5.357481	4.399961	4.231578
17	O	1.980478	1.972249	3.716552	4.124599	4.570455
18	O	4.046154	3.659635	1.965822	1.958956	5.739990
19	O	4.455427	4.446985	5.397267	5.779020	2.003932
20	O	5.742815	5.427785	4.387976	4.448886	4.089564
21	H	2.605248	4.631850	2.601782	4.942738	4.833425
22	H	4.967664	2.606796	4.641826	2.611745	6.512102
23	H	2.583147	2.588341	3.964759	4.332023	5.430680
24	H	4.242332	3.897446	2.591227	2.583449	6.360352
25	H	5.443412	6.101816	5.359816	6.381019	2.551712
26	H	6.374464	4.708393	5.997390	4.664758	5.060372
27	H	4.690824	4.667701	6.009826	6.347460	2.612713
28	H	6.386201	6.056086	5.272074	5.287450	4.327930

		6	7	8	9	10
6	Fe	0.000000				
7	Fe	3.054845	0.000000			
8	Fe	2.661618	2.555521	0.000000		
9	O	3.609127	3.619648	5.219609	0.000000	
10	O	1.762481	4.173530	3.543873	3.729520	0.000000
11	O	4.333905	1.763287	3.730234	3.627500	4.924655
12	O	3.624946	3.806186	1.761029	5.904231	3.665417
13	O	5.505399	4.436347	5.722564	3.441039	5.078705
14	O	4.559574	5.383227	4.464208	5.431648	3.290480
15	O	3.584831	2.017728	4.108172	3.503688	5.002549

16	O	1.973768	3.634682	2.008801	5.459904	3.197314
17	O	4.553859	5.369935	5.763954	3.318545	3.297202
18	O	5.439190	4.387799	4.367298	5.426529	5.009832
19	O	1.976409	3.679230	4.290951	3.232352	3.193135
20	O	3.590304	1.998557	1.943879	5.456975	4.960427
21	H	6.173280	4.758384	6.353261	3.741062	5.909149
22	H	4.891854	6.066844	4.800114	6.179798	3.533517
23	H	5.420087	6.020528	6.365680	4.116100	4.110426
24	H	6.104176	5.249413	5.247193	5.806876	5.442833
25	H	3.762390	2.676669	4.328732	4.240018	5.358948
26	H	2.571520	4.545425	2.606380	6.163939	3.377328
27	H	2.572122	4.575756	5.103253	3.423107	3.355809
28	H	3.784140	2.656583	2.537121	5.876960	5.339833

		11	12	13	14	15
11	O	0.000000				
12	O	4.362284	0.000000			
13	O	3.128516	5.586192	0.000000		
14	O	5.232138	3.250226	4.397380	0.000000	
15	O	3.166066	5.607746	5.507097	6.985388	0.000000
16	O	5.168492	3.196226	6.928927	5.312720	4.355157
17	O	4.996835	5.431175	3.067383	3.170773	6.255467
18	O	3.435849	3.486961	3.105517	3.036452	6.249996
19	O	4.975204	5.522878	6.157245	6.236559	3.034978
20	O	3.422494	3.531537	6.217732	6.150188	3.093909
21	H	3.275137	6.350911	0.971741	5.356599	5.632335
22	H	6.084367	3.455375	5.360636	0.971561	7.645296
23	H	5.427232	5.821172	3.053340	3.188585	7.035874
24	H	4.193407	4.237535	3.102426	3.036900	7.035564
25	H	4.043184	5.969850	6.446054	7.592753	0.971220
26	H	5.996091	3.348886	7.542964	5.355009	5.314501
27	H	5.742768	6.188767	6.539658	6.529666	3.882846
28	H	4.227080	4.223319	7.029407	6.890947	3.149000

		16	17	18	19	20
16	O	0.000000				
17	O	6.229433	0.000000			
18	O	6.062577	4.356739	0.000000		
19	O	3.362096	5.306504	6.893909	0.000000	
20	O	2.986772	6.910902	5.312204	4.466032	0.000000
21	H	7.594712	3.895037	3.763014	6.624047	6.596003
22	H	5.434102	3.843862	3.857035	6.640743	6.620419
23	H	6.997280	0.971165	4.266656	6.261337	7.553678
24	H	6.847400	4.255178	0.970891	7.529674	6.265925
25	H	4.236577	6.983980	7.027539	3.001434	3.163967
26	H	0.971823	6.554714	6.478273	4.009083	3.822716
27	H	4.029497	5.313976	7.478661	0.971676	5.421973
28	H	2.931609	7.555205	6.259343	4.386372	0.971290

```
             21        22        23        24        25
   21  H    0.000000
   22  H    6.322610  0.000000
   23  H    3.863637  3.861328  0.000000
   24  H    3.763004  3.840964  3.950914  0.000000
   25  H    6.598261  8.175426  7.807755  7.845437  0.000000
   26  H    8.273349  5.300243  7.288618  7.207284  5.174876
   27  H    7.021189  6.879924  6.285022  8.033257  3.847869
   28  H    7.389789  7.298972  8.261646  7.206434  2.915567
             26        27        28
   26  H    0.000000
   27  H    4.524395  0.000000
   28  H    3.753613  5.334819  0.000000
Alpha  occ. eigenvalues --   -0.21710  -0.21456  -0.20761  -0.20559  -0.20384
 Alpha  occ. eigenvalues --   -0.19796  -0.19094  -0.18789  -0.18550  -0.18303
 Alpha  occ. eigenvalues --   -0.16887
 Alpha virt. eigenvalues --   -0.14099  -0.13084  -0.12789  -0.12347  -0.12201
gap = 0.76 eV
  Beta  occ. eigenvalues --   -0.21901  -0.21308  -0.21081  -0.20666  -0.20031
  Beta  occ. eigenvalues --   -0.19943  -0.19149  -0.18943  -0.18436  -0.18236
  Beta  occ. eigenvalues --   -0.17187
  Beta virt. eigenvalues --   -0.14214  -0.13165  -0.12839  -0.12486  -0.12192
gap = 0.81 eV
Mulliken atomic spin densities:
             1
    1  Fe  -3.421523
    2  Fe  -3.412373
    3  Fe  -3.221681
    4  Fe  -3.312042
    5  Fe   3.418583
    6  Fe   3.446903
    7  Fe   3.172259
    8  Fe   3.312845
    9  O    0.004292
   10  O    0.037824
   11  O   -0.028728
   12  O    0.000849
   13  O   -0.156012
   14  O   -0.161113
   15  O    0.131991
   16  O    0.164263
   17  O   -0.131082
   18  O   -0.116822
   19  O    0.159529
   20  O    0.117573
   21  H   -0.010141
```

22 H -0.009010
23 H -0.017863
24 H -0.018197
25 H 0.016098
26 H 0.008853
27 H 0.007982
28 H 0.016742
Sum of Mulliken atomic spin densities = 0.00000
Dipole moment (field-independent basis, Debye):
X= 0.7094 Y= 0.7629 Z= 1.9415 Tot= 2.2033

Isotropic polarizability for W= 0.000000 289.10 Bohr**3.

Frequencies --	45.8531	48.9485	51.4099
Frequencies --	54.8871	55.3942	63.9533
Frequencies --	73.8749	76.8620	78.6030
Frequencies --	85.5670	88.1822	97.2591
Frequencies --	102.9972	108.3303	111.0251
Frequencies --	119.2866	122.3925	126.0991
Frequencies --	131.2521	135.2205	137.9561
Frequencies --	143.8544	146.3760	149.2788
Frequencies --	162.7245	162.9053	186.6221
Frequencies --	195.2047	202.5796	213.9531
Frequencies --	322.1594	329.8484	347.0734
Frequencies --	351.8909	359.8041	364.4767
Frequencies --	370.1204	378.8827	426.9910
Frequencies --	428.6270	433.9395	435.0720
Frequencies --	438.2143	446.5220	454.4997
Frequencies --	470.7248	499.0788	514.4310
Frequencies --	529.5843	532.0772	540.8048
Frequencies --	541.8064	553.0789	559.0779
Frequencies --	571.1445	575.0032	582.3636
Frequencies --	604.3234	644.5161	676.1958
Frequencies --	681.3067	685.7621	691.8727
Frequencies --	699.5464	701.8563	715.2285
Frequencies --	717.6907	722.9065	743.4894
Frequencies --	752.1038	3698.8269	3699.3791
Frequencies --	3700.4091	3701.0258	3701.2847
Frequencies --	3702.1524	3709.5537	3711.8248

Zero-point vibrational energy 325966.9 (Joules/Mol)
77.90795 (Kcal/Mol) 3.378 eV

Atom No Natural Electron Configuration

Fe	1	[core]4S(0.26)3d(6.45)4p(0.36)4d(0.03)
Fe	2	[core]4S(0.26)3d(6.43)4p(0.41)4d(0.03)
Fe	3	[core]4S(0.28)3d(6.46)4p(0.45)4d(0.03)
Fe	4	[core]4S(0.27)3d(6.48)4p(0.38)4d(0.03)
Fe	5	[core]4S(0.27)3d(6.44)4p(0.35)4d(0.03)
Fe	6	[core]4S(0.26)3d(6.42)4p(0.41)4d(0.03)
Fe	7	[core]4S(0.29)3d(6.49)4p(0.48)4d(0.03)
Fe	8	[core]4S(0.28)3d(6.47)4p(0.38)4d(0.03)
O	9	[core]2S(1.79)2p(4.98)3S(0.01)3p(0.02)
O	10	[core]2S(1.78)2p(4.94)3S(0.01)3p(0.02)
O	11	[core]2S(1.77)2p(4.90)3S(0.01)3p(0.02)
O	12	[core]2S(1.78)2p(4.95)3S(0.01)3p(0.02)
O	13	[core]2S(1.74)2p(5.21)3S(0.01)3p(0.01)
O	14	[core]2S(1.73)2p(5.21)3S(0.01)3p(0.01)
O	15	[core]2S(1.73)2p(5.19)3S(0.01)3p(0.01)
O	16	[core]2S(1.73)2p(5.20)3S(0.01)3p(0.01)
O	17	[core]2S(1.73)2p(5.20)3S(0.01)3p(0.01)
O	18	[core]2S(1.72)2p(5.20)3S(0.01)3p(0.01)
O	19	[core]2S(1.74)2p(5.20)3S(0.01)3p(0.01)
O	20	[core]2S(1.72)2p(5.20)3S(0.01)3p(0.01)
H	21	1S(0.52)
H	22	1S(0.52)
H	23	1S(0.51)
H	24	1S(0.51)
H	25	1S(0.52)
H	26	1S(0.52)
H	27	1S(0.52)
H	28	1S(0.52)

****

******* Alpha spin orbitals *******

****

Atom	No	Natural Electron Configuration
Fe	1	[core]3d(1.62)4p(0.18)5S(0.11)4d(0.01)
Fe	2	[core]3d(1.61)4p(0.21)5S(0.13)4d(0.01)
Fe	3	[core]3d(1.66)4p(0.23)5S(0.13)4d(0.01)
Fe	4	[core]3d(1.67)4p(0.19)5S(0.12)4d(0.01)
Fe	5	[core]3d(4.82)4p(0.18)5S(0.15)4d(0.02)
Fe	6	[core]3d(4.83)4p(0.20)5S(0.13)4d(0.02)
Fe	7	[core]3d(4.80)4p(0.24)5S(0.15)4d(0.02)
Fe	8	[core]3d(4.80)4p(0.19)5S(0.16)4d(0.01)
O	9	[core]2S(0.89)2p(2.49)4S(0.01)4p(0.01)
O	10	[core]2S(0.89)2p(2.49)4S(0.01)4p(0.01)

O	11	[core]2S(0.89)2p(2.44)4S(0.01)4p(0.01)
O	12	[core]2S(0.89)2p(2.48)4p(0.01)
O	13	[core]2S(0.86)2p(2.50)
O	14	[core]2S(0.85)2p(2.50)
O	15	[core]2S(0.88)2p(2.68)3p(0.01)
O	16	[core]2S(0.88)2p(2.70)4p(0.01)
O	17	[core]2S(0.85)2p(2.51)
O	18	[core]2S(0.85)2p(2.53)
O	19	[core]2S(0.88)2p(2.70)4S(0.01)
O	20	[core]2S(0.87)2p(2.67)3p(0.01)
H	21	1S(0.26)
H	22	1S(0.26)
H	23	1S(0.25)
H	24	1S(0.25)
H	25	1S(0.26)
H	26	1S(0.26)
H	27	1S(0.26)
H	28	1S(0.26)

****

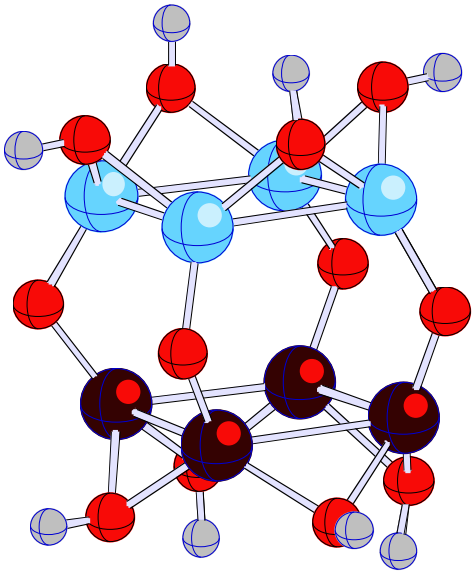
******* Beta spin orbitals *******

****

Atom	No	Natural Electron Configuration
Fe	1	[core]3d(4.83)4p(0.18)5S(0.15)4d(0.01)
Fe	2	[core]3d(4.82)4p(0.20)5S(0.14)4d(0.02)
Fe	3	[core]3d(4.80)4p(0.22)5S(0.15)4d(0.02)
Fe	4	[core]3d(4.81)4p(0.19)5S(0.15)4d(0.01)
Fe	5	[core]3d(1.62)4p(0.17)5S(0.11)4d(0.01)
Fe	6	[core]3d(1.59)4p(0.21)5S(0.12)4d(0.01)
Fe	7	[core]3d(1.69)4p(0.24)5S(0.14)4d(0.01)
Fe	8	[core]3d(1.67)4p(0.19)5S(0.12)4d(0.01)
O	9	[core]2S(0.89)2p(2.49)4S(0.01)4p(0.01)
O	10	[core]2S(0.89)2p(2.45)4S(0.01)4p(0.01)
O	11	[core]2S(0.89)2p(2.46)4S(0.01)4p(0.01)
O	12	[core]2S(0.89)2p(2.48)4p(0.01)
O	13	[core]2S(0.88)2p(2.70)4p(0.01)
O	14	[core]2S(0.88)2p(2.70)4p(0.01)
O	15	[core]2S(0.85)2p(2.51)
O	16	[core]2S(0.85)2p(2.50)
O	17	[core]2S(0.88)2p(2.69)
O	18	[core]2S(0.87)2p(2.68)3p(0.01)
O	19	[core]2S(0.86)2p(2.50)
O	20	[core]2S(0.85)2p(2.52)
H	21	1S(0.26)
H	22	1S(0.26)

H	23	1S(0.26)
H	24	1S(0.26)
H	25	1S(0.26)
H	26	1S(0.26)
H	27	1S(0.26)
H	28	1S(0.25)

HF= -11019.021259 4\S2=14.414356\S2-1=0.\S2A=44.80097



TITLE
Ga -0.0929643585,2.3152654532,-1.0308204817
Ga -0.1926688029,1.5718332205,1.4623929078
Ga -1.8527279082,0.4164635573,-1.0091121372
Ga -2.0490590392,-0.2745735361,1.4863097857
Fe 2.0354350068,0.1561421052,-1.6386262267
Fe 1.9114940215,-0.6136477778,0.9057635453
Fe 0.2000344627,-1.5659860321,-1.4385995586
Fe -0.0703467615,-2.3893027266,0.9655079584
O 1.453738065,1.8177748888,-1.7218669927
O 1.3151988398,0.7505569669,1.8490116047
O -1.1359128787,-0.6816420656,-2.1750511217
O -1.3260250387,-1.7836453334,2.0414606322
O -1.9529005963,2.3030743358,-1.7150389175
O -1.829767086,1.3813300462,2.582887915
O 1.8827104122,-1.5589992477,-2.5520533323
O 1.7918814849,-2.4083293102,1.7185185803
O -0.2949879006,3.361002991,0.638883724
O -3.3981693147,0.3342100144,0.203035783

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 O    3.4505225756,-0.281691912,-0.2889702996
 O    0.2777787224,-3.4032993221,-0.6559986678
 H    -2.118142837,2.4037123494,-2.6673241281
 H    -1.734892836,1.2998120915,3.5463636139
 H    -1.1025221359,3.8885070314,0.7519727795
 H    -3.9134679278,1.1361850193,0.3872433933
 H    2.6018882696,-2.2010962089,-2.4347363342
 H    1.887945625,-2.4715407359,2.683513645
 H    4.076491244,0.4142032349,-0.0281100056
 H    1.0790766926,-3.9520630972,-0.6696036644
END
```

$Fe_8O_{12}H_9$

```
$$$$$$$$$$$$$  Fe8O12H9    NEUTRAL    S = 6   head
fe8o12h9_Oh_8_GF.out
---------------------------------------------------------------------
# UBPW91/6-311+G*
scf=(VSHIFT=5,NoIncFock,Maxcycle=90,Tight,NoVarAcc)
 NOSYMM OPT=RFO IOP(5/13=1,5/36=1,8/11=1) INT=UltraFine
GUESS=READ GEOM
 =CHECKPOINT
 ---------------------------------------------------------------------
 Charge =  0 Multiplicity = 6
                    Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic           Coordinates (Angstroms)
 Number     Number       Type             X           Y           Z
 ---------------------------------------------------------------------
     1         26          0        0.168420    2.052359   -0.899334
     2         26          0       -0.209392    1.618263    1.798224
     3         26          0       -1.265220   -0.006924   -0.742703
     4         26          0       -1.965707   -0.269111    1.824505
     5         26          0        2.111403    0.356173   -1.641269
     6         26          0        1.166565   -0.121403    0.616531
     7         26          0        0.534138   -1.663487   -1.704029
     8         26          0       -0.425470   -2.220194    0.768682
     9          8          0        1.338408    1.855719   -2.204849
    10          8          0        1.504900    0.928876    2.356531
```

11	8	0	-0.998679	-0.941253	-2.214720
12	8	0	-1.545682	-1.978626	2.105813
13	8	0	-1.734766	1.903044	-1.437952
14	8	0	-1.748544	1.263672	3.006233
15	8	0	2.222029	-1.349315	-2.654304
16	8	0	1.411261	-1.873749	1.468157
17	8	0	-0.202654	3.206133	0.664901
18	8	0	-3.019658	0.060814	0.233038
19	8	0	3.099270	0.256871	0.036433
20	8	0	0.237876	-3.347718	-0.679814
21	1	0	-1.904704	1.883601	-2.395836
22	1	0	-1.624478	1.191399	3.965908
23	1	0	-1.039494	3.687922	0.544850
24	1	0	-3.388906	0.942777	0.041915
25	1	0	2.298107	-1.386623	-3.620812
26	1	0	1.465435	-1.729090	2.430961
27	1	0	3.691686	-0.495738	0.204132
28	1	0	1.032393	-3.837524	-0.404378
29	1	0	2.324990	1.450238	2.314777

Distance matrix (angstroms):

		1	2	3	4	5
1	Fe	0.000000				
2	Fe	2.758261	0.000000			
3	Fe	2.514061	3.195671	0.000000		
4	Fe	4.166896	2.578277	2.673945	0.000000	
5	Fe	2.683785	4.336943	3.512954	5.387522	0.000000
6	Fe	2.831852	2.513184	2.788226	3.360379	2.493684
7	Fe	3.819529	4.856799	2.627935	4.543574	2.563344
8	Fe	4.624900	3.980000	2.808564	2.700707	4.345257
9	O	1.764060	4.298450	3.519402	5.627413	1.778703
10	O	3.694463	1.930223	4.260814	3.709898	4.083900
11	O	3.471898	4.824709	1.763761	4.207406	3.418299
12	O	5.312052	3.849402	3.475674	1.782694	5.732903
13	O	1.983562	3.588969	2.086102	3.926222	4.150562
14	O	4.421564	1.988468	3.987798	1.947579	6.109175
15	O	4.343802	5.877358	4.197278	6.226051	1.986748
16	O	4.750157	3.863885	3.941635	3.755763	3.889894
17	O	1.978818	1.950845	3.665260	4.065755	4.335384
18	O	3.925858	3.573940	2.008659	1.937120	5.470654
19	O	3.562207	3.988050	4.441330	5.397022	1.949468
20	O	5.404983	5.567916	3.663899	4.539297	4.260669
21	H	2.562389	4.531515	2.591500	4.738056	4.362514
22	H	5.256074	2.623649	4.871966	2.614408	6.789318
23	H	2.493951	2.558027	3.919264	4.260692	5.080140
24	H	3.843396	3.694619	2.455117	2.582982	5.781922

25	H	4.875305	6.684522	4.783762	7.005742	2.644009
26	H	5.203122	3.796074	4.527083	3.777839	4.620460
27	H	4.485961	4.714716	5.070144	5.889233	2.574597
28	H	5.973454	6.013244	4.479619	5.166246	4.503471
29	H	3.917124	2.591940	4.935698	4.648291	4.110097

		6	7	8	9	10
6	Fe	0.000000				
7	Fe	2.857095	0.000000			
8	Fe	2.638683	2.710180	0.000000		
9	O	3.449454	3.644515	5.344738	0.000000	
10	O	2.060378	4.914354	4.020478	4.657569	0.000000
11	O	3.657379	1.769733	3.296202	3.644877	5.537295
12	O	3.608812	4.351995	1.761008	6.449961	4.221669
13	O	4.091088	4.235430	4.856396	3.167770	5.083555
14	O	4.015839	5.997122	4.346778	6.085653	3.334532
15	O	3.649676	1.962321	4.414128	3.354853	5.550937
16	O	1.963634	3.297927	1.995713	5.234999	2.941545
17	O	3.598555	5.465153	5.431891	3.526181	3.311080
18	O	4.207699	4.399422	3.495672	5.306385	5.072907
19	O	2.053035	3.646489	4.369878	3.268073	2.894211
20	O	3.598900	1.993344	1.951789	5.532871	5.395739
21	H	4.746271	4.359860	5.389197	3.248850	5.926373
22	H	4.553207	6.705086	4.826887	6.877373	3.528742
23	H	4.402589	6.014263	5.944154	4.070901	4.167548
24	H	4.713277	5.023068	4.394830	5.313089	5.413592
25	H	4.564674	2.619598	5.232626	3.665891	6.459051
26	H	2.442568	4.239076	2.565127	5.861547	2.659301
27	H	2.585815	3.869732	4.499272	4.107367	3.382955
28	H	3.856140	2.581431	2.473296	5.978993	5.528513
29	H	2.587672	5.390106	4.840198	4.643789	0.972682

		11	12	13	14	15
11	O	0.000000				
12	O	4.476870	0.000000			
13	O	3.038951	5.259409	0.000000		
14	O	5.716847	3.371114	4.489962	0.000000	
15	O	3.276081	6.103311	5.264369	7.391538	0.000000
16	O	4.498993	3.026734	5.710264	4.710993	4.234036
17	O	5.111427	5.546321	2.909879	3.412442	6.135822
18	O	3.328666	3.136751	2.799458	3.279209	6.148211
19	O	4.826631	5.554760	5.315223	5.773617	3.254143
20	O	3.110639	3.579834	5.660087	6.228782	3.439344
21	H	2.972118	5.942267	0.973037	5.439765	5.248664
22	H	6.568104	3.676305	5.451633	0.970357	8.067097
23	H	5.389449	5.899373	2.756936	3.526775	6.800432
24	H	3.788821	4.023897	2.418325	3.403078	6.633693
25	H	3.611681	6.922385	5.643655	8.204704	0.970215

26	H	5.317415	3.038885	6.196949	4.429134	5.155249
27	H	5.296117	5.765881	6.156052	6.367370	3.325529
28	H	3.973786	4.050066	6.455971	6.737068	3.559296
29	H	6.105928	5.175219	5.547037	4.136013	5.704372

		16	17	18	19	20
16	O	0.000000				
17	O	5.390282	0.000000			
18	O	4.990100	4.244414	0.000000		
19	O	3.072254	4.471668	6.125224	0.000000	
20	O	2.857131	6.704870	4.802387	4.657643	0.000000
21	H	6.328013	3.743552	3.387721	5.796718	5.907798
22	H	4.984937	4.120362	4.142351	6.215135	6.756824
23	H	6.147428	0.973054	4.144176	5.399997	7.254771
24	H	5.745310	3.957663	0.975054	6.524333	5.664167
25	H	5.188583	6.761253	6.725017	4.088811	4.091443
26	H	0.975117	5.500720	5.305722	3.513861	3.715344
27	H	2.949070	5.392777	6.734444	0.972369	4.565518
28	H	2.739770	7.230616	5.658839	4.607642	0.973156
29	H	3.549727	3.492025	5.901644	2.685979	6.028599

		21	22	23	24	25
21	H	0.000000				
22	H	6.405424	0.000000			
23	H	3.556937	4.275333	0.000000		
24	H	3.005102	4.309610	3.648082	0.000000	
25	H	5.464297	8.921389	7.365007	7.154285	0.000000
26	H	6.907051	4.520274	6.259082	6.034157	6.118381
27	H	6.613673	6.727480	6.324806	7.227063	4.167245
28	H	6.732289	7.172756	7.862957	6.526741	4.237262
29	H	6.345707	4.288535	4.411306	6.170254	6.578732

		26	27	28	29
26	H	0.000000			
27	H	3.381734	0.000000		
28	H	3.559799	4.313891	0.000000	
29	H	3.295522	3.179545	6.084821	0.000000

Alpha occ. eigenvalues -- -0.21148 -0.21089 -0.20548 -0.20380 -0.19978
Alpha occ. eigenvalues -- -0.19785 -0.19363 -0.18828 -0.18281 -0.16527
Alpha virt. eigenvalues -- -0.14044 -0.13850 -0.13335 -0.12859 -0.12715
gap = 0.68 eV
Beta occ. eigenvalues -- -0.20536 -0.19826 -0.19738 -0.19009 -0.18201
Beta occ. eigenvalues -- -0.17558 -0.17023 -0.16128
Beta virt. eigenvalues -- -0.14558 -0.13981 -0.13741 -0.13151 -0.12928
gap = 0.43 eV
Mulliken atomic spin densities:

		1
1	Fe	-3.286043
2	Fe	3.471707

3	Fe	-3.263359
4	Fe	3.410140
5	Fe	3.344280
6	Fe	3.021764
7	Fe	3.231376
8	Fe	-3.299162
9	O	-0.080628
10	O	0.200096
11	O	-0.066205
12	O	-0.008020
13	O	-0.170539
14	O	0.162532
15	O	0.163504
16	O	-0.022438
17	O	0.009444
18	O	0.024561
19	O	0.139159
20	O	-0.022067
21	H	-0.011181
22	H	0.009313
23	H	-0.000056
24	H	0.009296
25	H	0.005710
26	H	-0.000533
27	H	0.015240
28	H	0.005276
29	H	0.006833

Sum of Mulliken atomic spin densities = 7.00000

Dipole moment (field-independent basis, Debye):
X= 1.5862 Y= 1.1378 Z= 1.8488 Tot= 2.6886

Isotropic polarizability for W= 0.000000 292.80 Bohr**3. 1,496 A**3

Frequencies --	33.2881	52.3536	56.7053
Frequencies --	68.0998	71.7189	76.0648
Frequencies --	86.7656	92.5856	96.8397
Frequencies --	103.9302	105.8144	109.1432
Frequencies --	115.7804	118.4237	121.7590
Frequencies --	130.0599	130.9277	137.6031
Frequencies --	141.9476	144.3323	149.3753
Frequencies --	152.3571	154.2472	164.0759
Frequencies --	169.9198	177.4958	186.5896

Frequencies -- 202.9739 205.3460 215.8842
Frequencies -- 274.1807 291.8749 330.0461
Frequencies -- 356.5516 357.1909 359.2388
Frequencies -- 365.5587 376.8094 384.2094
Frequencies -- 407.2673 427.7595 447.6602
Frequencies -- 448.8196 452.1594 461.4895
Frequencies -- 464.3237 479.5418 484.9096
Frequencies -- 528.4078 535.3527 557.7879
Frequencies -- 563.0945 579.4354 585.9709
Frequencies -- 595.7063 602.4077 607.7235
Frequencies -- 610.9006 627.9786 639.0016
Frequencies -- 643.1626 643.6986 657.0465
Frequencies -- 659.6972 688.7087 691.5277
Frequencies -- 696.9490 698.0112 711.1289
Frequencies -- 731.6332 737.1272 743.2670
Frequencies -- 3649.1888 3654.9649 3683.9736
Frequencies -- 3686.5861 3688.2822 3689.2445
Frequencies -- 3690.9010 3717.1199 3717.9815
Zero-point vibrational energy 355625.7 (Joules/Mol)
84.99657 (Kcal/Mol) 3.686 eV

Atom	No	Natural Electron Configuration
Fe	1	[core]4S(0.27)3d(6.46)4p(0.44)4d(0.03)
Fe	2	[core]4S(0.25)3d(6.48)4p(0.40)4d(0.03)
Fe	3	[core]4S(0.32)3d(6.56)4p(0.62)4d(0.04)5p(0.01)
Fe	4	[core]4S(0.25)3d(6.45)4p(0.40)4d(0.03)
Fe	5	[core]4S(0.24)3d(6.48)4p(0.40)4d(0.03)
Fe	6	[core]4S(0.35)3d(6.66)4p(0.69)4d(0.04)5p(0.01)
Fe	7	[core]4S(0.25)3d(6.52)4p(0.42)4d(0.03)
Fe	8	[core]4S(0.28)3d(6.45)4p(0.42)4d(0.03)
O	9	[core]2S(1.78)2p(4.88)3S(0.01)3p(0.01)
O	10	[core]2S(1.71)2p(5.17)3S(0.01)3p(0.01)
O	11	[core]2S(1.76)2p(4.81)3S(0.01)3p(0.02)
O	12	[core]2S(1.78)2p(4.89)3S(0.01)3p(0.02)
O	13	[core]2S(1.73)2p(5.16)3S(0.01)3p(0.01)
O	14	[core]2S(1.72)2p(5.21)3S(0.01)3p(0.01)
O	15	[core]2S(1.72)2p(5.20)3S(0.01)3p(0.01)
O	16	[core]2S(1.71)2p(5.11)3S(0.01)3p(0.01)
O	17	[core]2S(1.72)2p(5.17)3S(0.01)3p(0.01)
O	18	[core]2S(1.72)2p(5.12)3S(0.01)3p(0.01)
O	19	[core]2S(1.71)2p(5.17)3S(0.01)3p(0.01)
O	20	[core]2S(1.73)2p(5.16)3S(0.01)3p(0.01)
H	21	1S(0.52)
H	22	1S(0.51)
H	23	1S(0.51)

H	24	1S(0.51)
H	25	1S(0.51)
H	26	1S(0.51)
H	27	1S(0.52)
H	28	1S(0.51)
H	29	1S(0.51)

****
******* Alpha spin orbitals *******
****

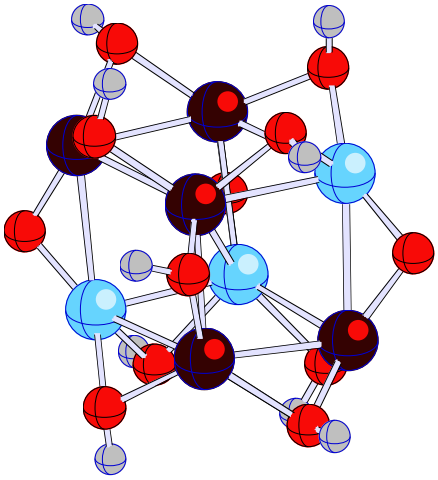
Atom	No	Natural Electron Configuration
Fe	1	[core]3d(1.69)4p(0.21)5S(0.12)4d(0.01)5d(0.01)
Fe	2	[core]3d(4.87)4p(0.21)5S(0.13)4d(0.01)
Fe	3	[core]3d(1.84)4p(0.30)5S(0.16)4d(0.02)
Fe	4	[core]3d(4.80)4p(0.20)5S(0.13)4d(0.01)
Fe	5	[core]3d(4.80)4p(0.21)5S(0.14)4d(0.01)5d(0.01)
Fe	6	[core]3d(4.75)4p(0.34)5S(0.18)4d(0.02)5d(0.01)
Fe	7	[core]3d(4.76)4p(0.21)5S(0.13)4d(0.01)
Fe	8	[core]3d(1.70)4p(0.20)5S(0.13)4d(0.02)
O	9	[core]2S(0.89)2p(2.41)
O	10	[core]2S(0.87)2p(2.69)4p(0.01)
O	11	[core]2S(0.88)2p(2.38)4p(0.01)
O	12	[core]2S(0.89)2p(2.44)
O	13	[core]2S(0.85)2p(2.48)
O	14	[core]2S(0.87)2p(2.70)3p(0.01)4S(0.01)
O	15	[core]2S(0.87)2p(2.70)3p(0.01)
O	16	[core]2S(0.86)2p(2.54)4p(0.01)
O	17	[core]2S(0.86)2p(2.60)
O	18	[core]2S(0.86)2p(2.58)
O	19	[core]2S(0.87)2p(2.67)3p(0.01)
O	20	[core]2S(0.86)2p(2.58)
H	21	1S(0.26)
H	22	1S(0.26)
H	23	1S(0.25)
H	24	1S(0.26)
H	25	1S(0.26)
H	26	1S(0.26)
H	27	1S(0.26)
H	28	1S(0.25)
H	29	1S(0.26)

NBO analysis skipped by request.

****
******* Beta spin orbitals *******
****

Atom	No	Natural Electron Configuration
Fe	1	[core]3d(4.76)4p(0.23)5S(0.15)4d(0.01)
Fe	2	[core]3d(1.62)4p(0.19)5S(0.12)4d(0.01)
Fe	3	[core]3d(4.72)4p(0.32)5S(0.16)4d(0.02)
Fe	4	[core]3d(1.64)4p(0.19)5S(0.11)4d(0.01)
Fe	5	[core]3d(1.68)4p(0.19)5S(0.11)4d(0.01)5d(0.01)
Fe	6	[core]3d(1.91)4p(0.34)5S(0.17)4d(0.01)
Fe	7	[core]3d(1.76)4p(0.21)5S(0.12)4d(0.01)
Fe	8	[core]3d(4.75)4p(0.21)5S(0.14)4d(0.01)
O	9	[core]2S(0.89)2p(2.47)4p(0.01)
O	10	[core]2S(0.84)2p(2.48)
O	11	[core]2S(0.88)2p(2.44)4S(0.01)4p(0.01)
O	12	[core]2S(0.89)2p(2.44)4p(0.01)
O	13	[core]2S(0.88)2p(2.69)3p(0.01)
O	14	[core]2S(0.85)2p(2.50)
O	15	[core]2S(0.85)2p(2.51)
O	16	[core]2S(0.86)2p(2.58)4p(0.01)
O	17	[core]2S(0.86)2p(2.58)
O	18	[core]2S(0.86)2p(2.55)
O	19	[core]2S(0.84)2p(2.50)
O	20	[core]2S(0.86)2p(2.59)
H	21	1S(0.26)
H	22	1S(0.25)
H	23	1S(0.25)
H	24	1S(0.25)
H	25	1S(0.25)
H	26	1S(0.26)
H	27	1S(0.25)
H	28	1S(0.26)
H	29	1S(0.25)

HF= -11019.5975525\S2=26.019094\S2-1=0.\S2A=55.006638



TITLE

Ga	0.1684195841,2.0523591522,-0.8993344838
Fe	-0.2093923657,1.61826276,1.7982240583
Ga	-1.265220176,-0.0069235994,-0.7427029512
Fe	-1.9657069419,-0.2691110781,1.8245052507
Fe	2.1114034762,0.3561726462,-1.6412685748
Fe	1.1665647896,-0.1214032613,0.6165314228
Fe	0.5341380361,-1.6634874371,-1.7040292859
Ga	-0.4254704133,-2.2201942475,0.7686822158
O	1.3384078538,1.8557192403,-2.204849489
O	1.5049003906,0.9288763924,2.3565309086
O	-0.9986785126,-0.9412531924,-2.2147204264
O	-1.5456824941,-1.9786262843,2.1058127388
O	-1.734765671,1.9030439339,-1.4379515245
O	-1.7485439834,1.2636724384,3.0062325445
O	2.2220293944,-1.3493147791,-2.654304235
O	1.4112606301,-1.8737489327,1.4681569576
O	-0.2026535055,3.2061328928,0.6649009889
O	-3.0196582252,0.0608143463,0.2330376179
O	3.0992695468,0.2568705261,0.0364332427
O	0.2378759618,-3.3477176928,-0.6798144287
H	-1.9047036096,1.8836010696,-2.3958364662
H	-1.6244777778,1.1913986726,3.9659077988
H	-1.0394935499,3.6879222009,0.5448504391
H	-3.3889062362,0.9427774456,0.0419149125
H	2.2981066484,-1.3866229002,-3.6208117714
H	1.4654351806,-1.7290903128,2.430961339
H	3.691686483,-0.4957383722,0.2041317032
H	1.0323930824,-3.8375240773,-0.4043782218
H	2.3249904042,1.4502384499,2.31477672

END

$Fe_8O_{12}H_{10}$

$$$$$$$$$$$$$ Fe8O12H10 NEUTRAL S = 1 head fe8o12h10_Oh_s_GF.out

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 # UBPW91/6-311+G* scf=(VSHIFT=5,NoIncFock,Maxcycle=90,Tight,NoVarAcc) NOSYMM OPT=RFO IOP(5/13=1,5/36=1,8/11=1) INT=UltraFine GUESS=READ GEOM=CHECKPOINT

Charge = 0 Multiplicity = 1

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	0.192555	2.205597	-0.833254
2	26	0	-0.375737	1.624876	1.699566
3	26	0	-1.193890	0.173995	-0.589625
4	26	0	-1.931240	-0.482529	1.666304
5	26	0	2.056276	0.388892	-1.669716
6	26	0	1.332659	-0.114272	0.636384
7	26	0	0.446715	-1.682110	-1.623579
8	26	0	0.073649	-2.204502	0.962594
9	8	0	1.529729	2.056850	-1.991952
10	8	0	1.380010	1.049232	2.274150
11	8	0	-1.274379	-1.010310	-2.199386
12	8	0	-1.359131	-2.128445	2.023238
13	8	0	-1.656640	1.983075	-1.467309
14	8	0	-1.940212	1.156239	2.788538
15	8	0	1.948079	-1.232299	-2.795893
16	8	0	1.881681	-1.850102	1.609305
17	8	0	-0.208842	3.334914	0.757263
18	8	0	-3.067208	-0.071020	0.122421
19	8	0	3.198152	0.050389	-0.108032
20	8	0	0.418002	-3.360965	-0.615397
21	1	0	-1.802619	1.852881	-2.420500
22	1	0	-1.879691	1.122285	3.756580
23	1	0	-0.971169	3.929329	0.661670
24	1	0	-3.612056	0.733910	0.103402
25	1	0	2.691817	-1.825869	-2.982086

26	1	0	1.994923	-1.628933	2.549902
27	1	0	3.695475	-0.774910	0.025332
28	1	0	-0.143387	-4.114551	-0.856121
29	1	0	2.084619	1.720938	2.279298
30	1	0	-2.050760	-1.596211	-2.203992

Distance matrix (angstroms):

		1	2	3	4	5
1	Fe	0.000000				
2	Fe	2.659956	0.000000			
3	Fe	2.471638	2.831046	0.000000		
4	Fe	4.240792	2.619514	2.462503	0.000000	
5	Fe	2.733779	4.335252	3.431670	5.271498	0.000000
6	Fe	2.973460	2.659625	2.823055	3.442293	2.468785
7	Fe	3.975359	4.759819	2.684356	4.232847	2.623332
8	Fe	4.763211	3.925456	3.110190	2.734955	4.193514
9	O	1.775596	4.176685	3.595798	5.639999	1.778531
10	O	3.521816	1.934983	3.948697	3.698669	4.055548
11	O	3.789495	4.790990	2.000097	3.956460	3.651244
12	O	5.417674	3.893488	3.486486	1.778694	5.624936
13	O	1.967502	3.434838	2.063308	3.996765	4.045756
14	O	4.332115	1.962922	3.596357	1.986215	6.036288
15	O	4.330467	5.811429	4.088673	5.960073	1.976926
16	O	5.026722	4.144822	4.288519	4.051157	3.974363
17	O	1.991537	1.959597	3.574331	4.285544	4.438473
18	O	4.089298	3.550700	2.019001	1.960443	5.447327
19	O	3.768884	4.303383	4.420095	5.453709	1.964007
20	O	5.575383	5.554069	3.885202	4.360102	4.225749
21	H	2.573807	4.366111	2.557600	4.708784	4.194999
22	H	5.151149	2.597264	4.501008	2.635781	6.743471
23	H	2.561309	2.596588	3.964578	4.625529	5.209173
24	H	4.185482	3.716897	2.577076	2.597601	5.949200
25	H	5.207352	6.575362	4.982172	6.692141	2.651677
26	H	5.421983	4.114653	4.824490	4.184465	4.677666
27	H	4.678786	5.013661	5.018414	5.868407	2.629562
28	H	6.329111	6.287014	4.423369	4.769762	5.077544
29	H	3.674613	2.529559	4.623026	4.621488	4.167717
30	H	4.622243	5.330934	2.544412	4.029114	4.592802

		6	7	8	9	10
6	Fe	0.000000				
7	Fe	2.889714	0.000000			
8	Fe	2.461824	2.664651	0.000000		
9	O	3.414785	3.910044	5.385966	0.000000	
10	O	2.009543	4.850110	3.743467	4.386038	0.000000
11	O	3.954885	1.935208	3.638872	4.160952	5.594642
12	O	3.636755	4.093845	1.784266	6.479502	4.202795

13	O	4.214297	4.228724	5.141413	3.230115	4.908342
14	O	4.117966	5.763716	4.322532	5.975338	3.361535
15	O	3.661864	1.957229	4.311020	3.411720	5.588686
16	O	2.064244	3.541030	1.952643	5.325147	3.016592
17	O	3.779911	5.591843	5.550414	3.494891	3.170133
18	O	4.429995	4.241672	3.888781	5.489101	5.065833
19	O	2.015276	3.587317	3.999162	3.218490	3.158817
20	O	3.597855	1.958522	1.986465	5.699435	5.359550
21	H	4.800438	4.265062	5.606074	3.365977	5.728414
22	H	4.645846	6.497916	4.763339	6.748568	3.581702
23	H	4.653920	6.222621	6.229452	4.099070	4.052542
24	H	5.045165	5.029239	4.791336	5.707769	5.452734
25	H	4.227316	2.628058	4.749597	4.172088	6.133112
26	H	2.528704	4.451710	2.557757	5.867694	2.761653
27	H	2.528384	3.754512	4.004974	4.096188	3.707567
28	H	4.517578	2.618010	2.646341	6.494275	6.227679
29	H	2.575385	5.431015	4.602911	4.320221	0.973493
30	H	4.659549	2.565471	3.861398	5.119542	6.230755

		11	12	13	14	15
11	O	0.000000				
12	O	4.368976	0.000000			
13	O	3.105224	5.401576	0.000000		
14	O	5.478745	3.422352	4.344686	0.000000	
15	O	3.284712	5.913098	5.009767	7.211781	0.000000
16	O	5.017179	3.278974	6.056279	5.003552	4.448804
17	O	5.362660	5.724871	2.978642	3.445337	6.175489
18	O	3.080144	3.280797	2.955715	3.143957	5.917620
19	O	5.049988	5.482559	5.399252	6.001317	3.229948
20	O	3.301325	3.411700	5.795572	6.128056	3.409827
21	H	2.919897	5.982846	0.973054	5.257216	4.871036
22	H	6.355147	3.720579	5.299030	0.970526	7.945488
23	H	5.716433	6.221014	2.964848	3.626657	6.864339
24	H	3.716164	4.117587	2.801999	3.191141	6.571681
25	H	4.124132	6.446316	5.975925	7.978017	0.969608
26	H	5.798859	3.431700	6.520621	4.826947	5.360693
27	H	5.450158	5.601136	6.203192	6.567009	3.349911
28	H	3.566484	3.703155	6.312252	6.655324	4.055160
29	H	6.229060	5.171338	5.301207	4.096031	5.873484
30	H	0.972661	4.316375	3.675502	5.702065	4.058755

		16	17	18	19	20
16	O	0.000000				
17	O	5.655144	0.000000			
18	O	5.465113	4.491512	0.000000		
19	O	2.879967	4.810869	6.270773	0.000000	
20	O	3.061758	6.863813	4.849206	4.429897	0.000000
21	H	6.597384	3.851588	3.430310	5.796913	5.947583

22	H	5.252979	4.084527	4.005158	6.470601	6.670315
23	H	6.514490	0.971395	4.548293	5.746465	7.530543
24	H	6.255079	4.332970	0.972180	6.847689	5.790168
25	H	4.662380	7.002160	6.773760	3.469424	3.623254
26	H	0.972862	5.719258	5.826228	3.366377	3.937732
27	H	2.637206	5.715774	6.799910	0.972745	4.223747
28	H	3.912411	7.622455	5.084920	5.391868	0.970050
29	H	3.639011	3.190842	5.865540	3.119301	6.081333
30	H	5.483593	6.039676	2.961683	5.886885	3.425314

		21	22	23	24	25
21	H	0.000000				
22	H	6.220613	0.000000			
23	H	3.808243	4.275906	0.000000		
24	H	3.300945	4.061728	4.182900	0.000000	
25	H	5.835113	8.660249	7.734127	7.470711	0.000000
26	H	7.158859	4.902847	6.577036	6.557943	5.579188
27	H	6.566310	6.971659	6.656752	7.462081	3.340121
28	H	6.388316	7.191398	8.227570	6.038205	4.218551
29	H	6.100502	4.272762	4.102627	6.177448	6.374221
30	H	3.464778	6.553465	6.317367	3.631965	4.811467

		26	27	28	29	30
26	H	0.000000				
27	H	3.161437	0.000000			
28	H	4.727754	5.164012	0.000000		
29	H	3.361980	3.728871	6.989120	0.000000	
30	H	6.242446	6.218009	3.434656	6.942962	0.000000

Alpha occ. eigenvalues -- -0.21586 -0.21009 -0.20622 -0.20370 -0.19852
Alpha occ. eigenvalues -- -0.19418 -0.18546 -0.18291 -0.17808 -0.17399
Alpha occ. eigenvalues -- -0.17031 -0.16308
Alpha virt. eigenvalues -- -0.13117 -0.12987 -0.12639 -0.12385 -0.12081
gap = 0.87 eV
Beta occ. eigenvalues -- -0.21650 -0.20846 -0.20575 -0.20246 -0.19917
Beta occ. eigenvalues -- -0.19250 -0.18637 -0.18415 -0.17794 -0.17244
Beta occ. eigenvalues -- -0.17083 -0.16622
Beta virt. eigenvalues -- -0.13249 -0.13072 -0.12427 -0.12332 -0.12255
0.92 eV
Mulliken atomic spin densities:

		1
1	Fe	3.362670
2	Fe	3.372158
3	Fe	3.282168
4	Fe	3.424147
5	Fe	-3.406061
6	Fe	-3.244334
7	Fe	-3.388736
8	Fe	-3.407812

9	O	0.008141
10	O	0.047537
11	O	-0.033918
12	O	-0.009108
13	O	0.191872
14	O	0.165850
15	O	-0.138286
16	O	-0.192171
17	O	0.143264
18	O	0.174443
19	O	-0.171950
20	O	-0.170781
21	H	0.007603
22	H	0.007004
23	H	0.014356
24	H	0.015494
25	H	-0.018913
26	H	-0.005917
27	H	-0.017365
28	H	-0.009539
29	H	0.000894
30	H	-0.002713

Sum of Mulliken atomic spin densities = 0.00000

Dipole moment (field-independent basis, Debye):

X= -0.7473 Y= -1.0146 Z= 0.5511 Tot= 1.3753

Isotropic polarizability for W= 0.000000 291.50 Bohr**3.

Frequencies --	30.5735	33.8773	58.4682
Frequencies --	64.7637	70.9130	74.3810
Frequencies --	89.7302	94.7614	99.8997
Frequencies --	104.2434	106.3143	111.3994
Frequencies --	114.5573	116.6341	119.8593
Frequencies --	123.3517	133.1414	134.1851
Frequencies --	135.9234	141.5691	144.3122
Frequencies --	147.1973	148.5472	152.6071
Frequencies --	167.7778	175.2590	199.1606
Frequencies --	201.0692	218.7191	228.7804
Frequencies --	305.7846	310.5026	320.0975
Frequencies --	330.2900	335.3715	363.7138
Frequencies --	366.6362	372.0774	372.3306
Frequencies --	379.5915	381.5514	383.4893
Frequencies --	431.1617	434.3577	455.6632

Frequencies -- 465.1301 465.7761 471.9829
Frequencies -- 478.0853 484.3740 500.1380
Frequencies -- 515.8553 521.2985 537.5454
Frequencies -- 554.4010 590.2984 598.3528
Frequencies -- 602.3079 610.1405 618.5805
Frequencies -- 623.5546 628.4100 629.2218
Frequencies -- 637.6737 639.7917 646.6637
Frequencies -- 656.5201 663.3652 673.7207
Frequencies -- 678.4682 690.5242 693.2807
Frequencies -- 698.8324 701.2022 3677.7987
Frequencies -- 3682.4285 3683.7918 3687.0245
Frequencies -- 3689.4507 3691.3977 3707.6302
Frequencies -- 3713.3904 3719.4522 3726.4955
Zero-point vibrational energy 380047.3 (Joules/Mol)
90.83349 (Kcal/Mol) 3.939 eV

Atom	No	Natural Electron Configuration
Fe	1	[core]4S(0.26)3d(6.48)4p(0.44)4d(0.03)
Fe	2	[core]4S(0.25)3d(6.48)4p(0.42)4d(0.03)5p(0.01)
Fe	3	[core]4S(0.34)3d(6.60)4p(0.64)4d(0.04)5p(0.01)
Fe	4	[core]4S(0.25)3d(6.48)4p(0.41)4d(0.03)
Fe	5	[core]4S(0.24)3d(6.47)4p(0.41)4d(0.03)
Fe	6	[core]4S(0.35)3d(6.63)4p(0.64)4d(0.04)5p(0.01)
Fe	7	[core]4S(0.25)3d(6.47)4p(0.42)4d(0.03)5p(0.01)
Fe	8	[core]4S(0.25)3d(6.47)4p(0.44)4d(0.03)
O	9	[core]2S(1.78)2p(4.91)3S(0.01)3p(0.02)
O	10	[core]2S(1.71)2p(5.15)3S(0.01)3p(0.01)
O	11	[core]2S(1.71)2p(5.16)3S(0.01)3p(0.01)
O	12	[core]2S(1.78)2p(4.93)3S(0.01)3p(0.02)
O	13	[core]2S(1.72)2p(5.16)3S(0.01)3p(0.01)
O	14	[core]2S(1.72)2p(5.20)3S(0.01)3p(0.01)
O	15	[core]2S(1.71)2p(5.21)3S(0.01)3p(0.01)
O	16	[core]2S(1.72)2p(5.15)3S(0.01)3p(0.01)
O	17	[core]2S(1.72)2p(5.19)3S(0.01)3p(0.01)
O	18	[core]2S(1.71)2p(5.16)3S(0.01)3p(0.01)
O	19	[core]2S(1.72)2p(5.15)3S(0.01)3p(0.01)
O	20	[core]2S(1.71)2p(5.20)3S(0.01)3p(0.01)
H	21	1S(0.52)
H	22	1S(0.51)
H	23	1S(0.51)
H	24	1S(0.52)
H	25	1S(0.51)
H	26	1S(0.52)
H	27	1S(0.51)
H	28	1S(0.51)

```
    H   29          1S( 0.51)
    H   30          1S( 0.51)


************************************************
*******        Alpha spin orbitals        *******
************************************************
  Atom  No         Natural Electron Configuration
--------------------------------------------------------------------------
    Fe    1     [core]3d( 4.79)4p( 0.23)5S( 0.14)4d( 0.01)
    Fe    2     [core]3d( 4.85)4p( 0.22)5S( 0.13)4d( 0.01)
    Fe    3     [core]3d( 4.81)4p( 0.32)5S( 0.17)4d( 0.02)
    Fe    4     [core]3d( 4.82)4p( 0.22)5S( 0.14)4d( 0.01)
    Fe    5     [core]3d( 1.65)4p( 0.19)5S( 0.10)4d( 0.01)
    Fe    6     [core]3d( 1.83)4p( 0.32)5S( 0.17)4d( 0.02)
    Fe    7     [core]3d( 1.62)4p( 0.20)5S( 0.12)4d( 0.01)
    Fe    8     [core]3d( 1.66)4p( 0.21)4d( 0.01)6S( 0.11)
     O    9    [core]2S( 0.89)2p( 2.46)4p( 0.01)
     O   10     [core]2S( 0.85)2p( 2.59)4p( 0.01)
     O   11     [core]2S( 0.85)2p( 2.57)
     O   12     [core]2S( 0.89)2p( 2.46)4p( 0.01)
     O   13     [core]2S( 0.87)2p( 2.69)4p( 0.01)
     O   14     [core]2S( 0.87)2p( 2.70)4S( 0.01)4p( 0.01)
     O   15     [core]2S( 0.84)2p( 2.52)
     O   16     [core]2S( 0.85)2p( 2.46)
     O   17     [core]2S( 0.87)2p( 2.69)3p( 0.01)4S( 0.01)
     O   18     [core]2S( 0.87)2p( 2.68)3p( 0.01)
     O   19     [core]2S( 0.84)2p( 2.47)
     O   20     [core]2S( 0.84)2p( 2.50)
     H   21          1S( 0.26)
     H   22          1S( 0.26)
     H   23          1S( 0.26)
     H   24          1S( 0.26)
     H   25          1S( 0.25)
     H   26          1S( 0.26)
     H   27          1S( 0.25)
     H   28          1S( 0.25)
     H   29          1S( 0.25)
     H   30          1S( 0.25)


NBO analysis skipped by request.


************************************************
*******        Beta  spin orbitals        *******
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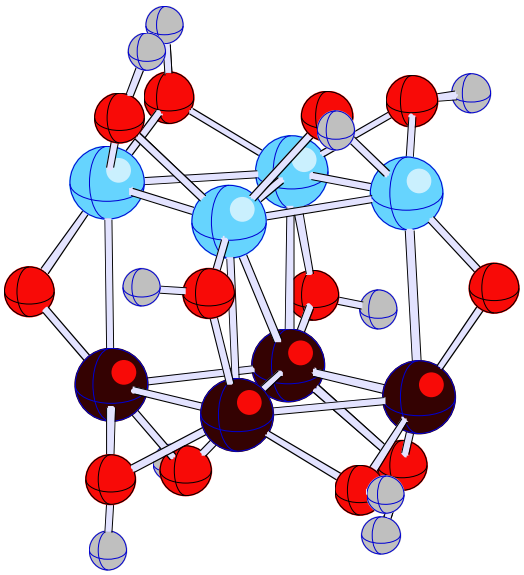
****

Atom	No	Natural Electron Configuration
Fe	1	[core]3d(1.69)4p(0.21)5S(0.11)4d(0.01)
Fe	2	[core]3d(1.62)4p(0.20)5S(0.12)4d(0.01)
Fe	3	[core]3d(1.79)4p(0.31)5S(0.16)4d(0.02)
Fe	4	[core]3d(1.66)4p(0.19)5S(0.11)4d(0.01)
Fe	5	[core]3d(4.82)4p(0.21)5S(0.14)4d(0.01)
Fe	6	[core]3d(4.80)4p(0.33)5S(0.18)4d(0.02)
Fe	7	[core]3d(4.86)4p(0.21)5S(0.13)4d(0.01)5d(0.01)
Fe	8	[core]3d(4.81)4p(0.23)4d(0.01)6S(0.14)
O	9	[core]2S(0.89)2p(2.45)4p(0.01)
O	10	[core]2S(0.85)2p(2.56)
O	11	[core]2S(0.85)2p(2.59)
O	12	[core]2S(0.89)2p(2.47)4p(0.01)
O	13	[core]2S(0.85)2p(2.47)
O	14	[core]2S(0.85)2p(2.50)
O	15	[core]2S(0.87)2p(2.69)4S(0.01)4p(0.01)
O	16	[core]2S(0.87)2p(2.68)3p(0.01)
O	17	[core]2S(0.85)2p(2.50)
O	18	[core]2S(0.84)2p(2.48)
O	19	[core]2S(0.87)2p(2.68)3p(0.01)
O	20	[core]2S(0.87)2p(2.70)3p(0.01)4S(0.01)
H	21	1S(0.26)
H	22	1S(0.25)
H	23	1S(0.25)
H	24	1S(0.25)
H	25	1S(0.26)
H	26	1S(0.26)
H	27	1S(0.26)
H	28	1S(0.26)
H	29	1S(0.25)
H	30	1S(0.26)

HF= -11020.202230\4\S2=14.284767\S2-1=0.\S2A=44.288344



TITLE

Fe	0.1925552087,2.2055972582,-0.8332537803
Fe	-0.3757368158,1.6248758223,1.6995657614
Fe	-1.1938895959,0.1739945634,-0.5896247064
Fe	-1.931240381,-0.4825288142,1.6663036582
Ga	2.0562764249,0.3888919012,-1.6697164936
Ga	1.3326586436,-0.1142723524,0.636384124
Ga	0.4467147232,-1.682110421,-1.6235789776
Ga	0.0736486429,-2.2045016725,0.9625943078
O	1.5297288211,2.0568497852,-1.9919516394
O	1.3800103396,1.0492320896,2.2741501452
O	-1.2743786683,-1.0103102666,-2.1993856584
O	-1.3591306501,-2.1284452595,2.0232375234
O	-1.6566402982,1.9830750085,-1.4673087795
O	-1.9402117868,1.1562390406,2.7885377418
O	1.9480789952,-1.2322985535,-2.7958925029
O	1.8816807636,-1.8501015273,1.6093054774
O	-0.2088419957,3.3349144108,0.7572632682
O	-3.0672084705,-0.0710204265,0.1224206887
O	3.1981524236,0.0503885672,-0.1080324928
O	0.4180018936,-3.3609647477,-0.6153967733
H	-1.8026193819,1.8528812859,-2.420499928
H	-1.8796907544,1.1222852204,3.756579819
H	-0.9711687503,3.9293290373,0.6616698949
H	-3.6120564671,0.7339101114,0.1034017381
H	2.6918166349,-1.8258692184,-2.9820861109
H	1.9949232588,-1.6289330852,2.5499018428
H	3.6954748479,-0.7749099635,0.0253319287
H	-0.1433871221,-4.114550603,-0.8561213915
H	2.0846188536,1.7209384795,2.279297983

H -2.0507603373,-1.5962106698,-2.2039916679
END

$Fe_8O_{12}H_{11}$

$$$$$$$$$$$$$ Fe8O12H11 NEUTRAL S = 22 head fe8o12h11_Oh_22_GF.out

---

UBPW91/GEN pseudo=read scf=(VSHIFT=4,Maxcycle=70,Tight,NoVarAcc) NOS YMM OPT=RFO IOP(5/13=1,5/36=1,8/11=1) INT=UltraFine GUESS=READ GEOM=CH ECKPOINT

Charge = 0 Multiplicity = 22

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	-0.073448	1.491403	-0.611133
2	26	0	0.061333	1.650245	1.922585
3	26	0	-2.076576	0.061440	-1.275509
4	26	0	-1.404065	-0.380466	1.177640
5	26	0	2.030948	0.238851	-1.390587
6	26	0	1.507923	-0.180337	1.046256
7	26	0	0.040118	-1.261894	-1.183469
8	26	0	0.203001	-2.459219	1.132216
9	8	0	1.387268	2.010053	-1.921151
10	8	0	1.797990	1.084740	2.600748
11	8	0	-1.483872	-1.263166	-2.552219
12	8	0	-1.324387	-2.037597	1.885868
13	8	0	-1.718072	1.947842	-1.691931
14	8	0	-1.596995	0.990140	2.650342
15	8	0	1.531713	-1.234631	-2.555507
16	8	0	1.827438	-1.957221	2.024421
17	8	0	0.057705	3.105635	0.617113
18	8	0	-3.200254	-0.075426	0.290950
19	8	0	3.270227	0.230656	0.102532
20	8	0	0.192646	-3.229577	-0.624110
21	1	0	-1.542573	2.231263	-2.604459
22	1	0	-2.389760	1.518278	2.830328

23	1	0	-0.661309	3.755820	0.563658
24	1	0	-3.763009	0.677435	0.533824
25	1	0	1.242779	-1.061416	-3.467056
26	1	0	1.787702	-1.802848	2.984863
27	1	0	3.979198	-0.425132	0.202354
28	1	0	1.011206	-3.597316	-1.001269
29	1	0	2.568124	1.667413	2.493974
30	1	0	-1.950041	-2.107707	-2.663335
31	1	0	1.894603	2.794708	-1.653444

Distance matrix (angstroms):

		1	2	3	4	5
1	Fe	0.000000				
2	Fe	2.542267	0.000000			
3	Fe	2.549256	4.162062	0.000000		
4	Fe	2.911038	2.612685	2.581761	0.000000	
5	Fe	2.570003	4.104695	4.112964	4.333435	0.000000
6	Fe	2.835910	2.492309	4.277579	2.921813	2.527345
7	Fe	2.814446	4.257766	2.498015	2.904723	2.501707
8	Fe	4.327020	4.187177	4.165013	2.627916	4.121348
9	O	2.029492	4.081895	4.026432	4.807143	1.957799
10	O	3.739497	1.948250	5.575372	3.798055	4.086631
11	O	3.653048	5.558731	1.932839	3.833716	3.994922
12	O	4.500411	3.939765	3.868598	1.803890	5.213026
13	O	2.020210	4.039749	1.964801	3.708646	4.131175
14	O	3.634512	1.927543	4.062609	2.021048	5.482290
15	O	3.713273	5.526105	4.042023	4.825430	1.943560
16	O	4.738408	4.017873	5.495985	3.694023	4.065271
17	O	2.032618	1.955103	4.171845	3.821500	4.017835
18	O	3.611872	4.034615	1.932661	2.026218	5.503799
19	O	3.644031	3.952825	5.524123	4.835115	1.940434
20	O	4.728490	5.505957	4.050245	3.730043	3.999604
21	H	2.584390	4.837792	2.599885	4.598325	4.267698
22	H	4.148454	2.617111	4.367878	2.703368	6.244654
23	H	2.617880	2.608129	4.362792	4.247060	4.841114
24	H	3.947952	4.183373	2.548959	2.664258	6.120919
25	H	4.050387	6.147938	4.133014	5.389126	2.573641
26	H	5.219880	4.004077	6.046403	3.934031	4.834487
27	H	4.556183	4.755633	6.252458	5.471078	2.602693
28	H	5.217637	6.081783	4.795425	4.574856	3.988436
29	H	4.080511	2.571143	6.193657	4.658844	4.173626
30	H	4.548266	6.260870	2.578231	4.246709	4.793172
31	H	2.580358	4.178356	4.835685	5.383120	2.572954

		6	7	8	9	10
6	Fe	0.000000				
7	Fe	2.880259	0.000000			

8	Fe	2.627454	2.611994	0.000000		
9	O	3.690240	3.614502	5.540752	0.000000	
10	O	2.025094	4.787181	4.154542	4.633839	0.000000
11	O	4.803372	2.048420	4.225062	4.399506	6.544949
12	O	3.489462	3.447378	1.754614	6.183036	4.473174
13	O	4.736440	3.694884	5.575708	3.114409	5.615580
14	O	3.685597	4.738133	4.176454	5.553791	3.396665
15	O	3.752972	2.026842	4.106628	3.309267	5.660155
16	O	2.053342	3.737452	1.920111	5.612535	3.096214
17	O	3.617307	4.724162	5.590531	3.067706	3.323765
18	O	4.769531	3.752549	4.239380	5.503450	5.627041
19	O	2.040893	3.783531	4.207559	3.287413	3.022916
20	O	3.717249	2.051322	1.917874	5.528395	5.620513
21	H	5.333766	4.089776	6.245830	3.016589	6.290315
22	H	4.610872	5.453827	5.042467	6.089690	4.216386
23	H	4.520155	5.359282	6.300555	3.663147	4.163238
24	H	5.364801	4.601507	5.091749	5.859020	5.946662
25	H	4.606146	2.588698	4.918159	3.441601	6.460068
26	H	2.543426	4.552106	2.524758	6.226358	2.913042
27	H	2.622841	4.258759	4.388829	4.142161	3.576265
28	H	4.014328	2.535825	2.549553	5.694751	5.959463
29	H	2.575673	5.338093	4.947452	4.583138	0.971604
30	H	5.425250	2.620331	4.377825	5.352047	7.207636
31	H	4.035938	4.485088	6.182651	0.971977	4.586009

		11	12	13	14	15
11	O	0.000000				
12	O	4.507970	0.000000			
13	O	3.332494	5.370229	0.000000		
14	O	5.670699	3.134634	4.448279	0.000000	
15	O	3.015722	5.341149	4.629795	6.468329	0.000000
16	O	5.691407	3.155893	6.452242	4.561299	4.646001
17	O	5.613158	5.474737	3.134574	3.368585	5.574597
18	O	3.527082	3.148452	3.197232	3.045094	5.642481
19	O	5.646297	5.425471	5.572428	5.545989	3.497809
20	O	3.224141	3.165785	5.621099	5.633015	3.082726
21	H	3.495313	6.199501	0.971512	5.399656	4.633148
22	H	6.126082	3.830309	4.592005	0.969433	7.208583
23	H	5.964522	5.979263	3.077859	3.588696	6.280377
24	H	4.299309	3.891825	3.278671	3.044512	6.421374
25	H	2.883098	6.016400	4.579666	7.049522	0.971806
26	H	6.453970	3.308776	6.944820	4.401006	5.575312
27	H	6.175363	5.793296	6.455866	6.252165	3.775085
28	H	3.752215	4.027813	6.218903	6.417299	2.875563
29	H	7.104296	5.408191	5.997659	4.222719	5.915510
30	H	0.971036	4.592559	4.176711	6.160882	3.591170
31	H	5.356140	6.799985	3.710806	5.828404	4.144995

		16	17	18	19	20
16	O	0.000000				
17	O	5.544815	0.000000			
18	O	5.641254	4.565065	0.000000		
19	O	3.249939	4.341727	6.480456	0.000000	
20	O	3.362462	6.457070	4.722052	4.687507	0.000000
21	H	7.094146	3.701884	4.056121	5.873098	6.062470
22	H	5.523887	3.661708	3.105677	6.413602	6.414366
23	H	6.400509	0.970865	4.604243	5.300603	7.136932
24	H	6.357388	4.527797	0.970815	7.060597	5.679151
25	H	5.594695	5.953919	5.902146	4.303714	3.726398
26	H	0.973580	5.717721	5.926285	3.826336	4.195766
27	H	3.208940	5.293056	7.188509	0.970908	4.783924
28	H	3.537082	6.961169	5.640030	4.579839	0.973407
29	H	3.729218	3.448665	6.415994	2.876841	6.272627
30	H	6.022213	6.478528	3.797499	6.353673	3.163563
31	H	6.009329	2.937057	6.162459	3.398553	6.344147

		21	22	23	24	25
21	H	0.000000				
22	H	5.546439	0.000000			
23	H	3.624620	3.623800	0.000000		
24	H	4.146510	2.804775	4.370112	0.000000	
25	H	4.398181	7.714091	6.563380	6.639922	0.000000
26	H	7.655410	5.339002	6.539011	6.555134	6.517202
27	H	6.739776	7.158681	6.256612	7.827343	4.621408
28	H	6.562343	7.239959	7.701617	6.589624	3.544647
29	H	6.573414	4.971517	4.303115	6.701156	6.688566
30	H	4.358459	6.597079	6.815810	4.611475	3.454677
31	H	3.610551	6.331607	3.517380	6.424606	4.310888

		26	27	28	29	30
26	H	0.000000				
27	H	3.800410	0.000000			
28	H	4.439855	4.507819	0.000000		
29	H	3.590646	3.409017	6.508309	0.000000	
30	H	6.779808	6.796992	3.708150	7.827080	0.000000
31	H	6.531680	4.261091	6.485653	4.350345	6.311485

		31
31	H	0.000000

Alpha occ. eigenvalues -- -0.19021 -0.18736 -0.18509 -0.18494 -0.17572
Alpha occ. eigenvalues -- -0.17483 -0.17216 -0.16940
Alpha virt. eigenvalues -- -0.13111 -0.12605 -0.11498 -0.09672 -0.09090
gap = 1.04 eV
Beta occ. eigenvalues -- -0.17941 -0.17592 -0.16624 -0.16415 -0.16315
Beta occ. eigenvalues -- -0.15769 -0.15723
Beta virt. eigenvalues -- -0.12983 -0.12833 -0.12664 -0.12288 -0.11264
gap = 0.75 eV

Mulliken atomic spin densities:

		1
1	Fe	3.170795
2	Fe	3.528476
3	Fe	3.513649
4	Fe	2.997052
5	Fe	3.574134
6	Fe	3.133996
7	Fe	3.075399
8	Fe	-3.251277
9	O	0.165269
10	O	0.149319
11	O	0.158893
12	O	-0.145370
13	O	0.165355
14	O	0.160629
15	O	0.160149
16	O	-0.075450
17	O	0.157877
18	O	0.158338
19	O	0.160770
20	O	-0.045132
21	H	0.009785
22	H	0.017010
23	H	0.013642
24	H	0.013302
25	H	0.009532
26	H	-0.003431
27	H	0.007929
28	H	-0.006637
29	H	0.010269
30	H	0.006436
31	H	0.009294

Sum of Mulliken atomic spin densities = 21.00000

Dipole moment (field-independent basis, Debye):

X= 1.0510 Y= 2.4889 Z= -1.5351 Tot= 3.1073

Isotropic polarizability for W= 0.000000 293.01 Bohr3.**

Frequencies --	**50.0919**	**52.5944**	**56.2494**
Frequencies --	**69.9448**	**72.5144**	**73.3765**
Frequencies --	**78.0189**	**85.0408**	**86.6972**

Frequencies --	91.1753	94.4799	96.2539
Frequencies --	104.5040	106.7856	110.1734
Frequencies --	116.5513	120.9743	127.3752
Frequencies --	129.1870	130.0566	138.4130
Frequencies --	143.2843	148.7224	153.1353
Frequencies --	160.5438	167.4067	176.8008
Frequencies --	226.8300	241.7064	247.3397
Frequencies --	279.1954	307.3650	320.4617
Frequencies --	323.8163	328.6387	329.9115
Frequencies --	342.9582	345.1988	350.0952
Frequencies --	352.9072	356.3694	372.6561
Frequencies --	434.3745	437.3069	452.0835
Frequencies --	456.3225	464.5698	467.1694
Frequencies --	475.6399	481.4737	491.1385
Frequencies --	505.2052	513.5980	523.2296
Frequencies --	533.9833	545.7625	554.3379
Frequencies --	568.7590	574.6940	584.5555
Frequencies --	597.1208	599.5905	605.6235
Frequencies --	617.8379	622.3243	625.5383
Frequencies --	636.4712	638.6805	643.8781
Frequencies --	660.7298	665.2408	671.8416
Frequencies --	672.4236	682.8999	689.6657
Frequencies --	694.1127	3677.9845	3678.9250
Frequencies --	3694.8813	3695.0361	3700.1494
Frequencies --	3701.2784	3702.1475	3707.1919
Frequencies --	3707.7774	3708.7637	3718.7312

Zero-point vibrational energy 405216.1 (Joules/Mol)
96.84898 (Kcal/Mol) 4.200 eV

Atom	No	Natural Electron Configuration
Fe	1	[core]4S(0.28)3d(6.56)4p(0.59)4d(0.03)5p(0.01)
Fe	2	[core]4S(0.24)3d(6.52)4p(0.38)4d(0.02)
Fe	3	[core]4S(0.25)3d(6.52)4p(0.38)4d(0.02)
Fe	4	[core]4S(0.27)3d(6.58)4p(0.59)4d(0.04)5p(0.01)
Fe	5	[core]4S(0.25)3d(6.52)4p(0.39)4d(0.02)
Fe	6	[core]4S(0.30)3d(6.59)4p(0.58)4d(0.03)5p(0.01)
Fe	7	[core]4S(0.30)3d(6.60)4p(0.59)4d(0.03)5p(0.01)
Fe	8	[core]4S(0.27)3d(6.43)4p(0.41)4d(0.03)
O	9	[core]2S(1.72)2p(5.18)3S(0.01)3p(0.01)
O	10	[core]2S(1.71)2p(5.18)3S(0.01)3p(0.01)
O	11	[core]2S(1.71)2p(5.19)3S(0.01)3p(0.01)
O	12	[core]2S(1.77)2p(4.84)3S(0.01)3p(0.02)
O	13	[core]2S(1.71)2p(5.19)3S(0.01)3p(0.01)
O	14	[core]2S(1.70)2p(5.19)3S(0.01)3p(0.01)
O	15	[core]2S(1.71)2p(5.18)3S(0.01)3p(0.01)

O	16	[core]2S(1.72)2p(5.15)3S(0.01)3p(0.01)
O	17	[core]2S(1.71)2p(5.20)3S(0.01)3p(0.01)
O	18	[core]2S(1.71)2p(5.17)3S(0.01)3p(0.01)
O	19	[core]2S(1.71)2p(5.19)3S(0.01)3p(0.01)
O	20	[core]2S(1.72)2p(5.14)3S(0.01)3p(0.01)
H	21	1S(0.52)
H	22	1S(0.52)
H	23	1S(0.52)
H	24	1S(0.52)
H	25	1S(0.52)
H	26	1S(0.51)
H	27	1S(0.52)
H	28	1S(0.51)
H	29	1S(0.52)
H	30	1S(0.52)
H	31	1S(0.52)

****

******* Alpha spin orbitals *******

****

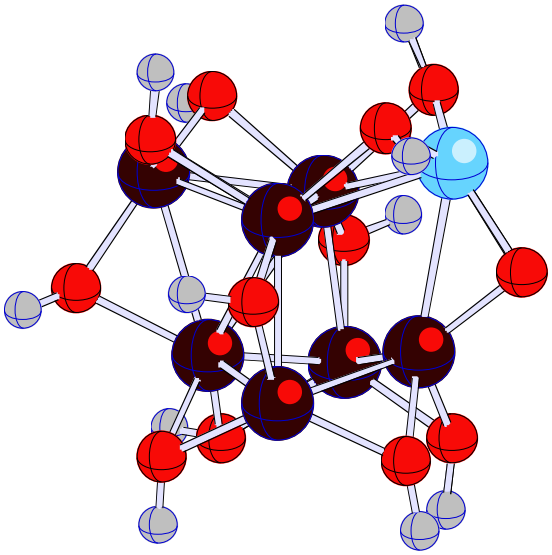
Atom	No	Natural Electron Configuration
Fe	1	[core]3d(4.88)4p(0.29)5S(0.14)4d(0.03)
Fe	2	[core]3d(4.87)4p(0.21)5S(0.14)4d(0.01)5d(0.01)
Fe	3	[core]3d(4.87)4p(0.21)5S(0.15)4d(0.01)5d(0.01)
Fe	4	[core]3d(4.75)4p(0.29)5S(0.14)4d(0.02)
Fe	5	[core]3d(4.87)4p(0.21)5S(0.14)4d(0.01)5d(0.01)
Fe	6	[core]3d(4.84)4p(0.29)5S(0.16)4d(0.02)
Fe	7	[core]3d(4.84)4p(0.30)5S(0.16)4d(0.02)
Fe	8	[core]3d(1.65)4p(0.19)5S(0.14)4d(0.01)5d(0.01)
O	9	[core]2S(0.87)2p(2.69)3p(0.01)4S(0.01)
O	10	[core]2S(0.87)2p(2.68)3p(0.01)
O	11	[core]2S(0.87)2p(2.69)3p(0.01)
O	12	[core]2S(0.89)2p(2.34)
O	13	[core]2S(0.87)2p(2.69)3p(0.01)4S(0.01)
O	14	[core]2S(0.86)2p(2.69)4S(0.01)4p(0.01)
O	15	[core]2S(0.87)2p(2.68)4p(0.01)
O	16	[core]2S(0.86)2p(2.53)
O	17	[core]2S(0.87)2p(2.70)3p(0.01)4S(0.01)4p(0.01)
O	18	[core]2S(0.87)2p(2.68)3p(0.01)4S(0.01)
O	19	[core]2S(0.87)2p(2.69)3p(0.01)4S(0.01)
O	20	[core]2S(0.86)2p(2.55)
H	21	1S(0.26)
H	22	1S(0.26)
H	23	1S(0.26)

H	24	1S(0.27)
H	25	1S(0.26)
H	26	1S(0.25)
H	27	1S(0.26)
H	28	1S(0.25)
H	29	1S(0.26)
H	30	1S(0.26)
H	31	1S(0.26)

****
******* Beta spin orbitals *******
****

Atom	No	Natural Electron Configuration
Fe	1	[core]3d(1.68)4p(0.30)5S(0.14)4d(0.01)
Fe	2	[core]3d(1.65)4p(0.18)5S(0.10)
Fe	3	[core]3d(1.66)4p(0.18)5S(0.10)
Fe	4	[core]3d(1.83)4p(0.29)5S(0.13)4d(0.01)
Fe	5	[core]3d(1.65)4p(0.18)5S(0.10)
Fe	6	[core]3d(1.75)4p(0.29)5S(0.14)4d(0.01)
Fe	7	[core]3d(1.76)4p(0.29)5S(0.14)4d(0.01)
Fe	8	[core]3d(4.77)4p(0.21)5S(0.13)4d(0.01)
O	9	[core]2S(0.85)2p(2.49)
O	10	[core]2S(0.85)2p(2.50)
O	11	[core]2S(0.84)2p(2.51)
O	12	[core]2S(0.88)2p(2.49)4p(0.01)
O	13	[core]2S(0.84)2p(2.49)
O	14	[core]2S(0.84)2p(2.50)
O	15	[core]2S(0.84)2p(2.49)
O	16	[core]2S(0.86)2p(2.61)
O	17	[core]2S(0.84)2p(2.50)
O	18	[core]2S(0.84)2p(2.49)
O	19	[core]2S(0.84)2p(2.50)
O	20	[core]2S(0.86)2p(2.60)
H	21	1S(0.26)
H	22	1S(0.26)
H	23	1S(0.26)
H	24	1S(0.26)
H	25	1S(0.26)
H	26	1S(0.26)
H	27	1S(0.26)
H	28	1S(0.26)
H	29	1S(0.26)
H	30	1S(0.26)
H	31	1S(0.26)

HF= -11020.7989981\S2=124.552873\S2-1=0.\S2A=122.353101



TITLE

Fe	-0.0734482402,1.4914025753,-0.6111326671
Fe	0.061333445,1.650245082,1.9225849953
Fe	-2.076575929,0.0614403637,-1.2755091246
Fe	-1.4040652081,-0.3804658651,1.177639805
Fe	2.0309479582,0.2388509518,-1.3905866895
Fe	1.5079234207,-0.1803371216,1.046255811
Fe	0.0401179059,-1.2618938719,-1.1834687085
Ga	0.2030009411,-2.4592190861,1.1322160954
O	1.3872675207,2.0100527541,-1.9211509581
O	1.7979904294,1.0847398932,2.6007479659
O	-1.4838719812,-1.2631661153,-2.5522189665
O	-1.3243873464,-2.0375968288,1.8858678658
O	-1.7180720765,1.9478421853,-1.6919309706
O	-1.5969945468,0.9901404672,2.6503421291
O	1.5317132379,-1.2346314409,-2.5555067491
O	1.8274375886,-1.9572205697,2.0244213195
O	0.0577051213,3.1056347132,0.6171133063
O	-3.2002535134,-0.0754256292,0.2909504912
O	3.2702270174,0.230655811,0.1025324466
O	0.1926458397,-3.2295767119,-0.6241101652
H	-1.5425727114,2.2312633631,-2.6044593943
H	-2.3897595038,1.5182782407,2.8303278204
H	-0.6613088641,3.7558195569,0.5636582071
H	-3.7630090728,0.6774354632,0.5338240254
H	1.2427792658,-1.0614159041,-3.4670555941
H	1.7877016291,-1.8028477126,2.984863328
H	3.9791977892,-0.4251320982,0.2023536748

H 1.0112058712,-3.5973161848,-1.0012689572
H 2.5681237791,1.6674129781,2.4939737599
H -1.9500407699,-2.1077074185,-2.663334683
H 1.8946030034,2.79470816,-1.6534444189
END

$Fe_8O_{12}H_{12}$

$$$$$$$$$$$$$ Fe_8O_12H_12 NEUTRAL S = 29 QB
fe8o12h12_29_GF.out

UBPW91/6-311+G* scf=(VSHIFT=-1,CDIIS,Maxcycle=80,Tight,NoVarAcc) NOS
YMM OPT=RFO IOP(5/13=1,5/36=1,8/11=1) INT=UltraFine GUESS=READ GEOM=CHECKPOINT

Charge = 0 Multiplicity = 29
Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	-0.083996	1.543609	-0.642522
2	26	0	0.193926	1.603641	2.009664
3	26	0	-2.193935	0.221235	-1.124296
4	26	0	-1.372782	-0.239284	1.137786
5	26	0	1.942699	0.577579	-1.535536
6	26	0	1.435900	-0.189895	0.970482
7	26	0	0.084138	-1.185633	-1.308523
8	26	0	0.193144	-2.393685	0.822600
9	8	0	1.277796	2.301594	-2.045661
10	8	0	1.844798	0.917145	2.703015
11	8	0	-1.659146	-1.254587	-2.271813
12	8	0	-1.502300	-2.135006	1.738339
13	8	0	-1.710187	1.991568	-1.751680
14	8	0	-1.605428	1.133042	2.584641
15	8	0	1.708651	-1.105206	-2.486708
16	8	0	1.790631	-1.977704	1.839859
17	8	0	0.182378	3.052055	0.693960
18	8	0	-3.316421	-0.232379	0.384219

19	8	0	3.134732	0.366417	0.002006
20	8	0	0.086701	-3.231351	-0.918433
21	1	0	-1.518048	2.136444	-2.693505
22	1	0	-2.305281	1.802901	2.522731
23	1	0	-0.491889	3.751325	0.692478
24	1	0	-4.013919	0.364918	0.698261
25	1	0	2.402502	-1.780031	-2.412017
26	1	0	1.757492	-1.960085	2.811195
27	1	0	3.864304	-0.274855	0.012258
28	1	0	0.773180	-3.839516	-1.235846
29	1	0	2.633888	1.472850	2.584635
30	1	0	-2.076149	-2.130731	-2.222484
31	1	0	1.750183	3.075595	-1.694610
32	1	0	-2.323086	-2.560209	1.439125

Distance matrix (angstroms):

		1	2	3	4	5
1	Fe	0.000000				
2	Fe	2.667384	0.000000			
3	Fe	2.536261	4.175480	0.000000		
4	Fe	2.830048	2.571209	2.450181	0.000000	
5	Fe	2.416232	4.084048	4.172271	4.336626	0.000000
6	Fe	2.813698	2.416437	4.211036	2.814093	2.669455
7	Fe	2.814353	4.336181	2.683810	3.000437	2.571906
8	Fe	4.210186	4.169860	4.040589	2.681959	4.177339
9	O	2.097097	4.255300	4.150870	4.859625	1.916911
10	O	3.912202	1.917653	5.607492	3.760331	4.253258
11	O	3.600776	5.471232	1.944440	3.569063	4.107581
12	O	4.605680	4.114398	3.771593	1.992787	5.472147
13	O	2.018761	4.233656	1.939510	3.666000	3.922965
14	O	3.591365	1.946725	3.864446	2.007683	5.465675
15	O	3.691994	5.463479	4.341174	4.835494	1.947119
16	O	4.698519	3.924835	5.431236	3.677253	4.236259
17	O	2.032868	1.956812	4.119036	3.667209	3.767282
18	O	3.828434	4.282006	1.934259	2.084621	5.656840
19	O	3.487320	3.769583	5.448333	4.687702	1.956928
20	O	4.785969	5.653529	4.142950	3.912875	4.281763
21	H	2.571865	5.033342	2.566567	4.510430	3.968339
22	H	3.875586	2.559097	3.976792	2.637830	6.001356
23	H	2.612014	2.611105	4.319626	4.110868	4.578638
24	H	4.316400	4.578227	2.579670	2.744786	6.365247
25	H	4.512246	5.989850	5.175957	5.406271	2.556945
26	H	5.253105	3.973328	5.988324	3.944625	5.036677
27	H	4.395978	4.581490	6.183860	5.356785	2.610533
28	H	5.483139	6.363711	5.030499	4.816736	4.579117
29	H	4.219769	2.510202	6.215352	4.591098	4.272595

30	H	4.468302	6.083571	2.598391	3.919657	4.894688
31	H	2.611146	4.279046	4.901908	5.363190	2.510468
32	H	5.117431	4.898827	3.784738	2.525980	6.073816

		6	7	8	9	10
6	Fe	0.000000				
7	Fe	2.830657	0.000000			
8	Fe	2.534364	2.452133	0.000000		
9	O	3.915307	3.758848	5.607944	0.000000	
10	O	2.096284	4.859428	4.150364	4.978767	0.000000
11	O	4.607098	1.992918	3.782051	4.617705	6.460879
12	O	3.606394	3.563912	1.944228	6.459954	4.631338
13	O	4.697532	3.675677	5.429551	3.018374	5.799708
14	O	3.688543	4.836074	4.333296	5.578368	3.459001
15	O	3.586691	2.008390	3.861148	3.462144	5.571505
16	O	2.019384	3.667670	1.939026	5.802815	3.021279
17	O	3.486836	4.688026	5.447270	3.044447	3.370132
18	O	4.788535	3.916360	4.144933	5.782056	5.773769
19	O	2.033091	3.665033	4.116367	3.374324	3.043465
20	O	3.826067	2.082580	1.934996	5.770860	5.780641
21	H	5.249996	3.939717	5.984416	2.874668	6.474400
22	H	4.514105	5.414718	5.171451	5.827293	4.247379
23	H	4.396233	5.358112	6.184444	3.568040	4.187475
24	H	5.484747	4.819281	5.032368	6.267541	6.216797
25	H	3.860589	2.635492	3.964918	4.249570	5.809419
26	H	2.573951	4.513532	2.567042	6.479280	2.880587
27	H	2.612003	4.106536	4.315497	4.190841	3.569235
28	H	4.315879	2.742837	2.581486	6.214794	6.268079
29	H	2.608714	5.359612	4.900214	4.895452	0.972361
30	H	5.127998	2.528908	3.806753	5.561089	6.994563
31	H	4.226691	4.591605	6.218822	0.972350	4.899691
32	H	4.468556	3.903045	2.596005	6.981920	5.573210

		11	12	13	14	15
11	O	0.000000				
12	O	4.108656	0.000000			
13	O	3.287958	5.408517	0.000000		
14	O	5.411913	3.377424	4.421732	0.000000	
15	O	3.377951	5.405712	4.671052	6.458441	0.000000
16	O	5.415691	3.298249	6.396093	4.665261	4.414426
17	O	5.543843	5.552879	3.269188	3.233193	5.452429
18	O	3.293323	2.957138	3.476779	3.103824	5.852812
19	O	5.547898	5.547435	5.402756	5.452232	3.223830
20	O	2.964323	3.284103	5.585874	5.846601	3.100113
21	H	3.420062	6.155223	0.972081	5.373386	4.578498
22	H	5.723057	4.094772	4.319759	0.970741	7.047214
23	H	5.933689	6.063303	3.248831	3.416966	6.207696
24	H	4.121783	3.693184	3.735690	3.154246	6.712161

25	H	4.097894	5.709548	5.619183	7.036767	0.970772
26	H	6.165072	3.436257	6.961336	4.574713	5.366655
27	H	6.056844	5.936325	6.270814	6.206231	3.403110
28	H	3.697471	4.114480	6.358832	6.706730	3.149002
29	H	7.032365	5.553458	6.159845	4.252914	5.763763
30	H	0.971572	4.002180	4.165205	5.829428	3.930169
31	H	5.541405	7.036629	3.626642	5.774568	4.255378
32	H	3.989552	0.971605	5.592456	3.932854	5.812410

		16	17	18	19	20
16	O	0.000000				
17	O	5.403522	0.000000			
18	O	5.589904	4.808850	0.000000		
19	O	3.267907	4.050660	6.490148	0.000000	
20	O	3.476087	6.487693	4.719319	4.804335	0.000000
21	H	6.958805	3.899322	4.279937	5.661019	5.877016
22	H	5.615673	3.330651	3.120577	6.165329	6.550334
23	H	6.272811	0.971399	4.893149	5.008665	7.189406
24	H	6.362698	4.982934	0.970510	7.182478	5.688755
25	H	4.300222	6.158336	6.551355	3.312236	3.114491
26	H	0.972061	5.664382	5.883857	3.898840	4.279928
27	H	3.246527	5.008955	7.190478	0.971397	4.886445
28	H	3.736510	7.181013	5.688663	4.979867	0.970500
29	H	3.629339	3.475406	6.569309	2.853947	6.394463
30	H	5.610529	6.361435	3.454984	6.191719	2.754965
31	H	6.166842	2.857243	6.398024	3.483551	6.568652
32	H	4.174035	6.191133	2.741958	6.357533	3.437380

		21	22	23	24	25
21	H	0.000000				
22	H	5.285840	0.000000			
23	H	3.889181	3.230259	0.000000		
24	H	4.568562	2.883735	4.885948	0.000000	
25	H	5.548759	7.704049	6.972180	7.446146	0.000000
26	H	7.603449	5.545214	6.493758	6.571097	5.265966
27	H	6.488855	6.977344	5.970699	7.933871	3.206171
28	H	6.564038	7.445851	7.933454	6.658405	2.877419
29	H	6.748163	4.950572	4.306064	6.998519	5.966684
30	H	4.329217	6.167903	6.753182	4.302786	4.496357
31	H	3.544168	5.987696	3.343903	6.804299	4.951495
32	H	6.307557	4.495693	6.614094	3.458926	6.145824

		26	27	28	29	30
26	H	0.000000				
27	H	3.887507	0.000000			
28	H	4.569428	4.880535	0.000000		
29	H	3.550274	3.344476	6.802907	0.000000	
30	H	6.329601	6.612664	3.465844	7.634045	0.000000
31	H	6.757249	4.313748	6.998840	4.654210	6.482692

```
  32  H    4.346704   6.748525   4.287069   6.492254   3.694971
                31         32
  31  H    0.000000
  32  H    7.627195   0.000000
Alpha  occ. eigenvalues --   -0.18388  -0.17709  -0.17216  -0.17061  -0.16873
 Alpha  occ. eigenvalues --   -0.16853  -0.16589
 Alpha virt. eigenvalues --   -0.13715  -0.05155  -0.04648  -0.04318  -0.04277
0.78 eV
  Beta  occ. eigenvalues --   -0.19787  -0.17991  -0.17358  -0.16362  -0.16053
  Beta  occ. eigenvalues --   -0.15746  -0.15480  -0.15382  -0.15193
  Beta virt. eigenvalues --   -0.12711  -0.12136  -0.11375  -0.11179  -0.10717
0.68 eV
Mulliken charges and spin densities:
           1         2
   1  Fe   1.101686   3.052370
   2  Fe   0.209009   3.415764
   3  Fe   0.192733   3.457075
   4  Fe   0.793837   3.145289
   5  Fe   0.208273   3.416466
   6  Fe   1.100204   3.054737
   7  Fe   0.794858   3.149210
   8  Fe   0.196149   3.455186   sum = ~26.2 e
   9  O   -0.744038   0.123346
  10  O   -0.743284   0.123291
  11  O   -0.726093   0.153019
  12  O   -0.723122   0.152364
  13  O   -0.773947   0.158656
  14  O   -0.694432   0.133373
  15  O   -0.690078   0.132854
  16  O   -0.775099   0.158513
  17  O   -0.809411   0.143349
  18  O   -0.784626   0.149558
  19  O   -0.808808   0.143098
  20  O   -0.785168   0.150461
  21  H    0.386102   0.006041
  22  H    0.342894   0.013380
  23  H    0.376506   0.016397
  24  H    0.370607   0.009409
  25  H    0.341234   0.013566
  26  H    0.386190   0.005982
  27  H    0.376149   0.016421
  28  H    0.371271   0.009328
  29  H    0.375201   0.011212
  30  H    0.380340   0.009497
  31  H    0.375276   0.011225
  32  H    0.379588   0.009563
```

Sum of Mulliken charges = 0.00000 28.00000
Dipole moment (field-independent basis, Debye):
X= 0.1013 Y= 0.1186 Z= 0.0105 Tot= 0.1563

Isotropic polarizability for W= 0.000000 294.27 Bohr**3. 1.36 A**3
Exact polarizability: 298.695 0.318 297.520 -2.048 4.079 286.598
Approx polarizability:1152.747 -0.6341147.152 -24.342 3.2451255.361

Frequencies --	39.3131	50.6187	59.0732
Frequencies --	59.2826	61.6455	67.9736
Frequencies --	71.0766	75.7011	79.1804
Frequencies --	82.2023	92.2315	92.4552
Frequencies --	95.9375	101.8959	103.6902
Frequencies --	114.2865	114.9040	119.5024
Frequencies --	124.1274	127.6257	128.9219
Frequencies --	130.1589	141.8665	144.8502
Frequencies --	153.2857	173.5429	222.6048
Frequencies --	246.4678	251.5421	252.6892
Frequencies --	290.8164	296.2766	299.2126
Frequencies --	301.6680	345.7519	347.8577
Frequencies --	350.6232	355.6439	360.5526
Frequencies --	364.2119	386.2771	387.7333
Frequencies --	404.4255	418.3292	428.3864
Frequencies --	432.0482	440.3726	450.0054
Frequencies --	457.7824	473.8254	474.1456
Frequencies --	475.2192	481.6991	489.3479
Frequencies --	495.6442	497.4341	506.6379
Frequencies --	514.3063	540.2625	550.9475
Frequencies --	554.7417	567.3180	577.7719
Frequencies --	586.1789	597.5083	609.8786
Frequencies --	614.9494	617.7402	621.1373
Frequencies --	627.5682	661.9548	666.5052
Frequencies --	670.9245	673.2441	677.5206
Frequencies --	684.7382	696.7914	699.5759
Frequencies --	3689.2845	3689.9181	3691.1186
Frequencies --	3691.2745	3699.4862	3699.7228
Frequencies --	3700.0358	3701.0877	3701.1303
Frequencies --	3701.2527	3703.6559	3703.7710

Zero-point vibrational energy 430499.4 (Joules/Mol)
102.89183 (Kcal/Mol) 4.462 eV

Atom	No	Natural Electron Configuration
Fe	1	[core]4S(0.29)3d(6.63)4p(0.58)4d(0.03)5p(0.01)

Fe	2	[core]4S(0.25)3d(6.54)4p(0.37)4d(0.02)
Fe	3	[core]4S(0.25)3d(6.54)4p(0.38)4d(0.02)
Fe	4	[core]4S(0.27)3d(6.60)4p(0.55)4d(0.03)5p(0.01)
Fe	5	[core]4S(0.26)3d(6.53)4p(0.37)4d(0.02)
Fe	6	[core]4S(0.29)3d(6.63)4p(0.58)4d(0.03)5p(0.01)
Fe	7	[core]4S(0.27)3d(6.60)4p(0.55)4d(0.03)5p(0.01)
Fe	8	[core]4S(0.25)3d(6.54)4p(0.38)4d(0.02)
O	9	[core]2S(1.72)2p(5.17)3S(0.01)3p(0.01)
O	10	[core]2S(1.72)2p(5.17)3S(0.01)3p(0.01)
O	11	[core]2S(1.71)2p(5.18)3S(0.01)3p(0.01)
O	12	[core]2S(1.71)2p(5.17)3S(0.01)3p(0.01)
O	13	[core]2S(1.71)2p(5.18)3S(0.01)3p(0.01)
O	14	[core]2S(1.71)2p(5.18)3S(0.01)3p(0.01)
O	15	[core]2S(1.71)2p(5.18)3S(0.01)3p(0.01)
O	16	[core]2S(1.71)2p(5.18)3S(0.01)3p(0.01)
O	17	[core]2S(1.71)2p(5.20)3S(0.01)3p(0.01)
O	18	[core]2S(1.72)2p(5.20)3S(0.01)3p(0.01)
O	19	[core]2S(1.71)2p(5.20)3S(0.01)3p(0.01)
O	20	[core]2S(1.72)2p(5.20)3S(0.01)3p(0.01)
H	21	1S(0.52)
H	22	1S(0.53)
H	23	1S(0.52)
H	24	1S(0.53)
H	25	1S(0.53)
H	26	1S(0.52)
H	27	1S(0.52)
H	28	1S(0.53)
H	29	1S(0.52)
H	30	1S(0.51)
H	31	1S(0.52)
H	32	1S(0.51)

****
******* Alpha spin orbitals *******
****

Atom	No	Natural Electron Configuration	
Fe	1	[core]3d(4.88)4p(0.28)5S(0.14)4d(0.02)	3.1
Fe	2	[core]3d(4.83)4p(0.20)5S(0.15)4d(0.01)5d(0.01)	3.2
Fe	3	[core]3d(4.85)4p(0.20)5S(0.14)4d(0.01)5d(0.01)	3.23
Fe	4	[core]3d(4.87)4p(0.17)5S(0.14)4d(0.02)5p(0.10)	3.14
Fe	5	[core]3d(4.83)4p(0.20)5S(0.15)4d(0.01)5d(0.01)	3.21
Fe	6	[core]3d(4.88)4p(0.28)5S(0.14)4d(0.02)	3.12
Fe	7	[core]3d(4.87)4p(0.17)5S(0.14)4d(0.02)5p(0.10)	3.14
Fe	8	[core]3d(4.85)4p(0.20)5S(0.14)4d(0.01)5d(0.01)	3.23

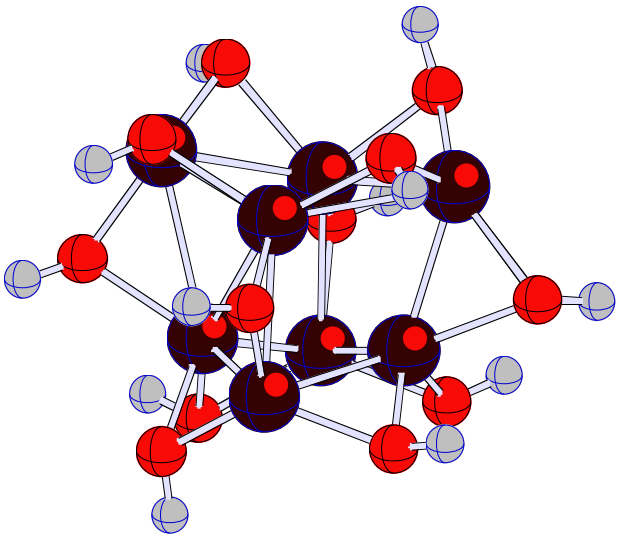
O	9	[core]2S(0.87)2p(2.66)3p(0.01)
O	10	[core]2S(0.87)2p(2.66)3p(0.01)
O	11	[core]2S(0.87)2p(2.68)4S(0.01)4p(0.01)
O	12	[core]2S(0.87)2p(2.68)4S(0.01)4p(0.01)
O	13	[core]2S(0.87)2p(2.68)3p(0.01)4S(0.01)
O	14	[core]2S(0.87)2p(2.67)4S(0.01)4p(0.01)
O	15	[core]2S(0.87)2p(2.67)4S(0.01)4p(0.01)
O	16	[core]2S(0.87)2p(2.68)3p(0.01)4S(0.01)
O	17	[core]2S(0.87)2p(2.69)3p(0.01)4S(0.01)4p(0.01)
O	18	[core]2S(0.87)2p(2.69)3p(0.01)4S(0.01)
O	19	[core]2S(0.87)2p(2.69)3p(0.01)4S(0.01)4p(0.01)
O	20	[core]2S(0.87)2p(2.69)3p(0.01)4S(0.01)
H	21	1S(0.26)
H	22	1S(0.27)
H	23	1S(0.26)
H	24	1S(0.26)
H	25	1S(0.27)
H	26	1S(0.26)
H	27	1S(0.26)
H	28	1S(0.26)
H	29	1S(0.26)
H	30	1S(0.26)
H	31	1S(0.26)
H	32	1S(0.26)

****
******* Beta spin orbitals *******
****

Atom	No	Natural Electron Configuration
Fe	1	[core]3d(1.75)4p(0.30)5S(0.14)4d(0.01)
Fe	2	[core]3d(1.71)4p(0.17)5S(0.11)
Fe	3	[core]3d(1.69)4p(0.18)5S(0.11)
Fe	4	[core]3d(1.73)4p(0.28)5S(0.14)4d(0.01)
Fe	5	[core]3d(1.71)4p(0.17)5S(0.11)
Fe	6	[core]3d(1.75)4p(0.30)5S(0.14)4d(0.01)
Fe	7	[core]3d(1.73)4p(0.28)5S(0.14)4d(0.01)
Fe	8	[core]3d(1.69)4p(0.18)5S(0.11)
O	9	[core]2S(0.85)2p(2.51)
O	10	[core]2S(0.85)2p(2.51)
O	11	[core]2S(0.84)2p(2.50)
O	12	[core]2S(0.84)2p(2.50)
O	13	[core]2S(0.84)2p(2.50)
O	14	[core]2S(0.84)2p(2.51)
O	15	[core]2S(0.84)2p(2.51)

O	16	[core]2S(0.84)2p(2.50)
O	17	[core]2S(0.84)2p(2.51)
O	18	[core]2S(0.85)2p(2.51)
O	19	[core]2S(0.84)2p(2.51)
O	20	[core]2S(0.85)2p(2.51)
H	21	1S(0.26)
H	22	1S(0.26)
H	23	1S(0.26)
H	24	1S(0.26)
H	25	1S(0.26)
H	26	1S(0.26)
H	27	1S(0.26)
H	28	1S(0.26)
H	29	1S(0.26)
H	30	1S(0.25)
H	31	1S(0.26)
H	32	1S(0.25)

HF= -11021.3950817\S2=210.315748\S2-1=0.\S2A=210.006176



TITLE

Fe	-0.083996	1.543609	-0.642522
Fe	0.193926	1.603641	2.009664
Fe	-2.193935	0.221235	-1.124296
Fe	-1.372782	-0.239284	1.137786
Fe	1.942699	0.577579	-1.535536
Fe	1.435900	-0.189895	0.970482
Fe	0.084138	-1.185633	-1.308523
Fe	0.193144	-2.393685	0.822600
O	1.277796	2.301594	-2.045661

```
O       1.844798    0.917145    2.703015
O      -1.659146   -1.254587   -2.271813
O      -1.502300   -2.135006    1.738339
O      -1.710187    1.991568   -1.751680
O      -1.605428    1.133042    2.584641
O       1.708651   -1.105206   -2.486708
O       1.790631   -1.977704    1.839859
O       0.182378    3.052055    0.693960
O      -3.316421   -0.232379    0.384219
O       3.134732    0.366417    0.002006
O       0.086701   -3.231351   -0.918433
H      -1.518048    2.136444   -2.693505
H      -2.305281    1.802901    2.522731
H      -0.491889    3.751325    0.692478
H      -4.013919    0.364918    0.698261
H       2.402502   -1.780031   -2.412017
H       1.757492   -1.960085    2.811195
H       3.864304   -0.274855    0.012258
H       0.773180   -3.839516   -1.235846
H       2.633888    1.472850    2.584635
H      -2.076149   -2.130731   -2.222484
H       1.750183    3.075595   -1.694610
H      -2.323086   -2.560209    1.439125
END
```

$Fe_8O_{12}H_{13}$

```
$$$$$$$$$$$$$  Fe8O12H13    NEUTRAL    S = 30   head
fe8o12h13_30_GF.out
-----------------------------------------------------------------------
 # UBPW91/6-311+G*
scf=(VSHIFT=5,NoIncFock,Maxcycle=90,Tight,NoVarAcc)  NOSYMM
 OPT=RFO IOP(5/13=1,5/36=1,8/11=1) INT=UltraFine GUESS=READ
GEOM=CHECKPOINT
 ----------------------------------------------------------------------
 Charge =  0 Multiplicity = 30
                    Input orientation:
 ----------------------------------------------------------------------
 Center     Atomic      Atomic           Coordinates (Angstroms)
 Number     Number       Type             X           Y           Z
 ----------------------------------------------------------------------
```

1	26	0	2.540392	0.210175	0.220991
2	26	0	0.943241	2.127336	-0.697229
3	26	0	1.263440	-1.913237	-0.847199
4	26	0	-0.160788	0.045573	-1.201711
5	26	0	0.529317	-0.150941	1.604263
6	26	0	-1.165323	1.708636	0.912749
7	26	0	-0.886886	-2.047337	0.719354
8	26	0	-2.498883	-0.193860	-0.475120
9	8	0	2.453886	-0.080686	2.167498
10	8	0	-0.243875	3.348559	0.293625
11	8	0	0.257462	-3.439103	-0.101720
12	8	0	-2.000881	0.118014	-2.307793
13	8	0	3.165479	-1.475042	-0.583519
14	8	0	0.540331	1.536495	-2.491217
15	8	0	-0.192932	-1.816026	2.552224
16	8	0	-3.092643	1.376124	0.574376
17	8	0	2.890062	2.061908	-0.325921
18	8	0	0.535366	-1.372756	-2.570899
19	8	0	-0.350750	1.338398	2.665172
20	8	0	-2.822133	-1.994386	0.268719
21	1	0	3.823686	-1.535503	-1.292753
22	1	0	-0.257460	1.853585	-2.948922
23	1	0	3.342450	2.671230	0.277631
24	1	0	1.068707	-0.860260	-3.202713
25	1	0	0.367024	-2.521294	2.914987
26	1	0	-3.686207	2.063480	0.234824
27	1	0	-0.846711	1.099479	3.464392
28	1	0	-3.546006	-2.223121	0.871741
29	1	0	0.089490	3.951438	0.977377
30	1	0	-0.123871	-4.101945	-0.699272
31	1	0	2.905438	-0.859086	2.531458
32	1	0	-1.969864	-0.621313	-2.938540
33	1	0	-0.887029	-0.144208	0.459512

Distance matrix (angstroms):

		1	2	3	4	5
1	Fe	0.000000				
2	Fe	2.658858	0.000000			
3	Fe	2.698242	4.056014	0.000000		
4	Fe	3.057376	2.409797	2.447660	0.000000	
5	Fe	2.467441	3.264773	3.107135	2.896265	0.000000
6	Fe	4.056629	2.685774	4.702581	2.871552	2.609219
7	Fe	4.134121	4.773255	2.663826	2.932231	2.526858
8	Fe	5.103147	4.157584	4.153285	2.460071	3.673646
9	O	1.970019	3.919703	3.723413	4.266618	2.006523
10	O	4.196055	1.970386	5.591062	3.626658	3.816032

11	O	4.316612	5.640050	1.973828	3.678026	3.714336
12	O	5.198692	3.911412	4.112797	2.148163	4.666735
13	O	1.969245	4.234194	1.969593	3.709243	3.672735
14	O	3.621525	1.931275	3.889258	2.092186	4.429505
15	O	4.124463	5.234495	3.699533	4.190300	2.047628
16	O	5.763280	4.297634	5.640587	3.677040	4.063396
17	O	1.962218	1.982993	4.326593	3.760359	3.767682
18	O	3.784236	3.990945	1.947653	2.090685	4.350269
19	O	3.950393	3.688167	5.051286	4.081699	2.029329
20	O	5.798193	5.665659	4.236008	3.661469	4.051442
21	H	2.643039	4.697659	2.626035	4.287671	4.600280
22	H	4.536202	2.566466	4.573765	2.516148	5.036729
23	H	2.589073	2.646200	5.157990	4.621169	4.199800
24	H	3.877297	3.901144	2.587494	2.517181	4.888874
25	H	4.409315	5.915225	3.915014	4.880020	2.713468
26	H	6.496573	4.722773	6.440811	4.308614	4.954762
27	H	4.773152	4.645375	5.667364	4.832569	2.630035
28	H	6.587006	6.445268	5.116791	4.572294	4.630203
29	H	4.536088	2.619264	6.253131	4.479603	4.173242
30	H	5.151656	6.320022	2.595565	4.178004	4.619888
31	H	2.571932	4.815947	3.901630	4.914947	2.647094
32	H	5.569238	4.589633	4.061653	2.595008	5.206171
33	H	3.453939	3.138129	3.075951	1.822939	1.821136

		6	7	8	9	10
6	Fe	0.000000				
7	Fe	3.771242	0.000000			
8	Fe	2.706299	2.731424	0.000000		
9	O	4.227854	4.138309	5.614817	0.000000	
10	O	1.980336	5.450725	4.269048	4.748582	0.000000
11	O	5.436238	1.980077	4.274162	4.610054	6.817624
12	O	3.687835	3.885016	1.924567	6.317647	4.504539
13	O	5.579469	4.294958	5.808458	3.165232	5.971617
14	O	3.811282	5.018821	4.036781	5.289668	3.413781
15	O	4.007077	1.973446	4.136865	3.188270	5.637092
16	O	1.984847	4.075103	1.979607	5.951833	3.476320
17	O	4.255027	5.678365	5.843927	3.316338	3.443961
18	O	4.952083	3.647413	3.871531	5.272814	5.577054
19	O	1.967636	3.941682	4.101674	3.182367	3.110692
20	O	4.107574	1.987726	1.974761	5.924862	5.932546
21	H	6.346566	5.147818	6.514861	3.995771	6.551008
22	H	3.969601	5.391625	3.916083	6.104962	3.570609
23	H	4.652954	6.351950	6.549546	3.454589	3.649761
24	H	5.341081	4.540496	4.539995	5.600502	5.626848
25	H	4.924363	2.572495	5.012305	3.297014	6.457547
26	H	2.634454	4.996977	2.647516	6.784793	3.674852
28	H	4.596526	2.669277	2.651113	6.501363	6.502454

29	H	2.570777	6.083189	5.098326	4.823358	0.970624
30	H	6.119321	2.610767	4.578652	5.570793	7.517331
31	H	5.077845	4.367766	6.220026	0.970707	5.712297
32	H	4.572568	4.072662	2.555585	6.777424	5.402390
33	H	1.927668	1.920786	1.863888	3.752728	3.555360

		11	12	13	14	15
11	O	0.000000				
12	O	4.756043	0.000000			
13	O	3.542066	5.674700	0.000000		
14	O	5.526869	2.916075	4.427197	0.000000	
15	O	3.143350	5.534343	4.607394	6.100276	0.000000
16	O	5.904804	3.328916	6.973805	4.756267	4.744473
17	O	6.102620	5.623865	3.556997	3.238178	5.729480
18	O	3.231697	2.953670	3.298126	2.910346	5.193582
19	O	5.554289	5.379837	5.552775	5.236565	3.160388
20	O	3.421744	3.431487	6.070217	5.602726	3.486962
21	H	4.214286	6.139218	0.969487	4.653376	5.567384
22	H	6.031936	2.542198	5.328359	0.972888	6.613079
23	H	6.855452	6.461773	4.238452	4.099513	6.148834
24	H	4.113965	3.343692	3.410951	2.555356	5.968628
25	H	3.155138	6.312713	4.600602	6.761858	0.970850
26	H	6.778215	3.618019	7.754768	5.056939	5.711731
27	H	5.876655	5.967704	6.253912	6.130591	3.124043
28	H	4.110061	4.240019	6.908071	6.491714	3.772646
29	H	7.470794	5.464168	6.429992	4.250453	5.985277
30	H	0.970486	4.890660	4.211157	5.953507	3.975226
31	H	4.538931	6.960247	3.185923	6.046470	3.242847
32	H	4.576950	0.972321	5.713731	3.340256	5.893498
33	H	3.532870	2.994562	4.391111	3.683602	2.766982

		16	17	18	19	20
16	O	0.000000				
17	O	6.088808	0.000000			
18	O	5.532770	4.730902	0.000000		
19	O	3.448308	4.469113	5.962549	0.000000	
20	O	3.395135	7.031095	4.441020	4.791469	0.000000
21	H	7.733004	3.840285	3.531740	6.430427	6.842198
22	H	4.547511	4.102490	3.343763	5.638455	5.633618
23	H	6.570827	0.969640	5.687500	4.595271	7.731115
24	H	6.048525	4.486907	0.972776	6.425032	5.336265
25	H	5.712934	6.154263	5.607354	3.933806	4.177449
26	H	0.969573	6.600132	6.123845	4.190180	4.148982
27	H	3.670549	5.408902	6.666844	0.970470	4.866890
28	H	3.639853	7.824247	5.406708	5.109841	0.969509
29	H	4.113468	3.621065	6.413743	3.141726	6.658271
30	H	6.359641	6.871410	3.374323	6.400648	3.558009
31	H	6.693527	4.086204	5.649349	3.930595	6.262105

32	H	4.194159	6.135498	2.641213	6.153340	3.591407
33	H	2.681294	4.444128	3.565940	2.711208	2.684062

		21	22	23	24	25
21	H	0.000000				
22	H	5.557389	0.000000			
23	H	4.516005	4.902911	0.000000		
24	H	3.419620	3.031186	5.454734	0.000000	
25	H	5.534020	7.342682	6.539963	6.377903	0.000000
26	H	8.466679	4.683652	7.055012	6.555465	6.680726
27	H	7.168415	6.484327	5.493170	7.208307	3.858108
28	H	7.711693	6.483173	8.471037	6.305089	4.424428
29	H	7.014573	4.465107	3.565154	6.448601	6.762220
30	H	4.745740	6.367662	7.671090	4.265909	3.975211
31	H	3.990653	6.884553	4.211158	6.021154	3.058362
32	H	6.091763	3.009577	7.028888	3.059379	6.582913
33	H	5.215071	4.000620	5.084118	4.213019	3.640404

		26	27	28	29	30
26	H	0.000000				
27	H	4.407056	0.000000			
28	H	4.335928	5.004768	0.000000		
29	H	4.286217	3.898126	7.166113	0.000000	
30	H	7.181590	6.701747	4.208215	8.228831	0.000000
31	H	7.567410	4.334162	6.799734	5.786697	5.489123
32	H	4.497131	6.724592	4.423602	6.362813	4.531756
33	H	3.572081	3.252335	3.400290	4.242180	4.193909

		31	32	33
31	H	0.000000		
32	H	7.331165	0.000000	
33	H	4.380276	3.598183	0.000000

Alpha occ. eigenvalues -- -0.19671 -0.19158 -0.18812 -0.18551 -0.18191
Alpha occ. eigenvalues -- -0.18094 -0.17860 -0.17460 -0.16916 -0.16810
Alpha occ. eigenvalues -- -0.16606 -0.16293 -0.15797
Alpha virt. eigenvalues -- -0.07369 -0.05449 -0.04747 -0.03041 -0.01811
Beta occ. eigenvalues -- -0.17835 -0.17625 -0.17036 -0.16219 -0.16191
Beta occ. eigenvalues -- -0.15609 -0.15328 -0.14990 -0.13952
Beta virt. eigenvalues -- -0.11650 -0.11521 -0.11207 -0.11011 -0.10344
Mulliken atomic spin densities:

		1
1	Fe	3.568923
2	Fe	3.544133
3	Fe	3.557562
4	Fe	2.524255
5	Fe	3.058677
6	Fe	3.546945
7	Fe	3.552640
8	Fe	3.502223

```
     9  O    0.187810
    10  O    0.157721
    11  O    0.151453
    12  O    0.171254
    13  O    0.142951
    14  O    0.186341
    15  O    0.185915
    16  O    0.160539
    17  O    0.142069
    18  O    0.183041
    19  O    0.203800
    20  O    0.166101
    21  H    0.012717
    22  H    0.009397
    23  H    0.011257
    24  H    0.011311
    25  H    0.010355
    26  H    0.012358
    27  H    0.012498
    28  H    0.011366
    29  H    0.011556
    30  H    0.011379
    31  H    0.007179
    32  H    0.010777
    33  H   -0.026502
 Sum of Mulliken atomic spin densities =  29.00000
Dipole moment (field-independent basis, Debye):
    X=           -0.1307    Y=           -0.6559    Z=            0.9891  Tot=
1.1940

Isotropic polarizability for W=    0.000000      295.38 Bohr**3.   1.33 A**3


Frequencies --    45.2687           55.6540           65.1044
 Frequencies --    68.1669           71.1687           76.3022
 Frequencies --    82.0449           92.0746           95.4624
 Frequencies --   101.4391          104.6920          107.1136
 Frequencies --   110.3947          112.6191          121.9795
 Frequencies --   123.1861          125.3636          128.9078
 Frequencies --   131.5843          132.7646          139.3857
 Frequencies --   143.3994          149.3808          152.5926
 Frequencies --   170.9164          188.5530          198.9504
 Frequencies --   213.0027          219.3509          225.5701
 Frequencies --   272.5070          285.4146          314.2024
 Frequencies --   322.8759          342.2690          345.3580
 Frequencies --   353.0990          356.1471          376.1367
```

```
Frequencies --   379.3457            382.6444            385.3916
Frequencies --   388.6877            392.2614            393.5653
Frequencies --   398.8006            403.5566            421.6764
Frequencies --   431.2289            450.0368            454.0493
Frequencies --   463.5959            471.5029            475.9613
Frequencies --   489.4218            504.6831            507.7133
Frequencies --   518.4921            524.7935            528.6345
Frequencies --   534.2877            538.3977            543.7279
Frequencies --   555.7814            584.6105            610.9877
Frequencies --   617.3734            631.0134            660.6471
Frequencies --   669.2950            675.3437            680.1014
Frequencies --   682.1742            697.0201            705.6324
Frequencies --   708.4522            714.8004            734.0029
Frequencies --   803.1384            916.2842           1176.4378
Frequencies --  3682.6138           3683.6319           3690.7789
Frequencies --  3700.0072           3704.8506           3710.3988
Frequencies --  3713.5514           3714.0726           3720.1821
Frequencies --  3721.5650           3723.6613           3724.5798
[headnode:~/feon] ggutsev% grep "Inten" fe8o12h13_30_GF.out
IR Inten    --     0.6960              0.0701              3.9964
IR Inten    --     2.1253              3.0120              0.4398
IR Inten    --     0.3324              0.2767              4.7173
IR Inten    --     2.5572              0.9972              0.1654
IR Inten    --     3.7824              6.0422              0.7979
IR Inten    --     0.4375              2.0622              4.1678
IR Inten    --     0.4241              9.2304              8.4977
IR Inten    --     5.5601              3.2538              3.1343
IR Inten    --    10.2042              3.6813              1.2494
IR Inten    --     8.3219             17.5129             15.9702
IR Inten    --     8.7857              5.2238             10.9251
IR Inten    --     8.1355             12.3800             23.8693
IR Inten    --   140.1447             94.4870             15.3356
IR Inten    --    48.9751             12.6984              0.6715
IR Inten    --    28.4185            123.7968             47.2813
IR Inten    --    27.7018             55.6006            147.3305
IR Inten    --   125.9555             64.2076            314.7399
IR Inten    --   155.3931             57.8019             31.3175
IR Inten    --    40.6016              2.5629              4.4944
IR Inten    --     4.1836             12.6253             34.3104
IR Inten    --    14.9716             57.4806             32.1449
IR Inten    --    54.9979             47.3640              1.9387
IR Inten    --    71.0832             50.1880             47.7029
IR Inten    --    11.9401             62.6378             57.8849
IR Inten    --    27.2889             52.5441             74.4050
IR Inten    --    31.4508             40.5648            125.4884
IR Inten    --     0.7805              5.9524              3.2089
```

IR Inten -- 49.7248 13.6590 25.3920
IR Inten -- 25.5031 10.3374 43.8576
IR Inten -- 30.5272 45.9295 41.5612
IR Inten -- 38.7036 44.2670 44.1853
Zero-point vibrational energy 448694.4 (Joules/Mol)
107.24054 (Kcal/Mol) 4.650 eV

Atom	No	Natural Electron Configuration
Fe	1	[core]4S(0.24)3d(6.51)4p(0.40)4d(0.02)5p(0.01)
Fe	2	[core]4S(0.24)3d(6.48)4p(0.40)4d(0.03)5p(0.01)
Fe	3	[core]4S(0.23)3d(6.49)4p(0.40)4d(0.03)5p(0.01)
Fe	4	[core]4S(0.32)3d(6.88)4p(0.72)4d(0.04)5p(0.01)
Fe	5	[core]4S(0.25)3d(6.64)4p(0.60)4d(0.03)5p(0.01)
Fe	6	[core]4S(0.22)3d(6.54)4p(0.44)4d(0.03)5p(0.01)
Fe	7	[core]4S(0.22)3d(6.54)4p(0.45)4d(0.03)5p(0.01)
Fe	8	[core]4S(0.21)3d(6.52)4p(0.41)4d(0.02)
O	9	[core]2S(1.71)2p(5.17)3S(0.01)3p(0.01)
O	10	[core]2S(1.71)2p(5.20)3S(0.01)3p(0.01)
O	11	[core]2S(1.71)2p(5.21)3S(0.01)3p(0.01)
O	12	[core]2S(1.72)2p(5.17)3S(0.01)3p(0.01)
O	13	[core]2S(1.71)2p(5.23)3S(0.01)3p(0.01)
O	14	[core]2S(1.71)2p(5.17)3S(0.01)3p(0.01)
O	15	[core]2S(1.71)2p(5.18)3S(0.01)3p(0.01)
O	16	[core]2S(1.71)2p(5.22)3S(0.01)3p(0.01)
O	17	[core]2S(1.71)2p(5.22)3S(0.01)3p(0.01)
O	18	[core]2S(1.71)2p(5.17)3S(0.01)3p(0.01)
O	19	[core]2S(1.70)2p(5.19)3S(0.01)3p(0.01)
O	20	[core]2S(1.71)2p(5.22)3S(0.01)3p(0.01)
H	21	1S(0.52)
H	22	1S(0.52)
H	23	1S(0.52)
H	24	1S(0.52)
H	25	1S(0.53)
H	26	1S(0.52)
H	27	1S(0.52)
H	28	1S(0.52)
H	29	1S(0.52)
H	30	1S(0.52)
H	31	1S(0.53)
H	32	1S(0.52)
H	33	1S(1.04)2S(0.02)

****
******* Alpha spin orbitals *******

****

Atom	No	Natural Electron Configuration	
Fe	1	[core]3d(4.89)4p(0.21)5S(0.13)4d(0.02)	3.32
Fe	2	[core]3d(4.89)4p(0.21)4d(0.01)6S(0.13)	
Fe	3	[core]3d(4.90)4p(0.21)4d(0.02)6S(0.13)	
Fe	4	[core]3d(4.85)4p(0.36)5S(0.17)4d(0.02)5d(0.01)	
Fe	5	[core]3d(4.86)4p(0.31)4d(0.02)6S(0.14)5d(0.01)	
Fe	6	[core]3d(4.89)4p(0.24)5S(0.12)4d(0.01)	
Fe	7	[core]3d(4.89)4p(0.24)4d(0.01)6S(0.12)	
Fe	8	[core]3d(4.89)4p(0.22)5S(0.13)4d(0.01)	
O	9	[core]2S(0.87)2p(2.69)3p(0.01)4S(0.01)	
O	10	[core]2S(0.87)2p(2.70)4S(0.01)4p(0.01)	
O	11	[core]2S(0.87)2p(2.70)4S(0.01)4p(0.01)	
O	12	[core]2S(0.87)2p(2.68)3p(0.01)	
O	13	[core]2S(0.87)2p(2.71)4S(0.01)4p(0.01)	
O	14	[core]2S(0.87)2p(2.68)3p(0.01)4p(0.01)	
O	15	[core]2S(0.87)2p(2.70)3p(0.01)4S(0.01)	
O	16	[core]2S(0.87)2p(2.70)3p(0.01)4S(0.01)	
O	17	[core]2S(0.87)2p(2.70)4S(0.01)4p(0.01)	
O	18	[core]2S(0.87)2p(2.69)3p(0.01)	
O	19	[core]2S(0.87)2p(2.71)4S(0.01)4p(0.01)	
O	20	[core]2S(0.87)2p(2.71)4S(0.01)4p(0.01)	
H	21	1S(0.26)	
H	22	1S(0.26)	
H	23	1S(0.26)	
H	24	1S(0.26)	
H	25	1S(0.26)	
H	26	1S(0.26)	
H	27	1S(0.26)	
H	28	1S(0.26)	
H	29	1S(0.26)	
H	30	1S(0.26)	
H	31	1S(0.26)	
H	32	1S(0.26)	
H	33	1S(0.55)3S(0.01)	

NBO analysis skipped by request.

****

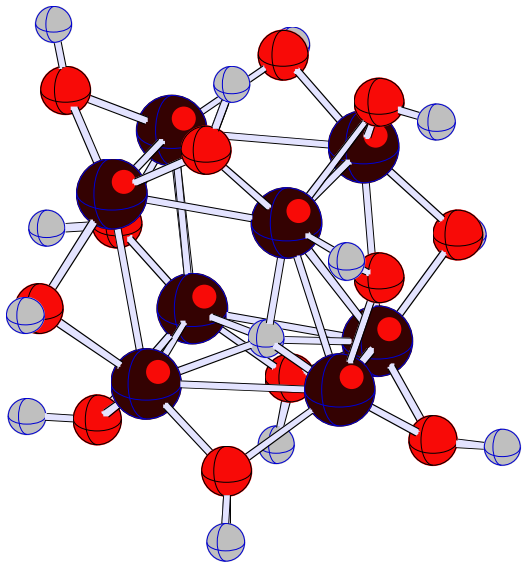
******* Beta spin orbitals *******

****

Atom	No	Natural Electron Configuration

Fe	1	[core]3d(1.62)4p(0.19)5S(0.11)4d(0.01)
Fe	2	[core]3d(1.59)4p(0.19)4d(0.01)6S(0.11)
Fe	3	[core]3d(1.60)4p(0.19)4d(0.01)6S(0.11)
Fe	4	[core]3d(2.03)4p(0.36)5S(0.15)4d(0.01)
Fe	5	[core]3d(1.79)4p(0.29)4d(0.01)6S(0.12)
Fe	6	[core]3d(1.65)4p(0.21)4d(0.01)6S(0.10)
Fe	7	[core]3d(1.65)4p(0.21)4d(0.01)6S(0.09)
Fe	8	[core]3d(1.63)4p(0.19)4d(0.01)6S(0.08)
O	9	[core]2S(0.84)2p(2.49)
O	10	[core]2S(0.84)2p(2.50)
O	11	[core]2S(0.84)2p(2.51)
O	12	[core]2S(0.85)2p(2.49)
O	13	[core]2S(0.84)2p(2.52)
O	14	[core]2S(0.85)2p(2.49)
O	15	[core]2S(0.84)2p(2.48)
O	16	[core]2S(0.84)2p(2.51)
O	17	[core]2S(0.85)2p(2.52)
O	18	[core]2S(0.84)2p(2.49)
O	19	[core]2S(0.84)2p(2.48)
O	20	[core]2S(0.84)2p(2.51)
H	21	1S(0.25)
H	22	1S(0.25)
H	23	1S(0.26)
H	24	1S(0.25)
H	25	1S(0.26)
H	26	1S(0.26)
H	27	1S(0.26)
H	28	1S(0.26)
H	29	1S(0.26)
H	30	1S(0.26)
H	31	1S(0.26)
H	32	1S(0.26)
H	33	1S(0.49)

HF=-11021.98748816\S2=224.981106\S2-1=0.\S2A=224.75316



TITLE

Fe	2.5403916601,0.2101745007,0.2209911944
Fe	0.9432411276,2.1273361047,-0.6972288335
Fe	1.2634397297,-1.9132366823,-0.8471989724
Fe	-0.1607880813,0.0455729186,-1.2017108616
Fe	0.5293171224,-0.1509410864,1.6042629382
Fe	-1.1653234849,1.7086361406,0.9127489898
Fe	-0.8868859933,-2.0473370182,0.7193538856
Fe	-2.4988833908,-0.1938604694,-0.47512037
O	2.4538859992,-0.0806856116,2.1674983552
O	-0.2438746985,3.3485592333,0.2936251662
O	0.2574616193,-3.4391028345,-0.1017196392
O	-2.0008808616,0.1180138848,-2.3077926928
O	3.1654793057,-1.475042221,-0.583518771
O	0.5403309542,1.5364950709,-2.4912167612
O	-0.1929317644,-1.8160257244,2.5522241679
O	-3.0926426274,1.3761241486,0.574375983
O	2.8900619108,2.0619084344,-0.325921341
O	0.5353663961,-1.3727556086,-2.5708986258
O	-0.3507499978,1.338398391,2.6651718758
O	-2.8221329717,-1.9943863535,0.2687191843
H	3.8236857233,-1.5355033248,-1.2927532615
H	-0.2574601322,1.8535850413,-2.9489222732
H	3.3424495038,2.671230203,0.2776305753
H	1.068707413,-0.8602604115,-3.2027128466
H	0.3670236321,-2.5212940824,2.9149867803
H	-3.6862066199,2.0634798908,0.2348240795
H	-0.8467113272,1.0994791298,3.4643919338
H	-3.5460062481,-2.2231211426,0.8717406833
H	0.0894901544,3.9514380279,0.9773766496

H -0.1238710676,-4.1019452956,-0.699272094
H 2.9054376912,-0.8590855229,2.5314583126
H -1.969863718,-0.6213130136,-2.9385402259
H -0.8870289654,-0.1442079093,0.4595122494
END

$Fe_8O_{12}H_{14}$

$$$$$$$$$$$$$ Fe_8O_12H_14 NEUTRAL S = 29 head fe8o12h14_29_GF.out GS

UBPW91/6-311+G* scf=(VSHIFT=5,NoIncFock,MAXCYC=77,Tight,NoVarAcc) NO SYMM OPT=RFO IOP(5/13=1,5/36=1,8/11=1) INT=UltraFine GUESS=READ GEOM=CHECKPOINT

Charge = 0 Multiplicity =29

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	2.592956	1.044421	0.145035
2	26	0	0.642648	1.130815	1.926505
3	26	0	0.666755	1.238149	-1.788182
4	26	0	-0.977985	0.934800	0.069410
5	26	0	1.188133	-1.013996	-0.051150
6	26	0	-0.583024	-1.146974	1.939531
7	26	0	-0.552103	-1.065674	-1.808182
8	26	0	-2.546577	-0.987730	-0.085749
9	8	0	3.192580	-0.795602	-0.128308
10	8	0	0.114930	-0.069608	3.433107
11	8	0	-0.084319	0.167669	-3.291080
12	8	0	-2.990234	0.906996	0.126364
13	8	0	2.493620	1.972593	-1.592320
14	8	0	-0.811346	2.387746	1.502563
15	8	0	0.839985	-2.438360	-1.500519
16	8	0	-2.417812	-1.890554	1.661739
17	8	0	2.534988	1.804492	1.952806
18	8	0	-1.002977	2.304778	-1.496789
19	8	0	0.882584	-2.357826	1.441492

20	8	0	-2.523262	-1.603226	-1.934993
21	1	0	2.792251	2.867121	-1.813437
22	1	0	-1.608426	2.440424	2.055294
23	1	0	3.197468	1.601280	2.630390
24	1	0	-0.891388	3.176740	-1.078136
25	1	0	1.480744	-2.578099	-2.216808
26	1	0	-3.119324	-1.820837	2.327668
27	1	0	0.703476	-3.254011	1.110448
28	1	0	-2.833501	-2.471747	-2.234012
29	1	0	0.774698	-0.501972	3.999724
30	1	0	-0.826429	0.624445	-3.724276
31	1	0	3.691977	-1.018679	-0.930440
32	1	0	-3.302986	1.417252	-0.641492
33	1	0	-0.730618	-0.830636	-0.020889
34	1	0	0.762498	0.945819	0.074677

Distance matrix (angstroms):

		1	2	3	4	5
1	Fe	0.000000				
2	Fe	2.642878	0.000000			
3	Fe	2.735893	3.716316	0.000000		
4	Fe	3.573424	2.472584	2.499568	0.000000	
5	Fe	2.499820	2.967977	2.891587	2.916232	0.000000
6	Fe	4.255500	2.586651	4.598544	2.826151	2.667862
7	Fe	4.261332	4.494427	2.606456	2.776441	2.473510
8	Fe	5.531519	4.325338	4.263604	2.486097	3.734963
9	O	1.954469	3.799407	3.642954	4.519624	2.017786
10	O	4.265336	1.997336	5.410786	3.676650	3.766122
11	O	4.443353	5.355308	1.992170	3.560902	3.675951
12	O	5.584913	4.060595	4.141101	2.013247	4.602225
13	O	1.972251	4.064088	1.978688	3.986277	3.605443
14	O	3.903419	1.968171	3.786207	2.047620	4.240730
15	O	4.232082	4.952014	3.691812	4.141003	2.061721
16	O	6.001855	4.308733	5.586170	3.548413	4.087197
17	O	1.961914	2.008852	4.219720	4.079771	3.711299
18	O	4.149075	3.975576	2.002652	2.080971	4.231441
19	O	4.022618	3.530357	4.838224	4.023147	2.031555
20	O	6.124723	5.692901	4.274479	3.584283	4.203630
21	H	2.682828	4.650023	2.678044	4.636125	4.554330
22	H	4.821776	2.607488	4.625389	2.570621	4.918421
23	H	2.617731	2.691450	5.104915	4.943402	4.250618
24	H	4.264222	3.945496	2.586525	2.520051	4.789716
25	H	4.465195	5.623654	3.925563	4.859280	2.687399
26	H	6.753053	4.798500	6.374324	4.156753	4.986376
27	H	4.793607	4.460532	5.346298	4.632193	2.569410
28	H	6.889829	6.509375	5.119950	4.511459	4.802444

29	H	4.533875	2.642285	6.044794	4.536913	4.103983
30	H	5.180747	5.860539	2.520851	3.809376	4.498311
31	H	2.573106	4.699028	3.870524	5.159876	2.653754
32	H	5.959846	4.716426	4.135918	2.478663	5.140974
33	H	3.819623	3.086339	3.058733	1.784967	1.927730
34	H	1.834462	1.864900	1.888086	1.740526	2.009446

		6	7	8	9	10
6	Fe	0.000000				
7	Fe	3.748723	0.000000			
8	Fe	2.825360	2.636434	0.000000		
9	O	4.319098	4.113097	5.742530	0.000000	
10	O	1.969423	5.376634	4.506541	4.762633	0.000000
11	O	5.416298	1.984677	4.203786	4.655007	6.731322
12	O	3.647058	3.684885	1.957501	6.418013	4.640081
13	O	5.627736	4.307445	6.036295	3.208548	5.923147
14	O	3.568938	4.791070	4.114316	5.368879	3.259383
15	O	3.940378	1.979099	3.946481	3.180617	5.520630
16	O	1.999131	4.025128	1.971138	5.989966	3.587251
17	O	4.293406	5.649161	6.146098	3.394695	3.400033
18	O	4.888685	3.414703	3.900556	5.393310	5.584917
19	O	1.965252	3.779995	3.996095	3.200140	3.129180
20	O	4.357135	2.047074	1.949124	6.048737	6.174831
21	H	6.449047	5.162518	6.807927	4.051600	6.581690
22	H	3.732864	5.323062	4.149268	6.187862	3.341944
23	H	4.724649	6.393188	6.861082	3.654515	3.596980
24	H	5.281658	4.318120	4.589912	5.775852	5.648253
25	H	4.856173	2.566490	4.825972	3.235663	6.330838
26	H	2.652839	4.926068	2.616617	6.850040	3.840468
27	H	2.604240	3.857940	4.138812	3.711324	3.985167
28	H	4.923224	2.713513	2.626723	6.599781	6.824937
29	H	2.550261	5.984140	5.287525	4.793018	0.971230
30	H	5.939350	2.569663	4.335539	5.576733	7.252310
31	H	5.150614	4.334149	6.295556	0.970864	5.721586
32	H	4.542590	3.885028	2.581655	6.881312	5.522251
33	H	1.991256	1.811498	1.823895	3.924825	3.636510
34	H	3.109323	3.052775	3.835925	2.996506	3.567841

		11	12	13	14	15
11	O	0.000000				
12	O	4.546413	0.000000			
13	O	3.576214	5.844829	0.000000		
14	O	5.332572	2.972221	4.546807	0.000000	
15	O	3.294212	5.339357	4.711628	5.919180	0.000000
16	O	5.849093	3.242118	7.045209	4.572737	4.573096
17	O	6.085911	5.888079	3.549350	3.426493	5.727154
18	O	2.937797	2.921918	3.513640	3.006612	5.088603
19	O	5.450712	5.233292	5.527384	5.039204	2.943421

20	O	3.305069	3.281534	6.170333	5.538529	3.492513
21	H	4.212496	6.406407	0.968635	4.920525	5.661924
22	H	6.006000	2.825166	5.509150	0.971403	6.514680
23	H	6.920201	6.711173	4.297040	4.238055	6.240259
24	H	3.821387	3.317787	3.629412	2.699801	5.891130
25	H	3.338072	6.134003	4.703690	6.614153	0.971169
26	H	6.688478	3.507631	7.826976	4.870290	5.541884
27	H	5.630449	5.650301	6.150362	5.854730	2.738808
28	H	3.954986	4.124542	6.967220	6.454904	3.746148
29	H	7.371713	5.582368	6.352096	4.135434	5.831513
30	H	0.973155	4.425981	4.169588	5.516276	4.135553
31	H	4.608736	7.033989	3.289658	6.148426	3.236409
32	H	4.352194	0.973538	5.900264	3.427404	5.724323
33	H	3.479722	2.854280	4.552274	3.561658	2.690888
34	H	3.556816	3.753289	2.613413	2.568073	3.733619

		16	17	18	19	20
16	O	0.000000				
17	O	6.186139	0.000000			
18	O	5.438645	4.966608	0.000000		
19	O	3.340579	4.507413	5.824835	0.000000	
20	O	3.609731	7.232802	4.216133	4.854880	0.000000
21	H	7.864927	3.921728	3.849708	6.445266	6.946470
22	H	4.423501	4.193184	3.605864	5.441056	5.754165
23	H	6.683006	0.969172	5.930620	4.737793	7.989889
24	H	5.959392	4.775953	0.973674	6.334582	5.123016
25	H	5.542074	6.140376	5.525376	3.713418	4.130601
26	H	0.969763	6.727167	6.010498	4.133876	4.309631
27	H	3.450417	5.445407	6.372581	0.972017	4.734093
28	H	3.960740	8.039674	5.168124	5.227963	0.969531
29	H	4.193621	3.550813	6.422587	3.162339	6.878238
30	H	6.153607	6.702306	2.795780	6.204822	3.323145
31	H	6.693958	4.197860	5.780026	3.913063	6.322975
32	H	4.126740	6.400178	2.609459	6.009079	3.377040
33	H	2.607928	4.637193	3.476101	2.659566	2.733909
34	H	4.547323	2.721473	2.726385	3.577243	4.618725

		21	22	23	24	25
21	H	0.000000				
22	H	5.874956	0.000000			
23	H	4.638335	4.912384	0.000000		
24	H	3.769049	3.297679	5.740556	0.000000	
25	H	5.615441	7.278695	6.626438	6.327856	0.000000
26	H	8.606533	4.529387	7.190576	6.445073	6.510478
27	H	7.097910	6.218056	5.666045	6.977682	3.483049
28	H	7.767205	6.635389	8.753545	6.083853	4.315590
29	H	7.015280	4.256499	3.488346	6.487945	6.591970
30	H	4.666449	6.108414	7.584704	3.677022	4.225138

31	H	4.085171	6.998162	4.448397	6.215351	2.996011
32	H	6.373969	3.345305	7.279765	3.016995	6.428726
33	H	5.412692	3.972520	5.326665	4.147611	3.572927
34	H	3.372873	3.431904	3.590317	3.006880	4.264361

		26	27	28	29	30
26	H	0.000000				
27	H	4.260213	0.000000			
28	H	4.616742	4.930270	0.000000		
29	H	4.438309	3.990828	7.467167	0.000000	
30	H	6.918294	6.384166	3.979401	7.968224	0.000000
31	H	7.592927	4.253595	6.811209	5.751871	5.560698
32	H	4.397142	6.398572	4.228576	6.469297	4.033043
33	H	3.493155	3.034682	3.466018	4.305732	3.980140
34	H	5.272465	4.326069	5.471838	4.183568	4.130377

		31	32	33	34
31	H	0.000000			
32	H	7.412607	0.000000		
33	H	4.519070	3.472063	0.000000	
34	H	3.667609	4.154913	2.322567	0.000000

Alpha occ. eigenvalues -- -0.19581 -0.19421 -0.19020 -0.18924 -0.18836
Alpha occ. eigenvalues -- -0.18326 -0.17828 -0.17508 -0.17395 -0.17179
Alpha occ. eigenvalues -- -0.16819 -0.16401 -0.16290
Alpha virt. eigenvalues -- -0.10569 -0.05604 -0.05199 -0.03765 -0.02716
1.556 eV
Beta occ. eigenvalues -- -0.19785 -0.18334 -0.17740 -0.17341 -0.16746
Beta occ. eigenvalues -- -0.15886 -0.15716 -0.15425 -0.14883 -0.13638
Beta virt. eigenvalues -- -0.12439 -0.12068 -0.11767 -0.10868 -0.10657
0.326 eV
Mulliken atomic spin densities:

		1
1	Fe	3.401666
2	Fe	3.477965
3	Fe	3.491885
4	Fe	2.417560
5	Fe	2.986927
6	Fe	3.556860
7	Fe	3.389761
8	Fe	3.406096
9	O	0.183488
10	O	0.159468
11	O	0.166846
12	O	0.143267
13	O	0.151372
14	O	0.174766
15	O	0.177895
16	O	0.140396

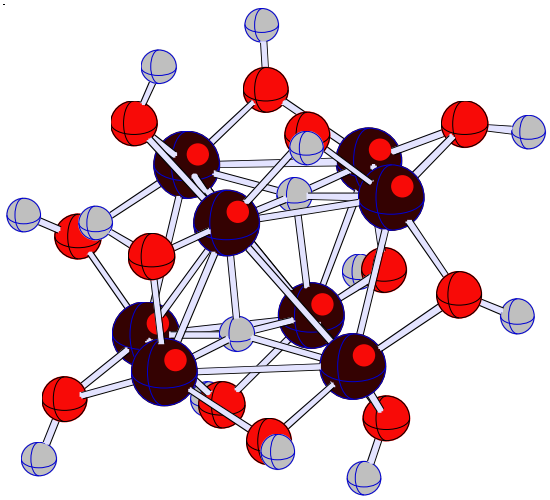
17	O	0.146076
18	O	0.169576
19	O	0.218750
20	O	0.150445
21	H	0.011829
22	H	0.010094
23	H	0.008815
24	H	0.008452
25	H	0.009896
26	H	0.013239
27	H	0.005988
28	H	0.012139
29	H	0.008039
30	H	0.002197
31	H	0.007934
32	H	0.008040
33	H	-0.096749
34	H	-0.120979

Sum of Mulliken atomic spin densities = 28.00000

Dipole moment (field-independent basis, Debye):

X= 0.5236 Y= -0.4556 Z= 0.3573 Tot= 0.7806

Isotropic polarizability for W= 0.000000 304.07 Bohr**3. 1.325 A**3



Frequencies --	45.1136	53.0028	59.1232
Frequencies --	69.5407	78.3164	78.7167
Frequencies --	85.2337	86.2052	96.2933
Frequencies --	97.6117	100.9419	109.7715
Frequencies --	111.5723	113.3540	116.7914
Frequencies --	122.4762	128.3950	131.7486
Frequencies --	134.0271	138.9682	142.7868

Frequencies --	150.4113	156.4147	166.8945
Frequencies --	167.7456	193.7310	212.9398
Frequencies --	222.3033	225.1365	236.7266
Frequencies --	274.3086	285.9731	296.6870
Frequencies --	314.2115	320.8153	338.1694
Frequencies --	340.3353	350.7069	352.1299
Frequencies --	356.7791	359.8216	366.0279
Frequencies --	372.2818	382.2298	386.5367
Frequencies --	388.1373	437.6846	445.6192
Frequencies --	450.0311	452.7145	455.9815
Frequencies --	469.0943	471.3596	477.5603
Frequencies --	484.2491	492.2146	515.0757
Frequencies --	516.5921	530.6091	552.8729
Frequencies --	570.6220	588.7381	590.3544
Frequencies --	607.6201	623.8761	625.5677
Frequencies --	627.6226	640.4564	654.2358
Frequencies --	662.6475	664.7882	672.1954
Frequencies --	678.4284	684.6816	697.2530
Frequencies --	712.8687	717.8181	727.4751
Frequencies --	736.1120	914.1816	928.6511
Frequencies --	961.0343	992.4555	1274.0841
Frequencies --	3670.2721	3670.9922	3673.0391
Frequencies --	3693.6584	3697.7272	3699.4500
Frequencies --	3701.0152	3702.3743	3722.1248
Frequencies --	3722.9190	3723.2843	3731.5375

Zero-point vibrational energy 466730.6 (Joules/Mol)
111.55129 (Kcal/Mol) 4.837 eV

Atom	No	Natural Electron Configuration
Fe	1	[core]4S(0.21)3d(6.57)4p(0.40)4d(0.02)
Fe	2	[core]4S(0.21)3d(6.55)4p(0.46)4d(0.03)5p(0.01)
Fe	3	[core]4S(0.21)3d(6.55)4p(0.43)4d(0.03)
Fe	4	[core]4S(0.26)3d(6.94)4p(0.75)4d(0.04)5p(0.01)
Fe	5	[core]4S(0.23)3d(6.72)4p(0.63)4d(0.04)5p(0.01)
Fe	6	[core]4S(0.21)3d(6.50)4p(0.41)4d(0.03)5p(0.01)
Fe	7	[core]4S(0.21)3d(6.60)4p(0.48)4d(0.03)5p(0.01)
Fe	8	[core]4S(0.21)3d(6.55)4p(0.39)4d(0.02)
O	9	[core]2S(1.70)2p(5.16)3S(0.01)3p(0.02)
O	10	[core]2S(1.71)2p(5.19)3S(0.01)3p(0.01)
O	11	[core]2S(1.72)2p(5.16)3S(0.01)3p(0.01)
O	12	[core]2S(1.70)2p(5.13)3S(0.01)3p(0.02)
O	13	[core]2S(1.70)2p(5.23)3S(0.01)3p(0.01)
O	14	[core]2S(1.70)2p(5.14)3S(0.01)3p(0.02)
O	15	[core]2S(1.71)2p(5.17)3S(0.01)3p(0.02)
O	16	[core]2S(1.71)2p(5.22)3S(0.01)3p(0.01)

O	17	[core]2S(1.71)2p(5.21)3S(0.01)3p(0.01)
O	18	[core]2S(1.71)2p(5.15)3S(0.01)3p(0.02)
O	19	[core]2S(1.70)2p(5.16)3S(0.01)3p(0.02)
O	20	[core]2S(1.71)2p(5.22)3S(0.01)3p(0.01)
H	21	1S(0.51)
H	22	1S(0.52)
H	23	1S(0.52)
H	24	1S(0.53)
H	25	1S(0.53)
H	26	1S(0.52)
H	27	1S(0.52)
H	28	1S(0.52)
H	29	1S(0.52)
H	30	1S(0.52)
H	31	1S(0.53)
H	32	1S(0.52)
H	33	1S(0.95)2S(0.01)
H	34	1S(0.95)2S(0.01)

****

******* Alpha spin orbitals *******

****

Atom	No	Natural Electron Configuration
Fe	1	[core]3d(4.87)4p(0.22)4d(0.01)6S(0.13)
Fe	2	[core]3d(4.88)4p(0.24)4d(0.02)6S(0.12)
Fe	3	[core]3d(4.88)4p(0.23)4d(0.02)6S(0.12)
Fe	4	[core]3d(4.70)4p(0.39)4d(0.03)6S(0.14)5d(0.01)
Fe	5	[core]3d(4.82)4p(0.33)4d(0.02)6S(0.12)5d(0.01)
Fe	6	[core]3d(4.89)4p(0.22)4d(0.02)6S(0.12)
Fe	7	[core]3d(4.87)4p(0.25)4d(0.02)6S(0.12)
Fe	8	[core]3d(4.87)4p(0.22)5S(0.13)4d(0.02)
O	9	[core]2S(0.86)2p(2.68)3p(0.01)4S(0.01)
O	10	[core]2S(0.87)2p(2.69)3p(0.01)4S(0.01)
O	11	[core]2S(0.87)2p(2.69)3p(0.01)4S(0.01)
O	12	[core]2S(0.86)2p(2.65)3p(0.01)
O	13	[core]2S(0.86)2p(2.71)4S(0.01)4p(0.01)
O	14	[core]2S(0.86)2p(2.67)4p(0.01)
O	15	[core]2S(0.87)2p(2.68)4S(0.01)4p(0.01)
O	16	[core]2S(0.87)2p(2.70)4S(0.01)4p(0.01)
O	17	[core]2S(0.86)2p(2.69)4S(0.01)4p(0.01)
O	18	[core]2S(0.87)2p(2.67)4p(0.01)
O	19	[core]2S(0.87)2p(2.70)4S(0.01)4p(0.01)
O	20	[core]2S(0.87)2p(2.69)3p(0.01)4S(0.01)
H	21	1S(0.26)

H	22	1S(0.26)
H	23	1S(0.26)
H	24	1S(0.27)
H	25	1S(0.27)
H	26	1S(0.26)
H	27	1S(0.26)
H	28	1S(0.26)
H	29	1S(0.26)
H	30	1S(0.26)
H	31	1S(0.26)
H	32	1S(0.26)
H	33	1S(0.48)3S(0.01)
H	34	1S(0.47)3S(0.01)

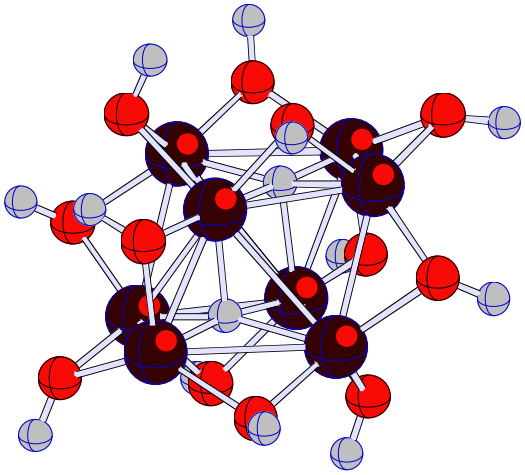
NBO analysis skipped by request.

****
******* Beta spin orbitals *******
****

Atom	No	Natural Electron Configuration
Fe	1	[core]3d(1.69)4p(0.18)4d(0.01)6S(0.08)
Fe	2	[core]3d(1.67)4p(0.22)4d(0.01)6S(0.09)
Fe	3	[core]3d(1.67)4p(0.20)4d(0.01)6S(0.09)
Fe	4	[core]3d(2.24)4p(0.36)4d(0.01)6S(0.12)
Fe	5	[core]3d(1.90)4p(0.30)4d(0.01)6S(0.11)
Fe	6	[core]3d(1.62)4p(0.19)4d(0.01)6S(0.09)
Fe	7	[core]3d(1.73)4p(0.22)4d(0.01)6S(0.09)
Fe	8	[core]3d(1.67)4p(0.17)5S(0.08)4d(0.01)
O	9	[core]2S(0.84)2p(2.48)
O	10	[core]2S(0.84)2p(2.49)
O	11	[core]2S(0.85)2p(2.48)
O	12	[core]2S(0.84)2p(2.48)
O	13	[core]2S(0.84)2p(2.52)
O	14	[core]2S(0.84)2p(2.47)
O	15	[core]2S(0.84)2p(2.48)
O	16	[core]2S(0.84)2p(2.52)
O	17	[core]2S(0.84)2p(2.52)
O	18	[core]2S(0.85)2p(2.49)
O	19	[core]2S(0.84)2p(2.46)
O	20	[core]2S(0.84)2p(2.52)
H	21	1S(0.25)
H	22	1S(0.26)
H	23	1S(0.26)

H	24	1S(0.26)
H	25	1S(0.26)
H	26	1S(0.25)
H	27	1S(0.26)
H	28	1S(0.26)
H	29	1S(0.26)
H	30	1S(0.26)
H	31	1S(0.26)
H	32	1S(0.26)
H	33	1S(0.47)
H	34	1S(0.48)

HF= -11022.5592526\S2=210.212229\S2-1=0.\S2A=210.002888



TITLE

Fe 2.5929563192,1.0444208999,0.1450349155
Fe 0.6426475364,1.1308147384,1.9265047133
Fe 0.6667552693,1.2381487737,-1.7881822965
Fe -0.9779850418,0.9348000551,0.0694101239
Fe 1.1881326903,-1.0139961286,-0.0511497718
Fe -0.583024153,-1.1469741755,1.9395310779
Fe -0.5521026441,-1.0656735057,-1.8081821789
Fe -2.5465774731,-0.9877296384,-0.0857485796
O 3.1925802737,-0.7956016503,-0.1283076455
O 0.1149301924,-0.0696082658,3.4331069812
O -0.0843191469,0.1676687266,-3.2910803193
O -2.9902341268,0.9069962187,0.1263635969
O 2.4936197792,1.9725930822,-1.5923197813
O -0.8113456857,2.3877460281,1.5025632122
O 0.83998491,-2.4383599253,-1.5005194167
O -2.4178120457,-1.890553923,1.6617389101
O 2.5349882735,1.8044924441,1.9528064016

O -1.0029772363,2.3047775911,-1.4967886654
O 0.8825844753,-2.3578258784,1.4414917047
O -2.5232618754,-1.6032259028,-1.9349927166
H 2.7922508238,2.8671205745,-1.8134372229
H -1.6084261992,2.440424084,2.0552936026
H 3.1974681763,1.6012802157,2.6303900219
H -0.8913881355,3.1767402694,-1.0781357595
H 1.4807442356,-2.5780990327,-2.2168078302
H -3.1193237569,-1.8208367164,2.3276676789
H 0.7034764474,-3.2540107908,1.1104476972
H -2.8335012085,-2.4717472777,-2.2340124405
H 0.7746980411,-0.5019719421,3.9997241037
H -0.8264291042,0.6244447023,-3.7242759068
H 3.6919767442,-1.0186785337,-0.9304404698
H -3.3029857492,1.4172520792,-0.6414915873
H -0.73061835,-0.8306357841,-0.0208892792
H 0.7624977445,0.9458185883,0.0746771262
END

$Fe_8O_{12}H_{15}$

$$$$$$$$$$$$$ Fe8O12H15 NEUTRAL S = 28 head fe8o12h15_28_GF.out

---

UBPW91/6-311+G* scf=(VSHIFT=5,NoIncFock,Maxcycle=90,Tight,NoVarAcc) NOSYMM OPT=RFO IOP(5/13=1,5/36=1,8/11=1) INT=UltraFine GUESS=READ GEOM=CHECKPOINT

Charge = 0 Multiplicity = 28

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	1.768138	0.325989	-0.121534
2	26	0	1.181673	-2.097914	0.041463
3	26	0	0.348712	1.136133	-2.194796
4	26	0	-0.556698	-1.111877	-1.425464
5	26	0	0.762401	1.433280	1.818903
6	26	0	-0.339514	-0.805147	1.554371

7	26	0	-0.990447	1.451985	-0.136641
8	26	0	-2.477086	-0.536392	0.097297
9	1	0	1.108756	-0.723784	-1.228392
10	1	0	-1.131856	0.654196	1.332764
11	1	0	-0.696622	-1.678761	0.185847
12	8	0	2.967881	-1.270524	0.296542
13	8	0	0.460614	0.071432	3.211734
14	8	0	-0.314768	-0.363719	-3.264232
15	8	0	-3.035797	1.326721	-0.150365
16	1	0	3.374690	-1.353389	1.174917
17	1	0	-0.128166	0.268822	3.958546
18	1	0	0.306298	-0.870378	-3.814580
19	1	0	-3.411882	1.601870	-1.003916
20	8	0	2.597618	1.627835	1.185033
21	8	0	-0.900058	2.574536	-1.815379
22	8	0	0.701386	-2.473472	1.933527
23	8	0	-2.517453	-1.593303	-1.545818
24	1	0	3.341623	1.291558	1.711109
25	1	0	-0.538334	3.448495	-1.586264
26	1	0	1.329356	-2.256064	2.645323
27	1	0	-2.783676	-2.527083	-1.525238
28	8	0	2.218249	1.476010	-1.713264
29	8	0	-0.241395	2.965931	1.062678
30	8	0	0.481134	-2.985152	-1.585887
31	8	0	-2.361603	-1.375340	1.891812
32	1	0	2.528339	2.353026	-1.430251
33	1	0	-0.904503	3.387677	1.635487
34	1	0	-0.002416	-3.820054	-1.470381
35	1	0	-2.852530	-0.940834	2.609407

Distance matrix (angstroms):

		1	2	3	4	5
1	Fe	0.000000				
2	Fe	2.499163	0.000000			
3	Fe	2.639984	4.019171	0.000000		
4	Fe	3.028622	2.479128	2.542674	0.000000	
5	Fe	2.450081	3.975477	4.045889	4.329408	0.000000
6	Fe	2.920672	2.504825	4.277672	3.003443	2.508935
7	Fe	2.979578	4.165526	2.475704	2.902170	2.626210
8	Fe	4.337455	3.978440	4.004518	2.517514	4.163870
9	H	1.661909	1.872453	2.229550	1.721392	3.749520
10	H	3.260777	3.820207	3.855907	3.325303	2.105116
11	H	3.191950	1.929903	3.831946	1.713844	3.805315
12	O	2.040349	1.984988	4.342673	3.925956	3.806873
13	O	3.589581	3.908530	5.511504	4.892724	1.971214
14	O	3.832851	4.021740	1.957921	1.999834	5.497978

15	O	4.907147	5.436173	3.958652	3.703859	4.279683
16	H	2.661223	2.578441	5.168097	4.719759	3.873538
17	H	4.499588	4.760320	6.232436	5.574722	2.593674
18	H	4.148115	4.140314	2.579067	2.551658	6.103361
19	H	5.407317	5.990156	3.972049	3.961591	5.041961
20	O	2.022364	4.146548	4.089326	4.926502	1.951324
21	O	3.878704	5.441806	1.942263	3.722844	4.156229
22	O	3.632935	1.987869	5.495150	3.836605	3.908910
23	O	4.906991	4.056800	4.010723	2.022577	5.589186
24	H	2.601300	4.352198	4.923186	5.550810	2.585361
25	H	4.149131	6.030802	2.550329	4.563243	4.165113
26	H	3.809859	2.612835	5.991278	4.630083	3.823044
27	H	5.552424	4.285175	4.866140	2.640491	6.280320
28	O	2.014634	4.114182	1.960244	3.805301	3.820671
29	O	3.522765	5.358221	3.782529	4.787357	1.982044
30	O	3.842442	1.981468	4.168129	2.147554	5.585182
31	O	4.899269	4.062106	5.509416	3.785685	4.201555
32	H	2.529728	4.877532	2.610772	4.639292	3.810705
33	H	4.427648	6.081509	4.616391	5.453107	2.575243
34	H	4.705733	2.579439	5.021141	2.764682	6.245147
35	H	5.514839	4.920158	6.135316	4.645458	4.396480

		6	7	8	9	10
6	Fe	0.000000				
7	Fe	2.894457	0.000000			
8	Fe	2.600866	2.493686	0.000000		
9	H	3.138133	3.214428	3.827641	0.000000	
10	H	1.675291	1.677979	2.180258	3.671334	0.000000
11	H	1.662403	3.160997	2.117286	2.484239	2.635818
12	O	3.568973	4.823698	5.497846	2.465906	4.646089
13	O	2.038492	3.901682	4.324263	4.557102	2.531028
14	O	4.838843	3.679014	4.000664	2.510122	4.778718
15	O	3.836786	2.049229	1.960787	4.748056	2.505385
16	H	3.773575	5.352077	6.006000	3.362552	4.936017
17	H	2.641616	4.349018	4.590755	5.423981	2.837365
18	H	5.408046	4.538960	4.812646	2.711789	5.557676
19	H	4.666691	2.576428	2.580442	5.088735	3.399511
20	O	3.831783	3.827787	5.623137	3.683944	3.857301
21	O	4.805381	2.021497	3.977841	3.906252	3.694893
22	O	2.002633	4.749432	4.150506	3.636632	3.674779
23	O	3.869855	3.686639	1.954103	3.742488	3.906068
24	H	4.239283	4.712404	6.308975	4.205706	4.534467
25	H	5.291181	2.508359	4.740513	4.499877	4.084250
26	H	2.465859	5.183670	4.892719	4.171596	4.031127
27	H	4.292200	4.580050	2.586401	4.300120	4.584454
28	O	4.735322	3.575198	5.419785	2.511010	4.601832
29	O	3.804264	2.071588	4.265741	4.548177	2.491984

30	O	3.909873	4.894287	4.192923	2.373920	4.936103
31	O	2.127869	3.740114	1.984301	4.712068	2.437997
32	H	5.206401	3.855795	5.977995	3.394513	4.890531
33	H	4.231498	2.625782	4.498596	5.399920	2.759574
34	H	4.283973	5.527157	4.400459	3.298507	5.399275
35	H	2.728875	4.090686	2.572008	5.519746	2.671078

		11	12	13	14	15
11	H	0.000000				
12	O	3.688833	0.000000			
13	O	3.682168	4.072539	0.000000		
14	O	3.711899	4.927189	6.536720	0.000000	
15	O	3.823311	6.556642	5.010425	4.467410	0.000000
16	H	4.202345	0.971547	3.830219	5.856415	7.073451
17	H	4.283629	5.036404	0.971263	7.252823	5.143600
18	H	4.202707	4.913804	7.090833	0.972271	5.424326
19	H	4.421619	7.116404	5.925384	4.308675	0.972469
20	O	4.773255	3.054013	3.331170	5.678401	5.797355
21	O	4.704979	5.848559	5.778306	3.327924	2.981727
22	O	2.374947	3.043649	2.858027	5.700906	5.722815
23	O	2.514238	5.795461	5.854445	3.052318	3.277577
24	H	5.239908	2.950415	3.469985	6.392429	6.643630
25	H	5.427171	6.173139	5.951743	4.171155	3.577856
26	H	3.238346	3.028667	2.548092	6.419264	6.301332
27	H	2.829003	6.162647	6.302111	3.714801	4.099469
28	O	4.696347	3.484927	5.414584	3.493749	5.483607
29	O	4.748603	5.369727	3.672789	5.460229	3.459360
30	O	2.496559	3.559128	5.688611	3.212820	5.746458
31	O	2.403028	5.564105	3.435149	5.638944	3.453427
32	H	5.409940	4.037960	5.570384	4.339060	5.800950
33	H	5.273848	6.203787	3.917344	6.199033	3.461101
34	H	2.794664	4.294739	6.105756	3.906625	6.118263
35	H	3.326577	6.271779	3.516305	6.424401	3.576553

		16	17	18	19	20
16	H	0.000000				
17	H	4.759218	0.000000			
18	H	5.877365	7.868165	0.000000		
19	H	7.716115	6.098019	5.276050	0.000000	
20	O	3.080851	4.119368	6.040476	6.395800	0.000000
21	O	6.530233	6.265009	4.161674	2.813150	4.704514
22	O	2.996102	3.508423	5.980530	6.492762	4.580029
23	O	6.494406	6.282851	3.693707	3.361963	6.633041
24	H	2.698952	4.258686	6.664864	7.285430	0.971279
25	H	6.781886	6.404957	4.932693	3.465030	4.563889
26	H	2.675875	3.197495	6.685590	7.118984	4.338849
27	H	6.825970	6.703783	4.187326	4.208880	7.318964
28	O	4.205288	6.255589	3.684647	5.676036	2.926960

29	O	5.634287	3.958948	6.229357	4.022868	3.140934
30	O	4.319416	6.457579	3.077322	6.044422	5.782486
31	O	5.780957	3.458742	6.319461	4.283936	5.840588
32	H	4.608766	6.359250	4.583975	6.002684	2.714850
33	H	6.403228	3.965673	7.021418	4.054936	3.945226
34	H	4.948422	6.797644	3.780366	6.421784	6.594763
35	H	6.403610	3.271941	7.158964	4.453574	6.191205

		21	22	23	24	25
21	O	0.000000				
22	O	6.488552	0.000000			
23	O	4.478785	4.820940	0.000000		
24	H	5.663392	4.603887	7.297861	0.000000	
25	H	0.973212	6.999681	5.416482	5.529839	0.000000
26	H	6.942826	0.973789	5.727377	4.184208	7.344153
27	H	5.445982	4.910355	0.971207	7.910452	6.383793
28	O	3.307722	5.585550	5.645848	3.608645	3.391987
29	O	2.978295	5.588767	5.724623	4.007743	2.708863
30	O	5.733279	3.563229	3.306112	6.110878	6.513918
31	O	5.610784	3.254156	3.448057	6.298554	6.220185
32	H	3.457065	6.160182	6.406784	3.414130	3.260196
33	H	3.545377	6.084471	6.126376	4.735929	3.243063
34	H	6.466496	3.727628	3.359988	6.887166	7.289201
35	H	5.979022	3.928882	4.219465	6.645152	6.498104

		26	27	28	29	30
26	H	0.000000				
27	H	5.863792	0.000000			
28	O	5.806530	6.409318	0.000000		
29	O	5.678138	6.582835	3.996944	0.000000	
30	O	4.376549	3.297346	4.789129	6.553803	0.000000
31	O	3.868672	3.630549	6.488590	4.901977	4.771482
32	H	6.268299	7.214013	0.972321	3.776476	5.719389
33	H	6.153187	6.964615	4.961873	0.972467	7.273940
34	H	4.599858	3.067603	5.747925	7.247282	0.971712
35	H	4.383980	4.429020	7.087976	4.947040	5.735246

		31	32	33	34	35
31	O	0.000000				
32	H	6.989159	0.000000			
33	H	4.987502	4.717379	0.000000		
34	H	4.779825	6.671825	7.900099	0.000000	
35	H	0.971981	7.491468	4.845548	5.749584	0.000000

Alpha occ. eigenvalues -- -0.20805 -0.20454 -0.20266 -0.20131 -0.20013
Alpha occ. eigenvalues -- -0.19615 -0.19421 -0.18537 -0.18301 -0.18068
Alpha occ. eigenvalues -- -0.17821 -0.17735 -0.17335
Alpha virt. eigenvalues -- -0.12728 -0.10715 -0.05811 -0.04934 -0.04681
gap = 1.25 eV
Beta occ. eigenvalues -- -0.23141 -0.21519 -0.20261 -0.19905 -0.18424

Beta occ. eigenvalues -- -0.17778 -0.17613 -0.17435 -0.17102 -0.16491
Beta occ. eigenvalues -- -0.15273
Beta virt. eigenvalues -- -0.13454 -0.13339 -0.13129 -0.12731 -0.12237
gap = 0.49 eV
Mulliken atomic spin densities:

		1
1	Fe	2.838685
2	Fe	3.424210
3	Fe	3.579892
4	Fe	2.793115
5	Fe	3.530617
6	Fe	2.538073
7	Fe	2.925851
8	Fe	3.636825
9	H	-0.083523
10	H	-0.070144
11	H	-0.056592
12	O	0.171217
13	O	0.125546
14	O	0.159320
15	O	0.168933
16	H	0.007334
17	H	0.006882
18	H	0.006762
19	H	0.008580
20	O	0.145903
21	O	0.150680
22	O	0.155981
23	O	0.174609
24	H	0.008637
25	H	0.008913
26	H	0.004389
27	H	0.006800
28	O	0.161132
29	O	0.133192
30	O	0.146189
31	O	0.151127
32	H	0.009486
33	H	0.009883
34	H	0.010126
35	H	0.011370

Sum of Mulliken atomic spin densities = 27.00000
Dipole moment (field-independent basis, Debye):
X= -0.3023 Y= 1.1787 Z= 3.3415 Tot= 3.5561

Isotropic polarizability for W= 0.000000 302.72 Bohr**3. 1.28 A**3

Frequencies --	44.6653	54.4356	60.1730
Frequencies --	63.3691	73.3266	84.3001
Frequencies --	89.9975	92.8767	100.0157
Frequencies --	107.4870	108.6763	114.4140
Frequencies --	118.0003	124.3524	125.8656
Frequencies --	132.9014	137.8135	138.1849
Frequencies --	145.8237	148.2402	153.1943
Frequencies --	168.1794	173.7630	180.3503
Frequencies --	187.0085	192.5804	209.3005
Frequencies --	220.6413	226.5342	234.8151
Frequencies --	250.2033	259.7237	300.9875
Frequencies --	305.7239	314.4026	319.9577
Frequencies --	326.2767	329.6765	337.7662
Frequencies --	343.2905	350.1991	357.7694
Frequencies --	398.8512	413.1403	434.7259
Frequencies --	446.5915	451.4525	458.9796
Frequencies --	460.4773	476.3085	477.2981
Frequencies --	484.1951	488.8707	494.1844
Frequencies --	507.3650	518.3989	534.9359
Frequencies --	560.3865	567.1364	570.9884
Frequencies --	577.7818	583.6254	606.5870
Frequencies --	611.0818	616.3219	625.3187
Frequencies --	629.0608	639.6122	647.6059
Frequencies --	665.0704	669.2359	671.9034
Frequencies --	674.1332	681.8617	686.6005
Frequencies --	690.0570	703.8160	710.7684
Frequencies --	726.3108	749.4292	772.7167
Frequencies --	987.0902	1023.3143	1113.2292
Frequencies --	1327.5541	1392.0803	1448.8894
Frequencies --	3659.3271	3678.6749	3683.8177
Frequencies --	3684.9896	3688.7503	3690.2774
Frequencies --	3690.8305	3691.7594	3694.1032
Frequencies --	3696.9503	3699.0614	3700.4511

[headnode:~/feon] ggutsev% grep "Inten" fe8o12h15_28_GF.out

IR Inten	--	0.7621	2.3782	1.9987
IR Inten	--	3.7794	0.8858	0.6966
IR Inten	--	0.5296	4.5989	1.2805
IR Inten	--	1.6606	1.9587	2.6185
IR Inten	--	1.6599	8.9502	0.6375
IR Inten	--	0.7289	3.2809	2.1173
IR Inten	--	2.6658	4.9389	2.4053

IR Inten	--	4.5998	3.2267	5.7345
IR Inten	--	1.5205	2.7720	8.4845
IR Inten	--	14.3163	1.9530	32.2501
IR Inten	--	11.0687	11.9034	8.7884
IR Inten	--	11.5747	0.1386	7.3134
IR Inten	--	2.9672	6.9378	10.9500
IR Inten	--	3.8454	7.6332	4.7534
IR Inten	--	91.6284	162.7061	64.6817
IR Inten	--	58.2335	55.2958	91.6875
IR Inten	--	104.6399	166.1419	25.9725
IR Inten	--	162.3580	149.4385	113.9999
IR Inten	--	132.3161	33.8852	79.4772
IR Inten	--	8.2617	70.2273	21.9393
IR Inten	--	19.0215	48.3532	22.2124
IR Inten	--	21.0496	54.1974	110.8611
IR Inten	--	32.9628	70.1560	11.3381
IR Inten	--	94.8522	48.0434	23.8328
IR Inten	--	94.1038	143.0643	39.9629
IR Inten	--	35.5568	56.8820	4.3746
IR Inten	--	13.1249	2.7570	8.7274
IR Inten	--	1.3733	2.5027	6.7780
IR Inten	--	6.7830	14.1050	1.3903
IR Inten	--	18.1314	38.9685	31.1279
IR Inten	--	8.3156	30.2375	44.3308
IR Inten	--	51.1244	49.9947	29.6382
IR Inten	--	24.6633	22.1494	28.0989

Zero-point vibrational energy 490717.7 (Joules/Mol)
117.28435 (Kcal/Mol) 5.086 eV

Atom	No	Natural Electron Configuration
Fe	1	[core]4S(0.24)3d(6.72)4p(0.59)4d(0.04)5p(0.01)
Fe	2	[core]4S(0.23)3d(6.52)4p(0.48)4d(0.03)
Fe	3	[core]4S(0.23)3d(6.45)4p(0.38)4d(0.02)
Fe	4	[core]4S(0.26)3d(6.80)4p(0.67)4d(0.04)5p(0.01)
Fe	5	[core]4S(0.24)3d(6.49)4p(0.40)4d(0.02)
Fe	6	[core]4S(0.27)3d(6.88)4p(0.70)4d(0.04)5p(0.01)
Fe	7	[core]4S(0.26)3d(6.72)4p(0.62)4d(0.04)5p(0.01)
Fe	8	[core]4S(0.23)3d(6.44)4p(0.42)4d(0.02)
H	9	1S(0.88)2S(0.01)
H	10	1S(0.89)2S(0.01)
H	11	1S(0.86)2S(0.01)
O	12	[core]2S(1.71)2p(5.14)3S(0.01)3p(0.02)
O	13	[core]2S(1.70)2p(5.17)3S(0.01)3p(0.02)
O	14	[core]2S(1.70)2p(5.13)3S(0.01)3p(0.01)

O	15	[core]2S(1.71)2p(5.16)3S(0.01)3p(0.01)
H	16	1S(0.53)
H	17	1S(0.53)
H	18	1S(0.52)
H	19	1S(0.52)
O	20	[core]2S(1.71)2p(5.16)3S(0.01)3p(0.01)
O	21	[core]2S(1.71)2p(5.15)3S(0.01)3p(0.01)
O	22	[core]2S(1.70)2p(5.11)3p(0.02)
O	23	[core]2S(1.69)2p(5.14)3S(0.01)3p(0.02)
H	24	1S(0.53)
H	25	1S(0.52)
H	26	1S(0.53)
H	27	1S(0.52)
O	28	[core]2S(1.71)2p(5.16)3S(0.01)3p(0.01)
O	29	[core]2S(1.72)2p(5.17)3S(0.01)3p(0.01)
O	30	[core]2S(1.71)2p(5.16)3p(0.01)
O	31	[core]2S(1.72)2p(5.15)3S(0.01)3p(0.01)
H	32	1S(0.51)
H	33	1S(0.53)
H	34	1S(0.53)
H	35	1S(0.53)

****

******* Alpha spin orbitals *******

****

Atom	No	Natural Electron Configuration
Fe	1	[core]3d(4.75)4p(0.31)5S(0.13)4d(0.03)
Fe	2	[core]3d(4.84)4p(0.26)4d(0.01)6S(0.14)5d(0.01)
Fe	3	[core]3d(4.88)4p(0.21)4d(0.01)6S(0.14)
Fe	4	[core]3d(4.74)4p(0.35)4d(0.03)6S(0.14)
Fe	5	[core]3d(4.88)4p(0.22)4d(0.01)6S(0.14)
Fe	6	[core]3d(4.67)4p(0.24)5S(0.15)4d(0.03)5p(0.13)
Fe	7	[core]3d(4.79)4p(0.20)5S(0.14)4d(0.03)5p(0.12)
Fe	8	[core]3d(4.88)4p(0.23)4d(0.02)6S(0.14)
H	9	1S(0.41)2S(0.01)
H	10	1S(0.42)2S(0.01)
H	11	1S(0.40)2S(0.01)
O	12	[core]2S(0.86)2p(2.67)4p(0.01)
O	13	[core]2S(0.86)2p(2.66)3p(0.01)
O	14	[core]2S(0.86)2p(2.66)3p(0.01)
O	15	[core]2S(0.87)2p(2.68)3p(0.01)
H	16	1S(0.27)
H	17	1S(0.26)
H	18	1S(0.26)

H	19	1S(0.26)
O	20	[core]2S(0.86)2p(2.67)3p(0.01)
O	21	[core]2S(0.87)2p(2.67)3p(0.01)
O	22	[core]2S(0.86)2p(2.64)3p(0.01)
O	23	[core]2S(0.86)2p(2.67)3p(0.01)
H	24	1S(0.26)
H	25	1S(0.26)
H	26	1S(0.26)
H	27	1S(0.26)
O	28	[core]2S(0.87)2p(2.68)3p(0.01)
O	29	[core]2S(0.87)2p(2.67)4p(0.01)
O	30	[core]2S(0.87)2p(2.66)3p(0.01)
O	31	[core]2S(0.87)2p(2.67)3p(0.01)
H	32	1S(0.26)
H	33	1S(0.27)
H	34	1S(0.27)
H	35	1S(0.27)

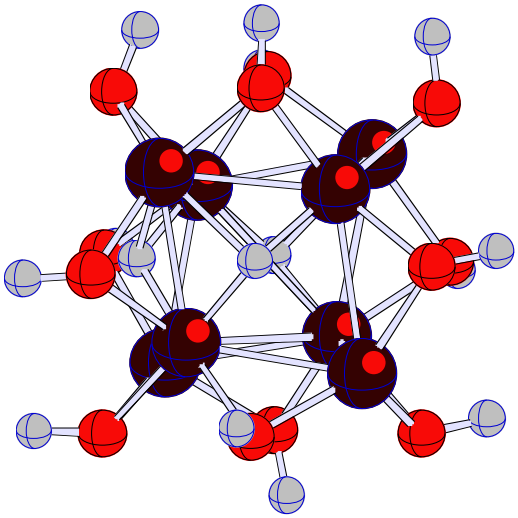
NBO analysis skipped by request.

****
******* Beta spin orbitals *******
****

Atom	No	Natural Electron Configuration
Fe	1	[core]3d(1.97)4p(0.28)5S(0.12)4d(0.01)
Fe	2	[core]3d(1.68)4p(0.14)4d(0.01)5p(0.07)6S(0.09)
Fe	3	[core]3d(1.57)4p(0.17)4d(0.01)6S(0.10)
Fe	4	[core]3d(2.07)4p(0.32)4d(0.01)6S(0.12)
Fe	5	[core]3d(1.61)4p(0.18)4d(0.01)6S(0.10)
Fe	6	[core]3d(2.21)4p(0.33)5S(0.12)4d(0.01)
Fe	7	[core]3d(1.93)4p(0.30)5S(0.13)4d(0.01)
Fe	8	[core]3d(1.56)4p(0.19)4d(0.01)6S(0.09)
H	9	1S(0.47)
H	10	1S(0.48)
H	11	1S(0.45)
O	12	[core]2S(0.84)2p(2.47)
O	13	[core]2S(0.84)2p(2.51)
O	14	[core]2S(0.84)2p(2.48)
O	15	[core]2S(0.84)2p(2.48)
H	16	1S(0.27)
H	17	1S(0.26)
H	18	1S(0.26)
H	19	1S(0.26)

O 20 [core]2S(0.84)2p(2.49)
O 21 [core]2S(0.84)2p(2.49)
O 22 [core]2S(0.84)2p(2.46)
O 23 [core]2S(0.84)2p(2.47)
H 24 1S(0.26)
H 25 1S(0.26)
H 26 1S(0.26)
H 27 1S(0.26)
O 28 [core]2S(0.84)2p(2.48)
O 29 [core]2S(0.85)2p(2.50)
O 30 [core]2S(0.85)2p(2.49)
O 31 [core]2S(0.85)2p(2.48)
H 32 1S(0.25)
H 33 1S(0.26)
H 34 1S(0.26)
H 35 1S(0.27)

HF= -11023.1290253\S2=196.000369\S2-1=0.\S2A=195.754166



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Fe 1.1816728543,-2.0979140363,0.0414632045
Fe 0.3487123155,1.13613315,-2.1947956539
Fe -0.5566979112,-1.1118770301,-1.4254640636
Fe 0.7624010523,1.4332804856,1.8189034573
Fe -0.3395144507,-0.8051474905,1.5543709645
Fe -0.9904467977,1.4519850568,-0.1366410654
Fe -2.4770862176,-0.5363922525,0.0972972095
H 1.1087561826,-0.7237842653,-1.228392136

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 H        -1.1318557305,0.6541961684,1.3327636529
 H        -0.6966215427,-1.6787610685,0.1858470363
 O        2.9678806864,-1.270524097,0.2965420081
 O        0.4606140814,0.0714318334,3.2117339965
 O        -0.3147682612,-0.3637185817,-3.2642317355
 O        -3.0357974221,1.32672099,-0.1503651427
 H        3.3746897091,-1.3533893387,1.1749174274
 H        -0.1281661718,0.2688215314,3.958545737
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 H        -3.4118820073,1.6018698472,-1.0039160943
 O        2.5976180157,1.6278354079,1.1850326108
 O        -0.9000580591,2.5745359682,-1.8153789359
 O        0.7013859988,-2.4734721692,1.9335268565
 O        -2.5174530726,-1.5933034679,-1.5458178161
 H        3.3416232621,1.2915581712,1.7111086454
 H        -0.5383344292,3.4484950571,-1.5862640846
 H        1.3293555627,-2.2560640202,2.6453226295
 H        -2.783675533,-2.5270832979,-1.5252382419
 O        2.2182487433,1.4760102947,-1.7132638157
 O        -0.2413947247,2.9659311234,1.0626783761
 O        0.4811344724,-2.9851518466,-1.5858870872
 O        -2.3616026419,-1.3753398537,1.8918117623
 H        2.5283388422,2.353025726,-1.430250946
 H        -0.9045034442,3.3876773103,1.6354871817
 H        -0.0024162756,-3.8200541751,-1.4703808124
 H        -2.8525297679,-0.9408340337,2.6094065275
END
```

$Fe_8O_{12}H_{16}$

```
$$$$$$$$$$$$$  Fe_8O_12H_16      NEUTRAL    S = 27 head
fe8o12h16_td_27_GF.out
---------------------------------------------------------------------
# UBPW91/6-311+G*
scf=(VSHIFT=5,NoIncFock,MAXCYC=77,Tight,NoVarAcc) NO
 SYMM OPT=RFO IOP(5/13=1,5/36=1,8/11=1) INT=UltraFine GUESS=READ
GEOM=CHECKPOINT
 ---------------------------------------------------------------------
Charge =  0 Multiplicity = 27
                    Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic           Coordinates (Angstroms)
```

Number	Number	Type	X	Y	Z
1	26	0	-1.370755	1.270706	-1.614776
2	26	0	1.027451	1.074201	-1.132352
3	26	0	-1.397705	-1.344920	-1.566858
4	26	0	1.178300	-1.402400	-1.203763
5	26	0	-1.175739	1.283011	0.928575
6	26	0	1.268344	1.223835	1.349619
7	26	0	-1.188046	-1.205332	0.989082
8	26	0	1.312205	-1.455172	1.432805
9	1	0	-0.021595	-0.005183	-1.806713
10	1	0	0.102671	1.873264	-0.030218
11	1	0	-1.624745	0.079137	-0.195415
12	1	0	1.133430	-0.122169	0.131871
13	8	0	0.146408	2.364260	-2.407255
14	8	0	-0.092964	2.316113	2.311876
15	8	0	0.002348	-2.503140	-2.362346
16	8	0	-0.194264	-2.381719	2.268952
17	1	0	0.191109	3.297241	-2.137239
18	1	0	-0.311003	2.146574	3.243577
19	1	0	0.150457	-2.530708	-3.321355
20	1	0	-0.286837	-3.343632	2.173281
21	8	0	-2.289395	2.478960	-0.300076
22	8	0	-2.230304	-2.475184	-0.172984
23	8	0	2.510304	1.976600	-0.068635
24	8	0	2.236961	-2.517571	0.066535
25	1	0	-2.054877	3.422103	-0.301604
26	1	0	-3.195366	-2.490190	-0.067587
27	1	0	2.554390	2.946115	-0.118308
28	1	0	3.197225	-2.644365	0.017341
29	8	0	-2.392505	-0.039387	-2.706732
30	8	0	-2.059179	0.089686	2.235465
31	8	0	2.400962	-0.020291	-2.040284
32	8	0	2.163009	-0.079868	2.552073
33	1	0	-3.354201	-0.010372	-2.823750
34	1	0	-1.692592	0.054407	3.135479
35	1	0	3.237943	0.212247	-1.596416
36	1	0	2.168895	-0.089295	3.520995

Distance matrix (angstroms):

		1	2	3	4	5
1	Fe	0.000000				
2	Fe	2.454127	0.000000			
3	Fe	2.616204	3.452872	0.000000		
4	Fe	3.716464	2.482218	2.602104	0.000000	
5	Fe	2.550847	3.024082	3.630768	4.159303	0.000000

6	Fe	3.969216	2.498120	4.712977	3.664011	2.480791
7	Fe	3.597808	3.821672	2.568320	3.232181	2.489109
8	Fe	4.890443	3.613702	4.043976	2.640493	3.733867
9	H	1.866806	1.649342	1.935485	1.937914	3.236246
10	H	2.246083	1.645728	3.868993	3.641999	1.703531
11	H	1.870544	2.983646	1.990060	3.326977	1.707124
12	H	3.355863	1.743787	3.284424	1.850655	2.818072
13	O	2.031173	2.016399	4.104701	4.086676	3.747657
14	O	4.259603	3.828888	5.490909	5.272870	2.037946
15	O	4.084873	3.919322	1.983538	1.984139	5.152959
16	O	5.459642	5.000484	4.151705	3.860408	4.023699
17	H	2.611365	2.578987	4.939567	4.892090	3.914666
18	H	5.049140	4.700022	6.042494	5.881502	2.617775
19	H	4.435905	4.307693	2.623196	2.610313	5.862180
20	H	6.067650	5.672020	4.383778	4.161662	4.872911
21	O	2.008038	3.696958	4.125762	5.282662	2.044531
22	O	4.104788	4.912381	1.978283	3.719134	4.055807
23	O	4.236916	2.035847	5.343192	3.805310	3.881032
24	O	5.494858	3.975056	4.153779	1.994499	5.180160
25	H	2.611695	3.962768	4.975666	5.877342	2.619530
26	H	4.457280	5.627681	2.605963	4.647918	4.394119
27	H	4.522519	2.619903	6.010851	4.688434	4.216129
28	H	6.233621	4.456170	5.031066	2.666389	5.947895
29	O	1.988135	3.926174	1.998339	4.106990	4.055208
30	O	4.085719	4.673194	4.117439	4.953370	1.977992
31	O	4.009186	1.977064	4.050758	2.026054	4.827578
32	O	5.627981	4.024470	5.589689	4.101834	3.954798
33	H	2.652704	4.820373	2.681171	5.010555	4.527525
34	H	4.914050	5.162654	4.914982	5.403085	2.578184
35	H	4.728718	2.417560	4.890284	2.646392	5.196413
36	H	6.383955	4.930544	6.339044	5.002886	4.448646

		6	7	8	9	10
6	Fe	0.000000				
7	Fe	3.473426	0.000000			
8	Fe	2.680657	2.551581	0.000000		
9	H	3.624480	3.258440	3.791565	0.000000	
10	H	1.919505	3.490369	3.831696	2.588424	0.000000
11	H	3.473820	1.800999	3.692002	2.274528	2.496027
12	H	1.820120	2.701352	1.871173	2.259619	2.251774
13	O	4.083309	5.104690	5.540145	2.450130	2.427611
14	O	1.993030	3.917851	4.119448	4.728243	2.391608
15	O	5.410340	3.785949	4.149353	2.559119	4.960020
16	O	3.998051	2.002388	1.956292	4.721099	4.845537
17	H	4.197336	5.652355	6.048760	3.325732	2.544616
18	H	2.633033	4.133670	4.345834	5.497203	3.311126
19	H	6.096250	4.704049	5.010835	2.949919	5.498076

20	H	4.894768	2.605155	2.582928	5.201533	5.676542
21	O	4.117565	4.055726	5.608191	3.685626	2.482272
22	O	5.314283	2.012268	4.020989	3.694370	4.936817
23	O	2.029917	4.992118	3.932788	3.654981	2.410155
24	O	4.072179	3.782028	1.962284	3.862930	4.883031
25	H	4.313086	4.881641	6.175211	4.259797	2.669750
26	H	5.977220	2.607057	4.862164	4.390061	5.469752
27	H	2.602877	5.697951	4.829110	4.265744	2.677628
28	H	4.523110	4.716534	2.640268	4.544586	5.476084
29	O	5.608166	4.058225	5.732808	2.536221	4.128906
30	O	3.625386	1.997352	3.794348	4.527687	3.603896
31	O	3.784457	4.843795	3.912368	2.433838	3.592778
32	O	1.986445	3.865123	1.966746	4.876175	3.837700
33	H	6.348874	4.545090	6.479279	3.484344	4.827202
34	H	3.650206	2.539396	3.769182	5.217379	4.068520
35	H	3.685343	5.318243	3.957895	3.273545	3.878387
36	H	2.692616	4.350308	2.638196	5.761059	4.553244

		11	12	13	14	15
11	H	0.000000				
12	H	2.784810	0.000000			
13	O	3.640193	3.688320	0.000000		
14	O	3.692820	3.493090	4.725443	0.000000	
15	O	3.743150	3.628979	4.869739	6.714360	0.000000
16	O	3.764996	3.381634	6.671378	4.699119	4.637060
17	H	4.174231	4.210605	0.972296	4.564859	5.807816
18	H	4.222189	4.112942	5.673492	0.971778	7.290021
19	H	4.442312	4.323432	4.979590	7.435335	0.970769
20	H	4.372192	4.069685	7.331373	5.664759	4.621901
21	O	2.492362	4.320669	3.222808	3.416596	5.858871
22	O	2.625217	4.116348	5.836176	5.805108	3.127111
23	O	4.551381	2.518097	3.347750	3.543883	5.623079
24	O	4.660931	2.638182	5.858526	5.816752	3.300480
25	H	3.372197	4.786967	3.224662	3.450013	6.602070
26	H	3.014072	4.938196	6.340914	6.195748	3.935919
27	H	5.068597	3.390587	3.372864	3.648449	6.422072
28	H	5.542032	3.260958	6.346060	6.379387	3.986238
29	O	2.628729	4.527332	3.509028	6.001890	3.453114
30	O	2.469418	3.829195	5.620778	2.971332	5.666790
31	O	4.429418	2.516998	3.302085	5.533511	3.467219
32	O	4.681992	2.630437	5.885183	3.299672	5.890010
33	H	3.147567	5.374665	4.250483	6.513283	4.206329
34	H	3.331677	4.127861	6.280067	2.890060	6.296026
35	H	5.062238	2.743682	3.853079	5.549409	4.292907
36	H	5.313359	3.543929	6.727149	3.516243	6.718205

		16	17	18	19	20
16	O	0.000000				

17	H	7.198168	0.000000			
18	H	4.633460	5.525336	0.000000		
19	H	5.602906	5.947165	8.073924	0.000000	
20	H	0.971081	7.931595	5.593610	5.571633	0.000000
21	O	5.883510	3.193376	4.072100	6.338595	6.635534
22	O	3.180762	6.560673	6.059476	3.947575	3.168000
23	O	5.636838	3.376667	4.354241	6.038616	6.415220
24	O	3.283284	6.546310	6.191927	3.978877	3.389736
25	H	6.614680	2.903377	4.151672	7.029819	7.417964
26	H	3.804970	7.017552	6.386152	4.667245	3.769535
27	H	6.452900	3.128014	4.489099	6.784836	7.272197
28	H	4.079330	6.998688	6.757911	4.521349	4.156409
29	O	5.922518	4.258223	6.672125	3.612631	6.258306
30	O	3.096267	5.871350	2.881527	6.528951	3.864289
31	O	5.557073	3.987338	6.322124	3.606675	6.001915
32	O	3.306873	6.105973	3.399405	6.674888	4.098460
33	H	6.445472	4.897022	7.122214	4.345381	6.744603
34	H	2.988405	6.470383	2.509510	7.195162	3.801136
35	H	5.783578	4.369540	6.305725	4.475689	6.267293
36	H	3.522405	6.884467	3.350517	7.540049	4.293910

		21	22	23	24	25
21	O	0.000000				
22	O	4.956127	0.000000			
23	O	4.831464	6.504047	0.000000		
24	O	6.751862	4.473882	4.504504	0.000000	
25	H	0.971864	5.901298	4.794229	7.337242	0.000000
26	H	5.056411	0.970916	7.246163	5.434051	6.025835
27	H	4.869654	7.230959	0.971787	5.476020	4.637402
28	H	7.513470	5.433499	4.672534	0.969847	8.030463
29	O	3.484924	3.518423	5.921257	5.938380	4.228539
30	O	3.491505	3.522566	5.454310	5.473469	4.188287
31	O	5.592319	5.564345	2.808367	3.271390	5.893011
32	O	5.874204	5.697778	3.349296	3.482207	6.180440
33	H	3.701286	3.790120	6.777251	6.775019	4.453240
34	H	4.247079	4.199273	5.623656	5.610247	4.825575
35	H	6.113097	6.257010	2.444691	3.349519	6.324054
36	H	6.408813	6.220201	4.155710	4.223086	6.691968

		26	27	28	29	30
26	H	0.000000				
27	H	7.913007	0.000000			
28	H	6.395014	5.628953	0.000000		
29	O	3.690001	6.331266	6.741778	0.000000	
30	O	3.640156	5.914765	6.326522	4.955106	0.000000
31	O	6.427349	3.537951	3.428356	4.839611	6.179561
32	O	6.433075	4.054711	3.751148	6.957684	4.237435
33	H	3.710952	7.139445	7.611235	0.969224	5.223290

34	H	4.358088	6.081609	6.396598	5.884735	0.972448
35	H	7.143385	3.182150	3.281174	5.744394	6.538947
36	H	6.886038	4.754666	4.456617	7.719679	4.422808

		31	32	33	34	35
31	O	0.000000				
32	O	4.598904	0.000000			
33	H	5.808254	7.703500	0.000000		
34	H	6.599340	3.901802	6.186886	0.000000	
35	H	0.975516	4.295436	6.709119	6.835636	0.000000
36	H	5.566547	0.968986	8.412290	3.883344	5.236572

		36
36	H	0.000000

Alpha occ. eigenvalues -- -0.18767 -0.18545 -0.18212 -0.17869 -0.17732
Alpha occ. eigenvalues -- -0.17168 -0.17066 -0.16621
Alpha virt. eigenvalues -- -0.12035 -0.10538 -0.10180 -0.05166 -0.03126
1.25 eV
Beta occ. eigenvalues -- -0.17606 -0.17451 -0.16650 -0.16063 -0.15916
Beta occ. eigenvalues -- -0.15233 -0.14906
Beta virt. eigenvalues -- -0.12814 -0.12227 -0.11939 -0.11839 -0.11463
0.57 eV
Mulliken atomic spin densities:

		1
1	Fe	3.313081
2	Fe	2.055029
3	Fe	3.334613
4	Fe	3.300318
5	Fe	2.667847
6	Fe	3.243423
7	Fe	3.128856
8	Fe	3.333073
9	H	-0.080844
10	H	-0.070223
11	H	-0.124215
12	H	-0.108066
13	O	0.142031
14	O	0.124705
15	O	0.179809
16	O	0.156937
17	H	0.004102
18	H	0.006275
19	H	0.010915
20	H	0.010261
21	O	0.164288
22	O	0.168623
23	O	0.108664
24	O	0.186560

25	H	0.006618
26	H	0.010949
27	H	0.006046
28	H	0.008935
29	O	0.168958
30	O	0.171705
31	O	0.170185
32	O	0.175889
33	H	0.012488
34	H	0.002473
35	H	0.000650
36	H	0.009042

Sum of Mulliken atomic spin densities = 26.00000

Dipole moment (field-independent basis, Debye):

X= -0.0769 Y= -0.0866 Z= 2.3326 Tot= 2.3355

Isotropic polarizability for W= 0.000000 306.20 Bohr**3. 1.26 A**3

Frequencies --	34.5918	56.2264	62.0029
Frequencies --	63.3940	72.1288	79.3968
Frequencies --	83.6987	94.9225	103.1250
Frequencies --	112.0640	114.0888	115.1942
Frequencies --	119.9300	128.3163	137.5324
Frequencies --	140.4938	146.4824	151.7624
Frequencies --	154.9593	158.2779	162.4328
Frequencies --	176.0559	176.2729	184.3526
Frequencies --	196.9315	203.7181	206.5214
Frequencies --	220.8616	228.5098	233.0057
Frequencies --	281.9657	292.5411	296.7554
Frequencies --	301.4756	313.5609	326.7452
Frequencies --	334.3706	343.4653	346.6502
Frequencies --	351.1286	359.5984	360.8053
Frequencies --	366.4869	372.0995	378.0774
Frequencies --	393.2661	419.2306	425.6929
Frequencies --	444.9910	450.1503	454.9991
Frequencies --	462.1612	472.9070	478.4252
Frequencies --	491.6295	505.5190	516.6012
Frequencies --	524.9615	528.9740	548.8792
Frequencies --	557.6698	565.6241	590.0217
Frequencies --	615.0929	625.5571	628.4162
Frequencies --	633.2104	639.1058	640.6064
Frequencies --	663.7307	666.0392	675.7371
Frequencies --	678.5629	681.3210	685.5885
Frequencies --	696.7258	708.4397	720.1884

```
Frequencies --   742.9390            761.5549            765.7109
Frequencies --   848.6092            998.2004           1006.0878
Frequencies --  1077.6700           1112.3741           1140.9816
Frequencies --  1164.0368           1388.7078           1434.7358
Frequencies --  3634.9894           3670.4551           3675.9019
Frequencies --  3680.4622           3685.0761           3692.3408
Frequencies --  3708.1243           3708.9912           3712.5972
Frequencies --  3716.1663           3727.0514           3729.5514
[headnode:~/feon] ggutsev% grep "Inten" fe8o12h16_td_27_GF.out
IR Inten    --     0.3286              2.1912              2.5266
IR Inten    --     1.7376              1.4671              1.5175
IR Inten    --     0.6037              0.8130              3.1595
IR Inten    --     4.4608              5.0510              3.1368
IR Inten    --     3.6577              5.0438              2.5482
IR Inten    --     5.7312              3.5826              8.2387
IR Inten    --     3.1914              4.3162              4.4982
IR Inten    --     9.6597              5.5151              7.8992
IR Inten    --     4.3420              3.6675              0.3694
IR Inten    --     3.3080              2.5930             17.4551
IR Inten    --     1.6362              1.2190              7.3110
IR Inten    --     4.3297              2.0669              4.1825
IR Inten    --   147.5721             49.8376              3.2823
IR Inten    --    55.0146             52.6191              6.2085
IR Inten    --    14.6349              0.3591              3.8463
IR Inten    --   101.8271            326.1017             80.9201
IR Inten    --    75.3927            242.0657             47.1708
IR Inten    --    20.1748            117.8509             43.5329
IR Inten    --    42.6495              5.7711             39.7396
IR Inten    --    11.6943             10.6604             56.8459
IR Inten    --   106.6363             10.2183             34.3627
IR Inten    --    22.0401             51.4876             60.9377
IR Inten    --    76.8233             31.1425             37.0722
IR Inten    --    61.8424             60.6303            145.1611
IR Inten    --    31.5046             69.1412             26.1115
IR Inten    --    67.4382             18.0083             14.2266
IR Inten    --    13.5674             14.8238             90.8262
IR Inten    --     8.1175              1.2731              2.2070
IR Inten    --     1.8093              1.7877              1.4081
IR Inten    --     2.5677              8.1595              5.8958
IR Inten    --    24.6460             10.9842             20.3583
IR Inten    --     0.8685             10.1920             24.6922
IR Inten    --    41.3289             60.4336             59.3085
IR Inten    --    34.7284             29.2037             50.3152
Zero-point vibrational energy     506716.1 (Joules/Mol)
                                  121.10806 (Kcal/Mol)   5.252 eV
```

Atom	No	Natural Electron Configuration
Fe	1	[core]4S(0.21)3d(6.57)4p(0.50)4d(0.03)5p(0.01)
Fe	2	[core]4S(0.25)3d(7.02)4p(0.76)4d(0.05)5p(0.01)
Fe	3	[core]4S(0.22)3d(6.55)4p(0.48)4d(0.03)5p(0.01)
Fe	4	[core]4S(0.21)3d(6.58)4p(0.50)4d(0.03)5p(0.01)
Fe	5	[core]4S(0.23)3d(6.82)4p(0.60)4d(0.04)5p(0.01)
Fe	6	[core]4S(0.21)3d(6.60)4p(0.48)4d(0.03)5p(0.01)
Fe	7	[core]4S(0.23)3d(6.60)4p(0.51)4d(0.03)5p(0.01)
Fe	8	[core]4S(0.22)3d(6.55)4p(0.43)4d(0.02)
H	9	1S(0.88)2S(0.01)
H	10	1S(0.84)2S(0.01)
H	11	1S(0.92)2S(0.01)
H	12	1S(0.92)2S(0.01)
O	13	[core]2S(1.70)2p(5.09)3S(0.01)3p(0.02)
O	14	[core]2S(1.71)2p(5.15)3S(0.01)3p(0.02)
O	15	[core]2S(1.70)2p(5.17)3S(0.01)3p(0.01)
O	16	[core]2S(1.71)2p(5.18)3S(0.01)3p(0.01)
H	17	1S(0.54)
H	18	1S(0.54)
H	19	1S(0.52)
H	20	1S(0.51)
O	21	[core]2S(1.71)2p(5.14)3S(0.01)3p(0.02)
O	22	[core]2S(1.70)2p(5.18)3S(0.01)3p(0.01)
O	23	[core]2S(1.70)2p(5.13)3p(0.02)
O	24	[core]2S(1.70)2p(5.19)3S(0.01)3p(0.01)
H	25	1S(0.53)
H	26	1S(0.52)
H	27	1S(0.53)
H	28	1S(0.52)
O	29	[core]2S(1.70)2p(5.20)3S(0.01)3p(0.01)
O	30	[core]2S(1.70)2p(5.12)3S(0.01)3p(0.02)
O	31	[core]2S(1.70)2p(5.08)3p(0.02)
O	32	[core]2S(1.70)2p(5.21)3S(0.01)3p(0.01)
H	33	1S(0.52)
H	34	1S(0.53)
H	35	1S(0.53)
H	36	1S(0.52)

****
******* Alpha spin orbitals *******
****

Atom	No	Natural Electron Configuration
Fe	1	[core]3d(4.82)4p(0.27)4d(0.01)6S(0.12)5d(0.01)

Fe	2	[core]3d(4.46)4p(0.41)4d(0.03)6S(0.14)
Fe	3	[core]3d(4.84)4p(0.26)4d(0.02)6S(0.12)5d(0.01)
Fe	4	[core]3d(4.84)4p(0.26)4d(0.02)6S(0.12)5d(0.01)
Fe	5	[core]3d(4.66)4p(0.32)4d(0.02)6S(0.13)
Fe	6	[core]3d(4.84)4p(0.26)4d(0.01)6S(0.12)5d(0.01)
Fe	7	[core]3d(4.82)4p(0.26)4d(0.02)6S(0.12)5d(0.01)
Fe	8	[core]3d(4.86)4p(0.23)4d(0.01)6S(0.12)5d(0.01)
H	9	1S(0.42)
H	10	1S(0.39)2S(0.01)
H	11	1S(0.43)
H	12	1S(0.45)3S(0.01)
O	13	[core]2S(0.86)2p(2.63)3p(0.01)
O	14	[core]2S(0.86)2p(2.65)3p(0.01)
O	15	[core]2S(0.86)2p(2.69)3p(0.01)4S(0.01)
O	16	[core]2S(0.87)2p(2.68)3p(0.01)4S(0.01)
H	17	1S(0.27)
H	18	1S(0.27)
H	19	1S(0.26)
H	20	1S(0.26)
O	21	[core]2S(0.86)2p(2.66)3p(0.01)4p(0.01)
O	22	[core]2S(0.86)2p(2.68)3p(0.01)4p(0.01)
O	23	[core]2S(0.86)2p(2.63)3p(0.01)
O	24	[core]2S(0.86)2p(2.70)3p(0.01)4S(0.01)4p(0.01)
H	25	1S(0.27)
H	26	1S(0.26)
H	27	1S(0.27)
H	28	1S(0.26)
O	29	[core]2S(0.86)2p(2.69)3p(0.01)4S(0.01)4p(0.01)
O	30	[core]2S(0.86)2p(2.65)3p(0.01)
O	31	[core]2S(0.86)2p(2.63)3p(0.01)
O	32	[core]2S(0.86)2p(2.70)3p(0.01)4S(0.01)4p(0.01)
H	33	1S(0.26)
H	34	1S(0.27)
H	35	1S(0.26)
H	36	1S(0.26)

****

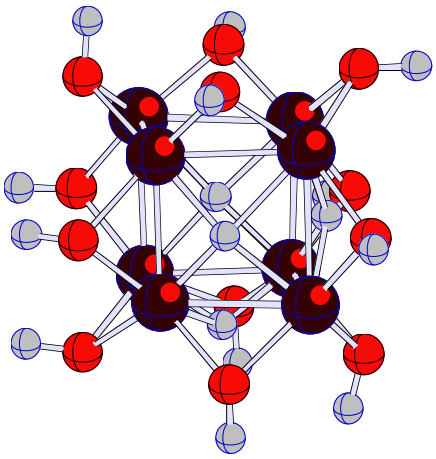
******* Beta spin orbitals *******

****

Atom	No	Natural Electron Configuration
Fe	1	[core]3d(1.75)4p(0.23)4d(0.01)6S(0.09)
Fe	2	[core]3d(2.56)4p(0.35)4d(0.01)6S(0.11)
Fe	3	[core]3d(1.71)4p(0.22)4d(0.01)6S(0.09)
Fe	4	[core]3d(1.74)4p(0.23)4d(0.01)6S(0.09)
Fe	5	[core]3d(2.17)4p(0.28)4d(0.01)6S(0.11)

Fe	6	[core]3d(1.76)4p(0.22)6S(0.09)
Fe	7	[core]3d(1.78)4p(0.24)4d(0.01)6S(0.11)
Fe	8	[core]3d(1.69)4p(0.20)6S(0.09)
H	9	1S(0.46)
H	10	1S(0.44)
H	11	1S(0.49)
H	12	1S(0.47)
O	13	[core]2S(0.84)2p(2.46)
O	14	[core]2S(0.84)2p(2.50)
O	15	[core]2S(0.84)2p(2.49)
O	16	[core]2S(0.84)2p(2.50)
H	17	1S(0.27)
H	18	1S(0.27)
H	19	1S(0.25)
H	20	1S(0.25)
O	21	[core]2S(0.84)2p(2.48)
O	22	[core]2S(0.84)2p(2.50)
O	23	[core]2S(0.84)2p(2.50)
O	24	[core]2S(0.84)2p(2.49)
H	25	1S(0.27)
H	26	1S(0.26)
H	27	1S(0.26)
H	28	1S(0.26)
O	29	[core]2S(0.83)2p(2.50)
O	30	[core]2S(0.84)2p(2.47)
O	31	[core]2S(0.84)2p(2.44)
O	32	[core]2S(0.83)2p(2.51)
H	33	1S(0.26)
H	34	1S(0.27)
H	35	1S(0.26)
H	36	1S(0.26)

HF=-11023.6943179\S2=182.230523\S2-1=0.\S2A=182.003658



TITLE

Fe	-1.3707549312,1.2707061527,-1.6147764058
Fe	1.0274507916,1.07420085,-1.1323524757
Fe	-1.3977049519,-1.3449203549,-1.5668576119
Fe	1.1782999718,-1.402399634,-1.2037630098
Fe	-1.1757394523,1.2830111441,0.9285748656
Fe	1.2683438795,1.2238350147,1.3496190059
Fe	-1.1880456993,-1.2053319987,0.9890818008
Fe	1.3122051355,-1.4551721332,1.432804578
H	-0.0215953981,-0.0051830882,-1.8067126589
H	0.1026714577,1.8732642345,-0.0302177149
H	-1.6247448183,0.0791367745,-0.1954150916
H	1.1334295942,-0.1221685019,0.131871331
O	0.1464075573,2.3642602508,-2.4072546209
O	-0.0929640554,2.3161125724,2.3118757325
O	0.0023479529,-2.5031398629,-2.3623462782
O	-0.1942637933,-2.3817186773,2.2689522269
H	0.1911087399,3.2972410618,-2.1372392206
H	-0.3110027507,2.1465735524,3.2435773564
H	0.1504574445,-2.5307084436,-3.3213545153
H	-0.2868365824,-3.3436315607,2.1732810094
O	-2.2893954902,2.4789603981,-0.3000764797
O	-2.2303040739,-2.4751843997,-0.1729837071
O	2.5103038948,1.9765995331,-0.0686351693
O	2.2369607846,-2.5175712705,0.0665349031
H	-2.0548765281,3.4221029746,-0.301604267
H	-3.1953659744,-2.4901903864,-0.0675871259
H	2.5543898112,2.9461148532,-0.1183076574
H	3.1972249119,-2.644365455,0.01734132
O	-2.3925046161,-0.0393867589,-2.7067319236
O	-2.0591785543,0.0896856229,2.2354651965
O	2.400961505,-0.0202907865,-2.0402843668
O	2.1630091965,-0.0798683823,2.5520727022

H -3.3542010803,-0.0103721353,-2.8237503625
H -1.6925924708,0.0544065971,3.1354789554
H 3.2379434424,0.2122471858,-1.5964157363
H 2.16889515,-0.0892949427,3.5209954154
END

$Fe_8O_{12}H_{17}$

$$$$$$$$$$$$$ Fe8O12H17 NEUTRAL S = 26 QB
fe8o12h17_18_26_GF.out

UBPW91/6-311+G* scf=(VSHIFT=5,NoIncFock,Maxcycle=90,Tight,NoVarAcc) NOSYMM OPT=RFO IOP(5/13=1,5/36=1,8/11=1) INT=UltraFine GUESS=READ GEOM=CHECKPOINT

Charge = 0 Multiplicity = 26
Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	2.342931	0.567918	-0.388101
2	26	0	1.153287	-1.563294	0.166899
3	26	0	0.501845	1.026394	-2.193103
4	26	0	-0.595724	-1.049748	-1.483001
5	26	0	0.674637	1.202442	1.464059
6	26	0	-0.396188	-0.960250	2.037010
7	26	0	-1.056587	1.579407	-0.282651
8	26	0	-2.359107	-0.577882	0.325087
9	1	0	1.060544	-0.490388	-1.186163
10	1	0	1.231117	-0.425703	1.417129
11	1	0	-1.328508	0.422015	-1.547359
12	1	0	0.718703	1.429755	-0.243550
13	1	0	-0.590624	-1.031023	0.248686
14	8	0	3.135353	-1.249113	0.020786
15	8	0	0.083211	0.500819	3.278091
16	8	0	-0.136090	-0.489341	-3.371354
17	8	0	-2.986506	1.298182	0.248385
18	1	0	3.658692	-1.328551	0.835685
19	1	0	-0.654061	0.963093	3.712316
20	1	0	0.566912	-1.060356	-3.729734
21	1	0	-3.683238	1.550409	-0.379209
22	8	0	2.645824	1.634645	1.292218

23	8	0	-0.649569	2.656297	-1.998079
24	8	0	0.509367	-2.742660	1.719646
25	8	0	-2.452232	-1.835686	-1.218937
26	1	0	3.217055	1.246410	1.976088
27	1	0	-0.193475	3.490821	-1.793258
28	1	0	1.171871	-3.003439	2.380941
29	1	0	-3.103639	-1.668799	-1.919862
30	8	0	2.472038	1.344251	-2.203122
31	8	0	-0.690666	2.632758	1.338928
32	8	0	0.388223	-2.753377	-1.244926
33	8	0	-2.370226	-1.242198	2.181630
34	1	0	2.947105	2.150243	-2.454830
35	1	0	-1.463884	2.599671	1.929979
36	1	0	-0.177745	-3.441817	-0.848595
37	1	0	-2.734849	-2.109804	2.418246

Distance matrix (angstroms):

		1	2	3	4	5
1	Fe	0.000000				
2	Fe	2.503067	0.000000			
3	Fe	2.618746	3.563771	0.000000		
4	Fe	3.528645	2.458645	2.453419	0.000000	
5	Fe	2.572221	3.092091	3.665472	3.920630	0.000000
6	Fe	3.964749	2.502369	4.758894	3.526798	2.480358
7	Fe	3.548372	3.868101	2.526729	2.926720	2.488018
8	Fe	4.891896	3.651434	4.135218	2.569311	3.697352
9	H	1.844297	1.729307	1.904390	1.773194	3.168324
10	H	2.341423	1.692113	3.959065	3.483896	1.721258
11	H	3.852873	3.611016	2.032843	1.645357	3.700040
12	H	1.844390	3.052159	2.002620	3.067880	1.723236
13	H	3.401154	1.825165	3.374727	1.731795	2.840138
14	O	2.024036	2.012125	4.124876	4.027661	3.761420
15	O	4.307180	3.883960	5.512300	5.053040	2.032922
16	O	4.020341	3.916006	2.023040	2.022671	5.186582
17	O	5.416761	5.033147	4.266536	3.771779	3.858886
18	H	2.612561	2.603735	4.968400	4.853256	3.962999
19	H	5.094265	4.713717	6.017815	5.571916	2.622477
20	H	4.119713	3.972472	2.592294	2.529752	5.666334
21	H	6.105741	5.778006	4.591266	4.184724	4.744449
22	O	2.013236	3.704163	4.136916	5.041372	2.025316
23	O	3.988535	5.073694	2.005087	3.742054	3.981660
24	O	4.331799	2.053427	5.432811	3.787364	3.956826
25	O	5.427816	3.872274	4.226946	2.033237	5.119180
26	H	2.610332	3.927690	4.980253	5.636924	2.593838
27	H	4.117181	5.585702	2.591669	4.568898	4.074360
28	H	4.668357	2.641277	6.132729	4.676681	4.333284

29	H	6.083940	4.742059	4.509794	2.619869	5.828407
30	O	1.978298	3.976169	1.995694	3.957394	4.086439
31	O	4.055724	4.730821	4.059277	4.640382	1.981291
32	O	3.947915	1.998716	3.898540	1.981712	4.803034
33	O	5.665146	4.071534	5.703822	4.076201	3.970184
34	H	2.672106	4.886881	2.703856	4.871964	4.628189
35	H	4.898300	5.223822	4.831056	5.071527	2.596652
36	H	4.758554	2.516290	4.715342	2.509815	5.257762
37	H	6.389806	4.526018	6.447982	4.573763	4.848303

		6	7	8	9	10
6	Fe	0.000000				
7	Fe	3.502402	0.000000			
8	Fe	2.632477	2.592258	0.000000		
9	H	3.568149	3.095582	3.739725	0.000000	
10	H	1.821570	3.484725	3.755719	2.609676	0.000000
11	H	3.953174	1.735795	2.359657	2.582733	4.007305
12	H	3.486554	1.782015	3.718449	2.166177	2.542272
13	H	1.800255	2.704401	1.827212	2.253316	2.247312
14	O	4.076810	5.066059	5.543667	2.517384	2.500778
15	O	1.976064	3.891193	3.981049	4.676242	2.374724
16	O	5.435055	3.829767	4.314316	2.491385	4.980249
17	O	3.874202	2.021306	1.979679	4.651401	4.703838
18	H	4.245101	5.651615	6.085895	3.397169	2.654493
19	H	2.563669	4.062220	4.093300	5.389580	3.278801
20	H	5.847472	4.635350	5.023538	2.652978	5.228207
21	H	4.790222	2.628585	2.603647	5.226805	5.593097
22	O	4.067190	4.023818	5.556973	3.629222	2.502405
23	O	5.424533	2.065925	4.333536	3.672237	4.969844
24	O	2.024286	5.014147	3.854763	3.717560	2.445554
25	O	3.949038	3.806222	1.993678	3.761715	4.743834
26	H	4.234216	4.845286	6.094869	4.203194	2.655625
27	H	5.875720	2.584646	5.072641	4.217956	5.260723
28	H	2.598407	5.750063	4.751596	4.364865	2.752665
29	H	4.846563	4.173935	2.604655	4.389463	5.609894
30	O	5.613927	4.024264	5.781557	2.528324	4.216496
31	O	3.672022	1.967985	3.757629	4.381422	3.612970
32	O	3.821218	4.667597	3.839992	2.361479	3.635254
33	O	1.999308	3.969860	1.971850	4.865946	3.771047
34	H	6.405421	4.590617	6.582286	3.484475	4.957033
35	H	3.718127	2.470336	3.670687	5.062760	4.083985
36	H	3.812166	5.128874	3.786554	3.218422	4.026827
37	H	2.633657	4.870492	2.620932	5.478985	4.423497

		11	12	13	14	15
11	H	0.000000				
12	H	2.628028	0.000000			
13	H	2.425195	2.830558	0.000000		

14	O	5.017749	3.617513	3.739306	0.000000	
15	O	5.028333	3.697125	3.460909	4.794566	0.000000
16	O	2.362073	3.767859	3.688457	4.773491	6.726339
17	O	2.596406	3.740038	3.341474	6.634582	4.386123
18	H	5.797891	4.173312	4.299974	0.971727	4.700639
19	H	5.330274	4.213209	3.997156	5.734187	0.972532
20	H	3.248507	4.286860	4.143498	4.549607	7.195891
21	H	2.860525	4.405683	4.077046	7.381768	5.353842
22	O	5.032791	2.472723	4.320803	3.189394	3.434565
23	O	2.378260	2.540659	4.318304	5.801179	5.746393
24	O	4.905739	4.615951	2.510659	3.465922	3.623605
25	O	2.543193	4.655031	2.503395	5.753442	5.666656
26	H	5.810030	3.346964	4.761201	3.171358	3.474492
27	H	3.281210	2.735262	4.977382	6.069500	5.893662
28	H	5.780759	5.171704	3.397547	3.535994	3.777550
29	H	2.767915	5.198207	3.380030	6.547311	6.471629
30	O	3.965438	2.630859	4.586195	3.480128	6.038342
31	O	3.691189	2.436755	3.823863	5.607570	2.984025
32	O	3.622395	4.313996	2.481032	3.378100	5.580368
33	O	4.214278	4.749980	2.635878	5.914448	3.203074
34	H	4.700122	3.220969	5.472201	4.209482	6.617317
35	H	4.105167	3.294938	4.095274	6.293737	2.935318
36	H	4.091665	4.990181	2.680750	4.066988	5.713319
37	H	4.910594	5.616107	3.235500	6.399053	3.936515

		16	17	18	19	20
16	O	0.000000				
17	O	4.941925	0.000000			
18	H	5.727463	7.169610	0.000000		
19	H	7.249569	4.189439	5.668023	0.000000	
20	H	0.974015	5.832230	5.520334	7.808280	0.000000
21	H	5.069099	0.971045	7.979243	5.124591	6.008817
22	O	5.830889	5.738113	3.164625	4.146938	6.066705
23	O	3.470530	3.514591	6.516928	5.956137	4.276910
24	O	5.604672	5.542034	3.563614	4.365422	5.703438
25	O	3.436577	3.501373	6.466998	5.948432	4.002558
26	H	6.546110	6.439861	2.850612	4.252093	6.700808
27	H	4.281982	4.095973	6.706480	6.075598	5.004132
28	H	6.412515	6.351680	3.373032	4.565081	6.440644
29	H	3.507748	3.676683	7.310126	6.681970	4.137485
30	O	3.395462	5.983955	4.217388	6.701507	3.426687
31	O	5.678188	2.870759	5.904417	2.902084	6.396243
32	O	3.149994	5.480320	4.129775	6.282734	3.012063
33	O	6.032727	3.251272	6.177935	3.186146	6.603338
34	H	4.160951	6.575799	4.841059	7.239573	4.195074
35	H	6.277672	2.615341	6.547457	2.551651	7.039338
36	H	3.883705	5.617837	4.692648	6.358618	3.811409

37	H	6.549727	4.047962	6.632664	3.930266	7.056956
		21	22	23	24	25
21	H	0.000000				
22	O	6.546586	0.000000			
23	O	3.612046	4.767541	0.000000		
24	O	6.357167	4.889575	6.656828	0.000000	
25	O	3.699481	6.658774	4.902507	4.269537	0.000000
26	H	7.297525	0.971961	5.721238	4.828045	7.200578
27	H	4.235938	4.585539	0.972833	7.189629	5.814078
28	H	7.206112	4.986950	7.384177	0.971714	5.239932
29	H	3.615639	7.367939	4.973433	5.239563	0.971328
30	O	6.423129	3.511685	3.392336	5.995251	5.943826
31	O	3.616484	3.482898	3.337343	5.520883	5.441763
32	O	5.987389	5.548747	5.559570	2.967066	2.985133
33	O	4.010057	5.850473	5.968994	3.279766	3.452942
34	H	6.973482	3.794336	3.660707	6.878178	6.824069
35	H	3.370287	4.269392	4.011977	5.698987	5.528553
36	H	6.118098	6.190806	6.223417	2.748964	2.808933
37	H	4.703441	6.651352	6.824078	3.378385	3.658430
		26	27	28	29	30
26	H	0.000000				
27	H	5.556713	0.000000			
28	H	4.733698	7.839867	0.000000		
29	H	7.976719	5.925096	6.209522	0.000000	
30	O	4.246224	3.446841	6.450308	6.344043	0.000000
31	O	4.195023	3.285431	6.026736	5.911476	4.920271
32	O	5.863063	6.295160	3.718003	3.718192	4.695847
33	O	6.119896	6.552820	3.960826	4.188332	7.025902
34	H	4.530212	3.478228	7.286740	7.175151	0.968850
35	H	4.872846	4.033681	6.208495	5.977450	5.843808
36	H	6.440727	6.996721	3.527540	3.584978	5.635826
37	H	6.847250	7.454016	4.007797	4.376034	7.771693
		31	32	33	34	35
31	O	0.000000				
32	O	6.070482	0.000000			
33	O	4.306548	4.651235	0.000000		
34	H	5.278144	5.661911	7.828118	0.000000	
35	H	0.973808	6.493492	3.955343	6.235813	0.000000
36	H	6.476790	0.975371	4.339074	6.604227	6.773050
37	H	5.275937	4.856603	0.970401	8.612751	4.902338
		36	37			
36	H	0.000000				
37	H	4.357211	0.000000			

Alpha occ. eigenvalues -- -0.20878 -0.20766 -0.20176 -0.19943 -0.19635
Alpha occ. eigenvalues -- -0.19618 -0.19422 -0.18963 -0.18431 -0.18038
Alpha occ. eigenvalues -- -0.17858 -0.17530 -0.17295

Alpha virt. eigenvalues -- -0.12914 -0.12541 -0.11129 -0.08725 -0.04808
gap = 1.19 eV
Beta occ. eigenvalues -- -0.18686 -0.18282 -0.17846 -0.17144 -0.16780
Beta occ. eigenvalues -- -0.16184 -0.15983 -0.15587
Beta virt. eigenvalues -- -0.13661 -0.13300 -0.12792 -0.12642 -0.12544
gap = 0.52 eV
Mulliken charges and spin densities:

		1	2
1	Fe	0.183549	3.224180
2	Fe	-0.320369	2.640554
3	Fe	0.159503	3.333355
4	Fe	-0.646027	2.361836
5	Fe	-0.040811	2.741169
6	Fe	0.155938	3.118389
7	Fe	-0.055092	2.848330
8	Fe	0.634147	3.410922
9	H	0.699408	-0.103891
10	H	0.611892	-0.108380
11	H	0.522249	-0.069974
12	H	0.719365	-0.129137
13	H	1.101550	-0.139127
14	O	-0.634936	0.161567
15	O	-0.654681	0.131602
16	O	-0.628661	0.140430
17	O	-0.751963	0.129514
18	H	0.365855	0.003809
19	H	0.373364	0.004765
20	H	0.390607	0.005276
21	H	0.376947	0.013282
22	O	-0.678261	0.157200
23	O	-0.630308	0.163551
24	O	-0.714227	0.128450
25	O	-0.747744	0.133352
26	H	0.380520	0.006673
27	H	0.374654	0.009125
28	H	0.371638	0.005581
29	H	0.389380	0.008714
30	O	-0.718549	0.178463
31	O	-0.648452	0.163810
32	O	-0.721448	0.140577
33	O	-0.782679	0.169061
34	H	0.424657	0.011295
35	H	0.360321	-0.000639
36	H	0.381724	-0.003206
37	H	0.396942	0.009518

Sum of Mulliken charges = 0.00000 25.00000

Dipole moment (field-independent basis, Debye):
X= -0.5250 Y= 0.2262 Z= 1.9582 Tot= 2.0399

Isotropic polarizability for W= 0.000000 309.53 Bohr**3. 1.24 A**3

Frequencies --	40.5761	58.3848	60.8962
Frequencies --	68.0809	79.8690	81.4747
Frequencies --	84.4272	90.8734	100.2170
Frequencies --	106.2382	114.2336	115.6549
Frequencies --	121.4651	124.6528	133.6185
Frequencies --	134.5494	144.4607	154.2795
Frequencies --	158.5043	164.4993	170.3228
Frequencies --	176.4206	186.3363	193.3554
Frequencies --	201.0847	204.5587	217.8986
Frequencies --	224.7032	229.2729	242.6205
Frequencies --	274.8953	283.3927	284.4271
Frequencies --	296.1868	297.7375	301.5010
Frequencies --	309.1227	313.0880	321.1015
Frequencies --	336.5224	344.1174	346.9333
Frequencies --	355.5373	390.5922	419.1125
Frequencies --	426.2035	436.3092	442.2541
Frequencies --	448.0934	455.0008	463.4284
Frequencies --	471.0573	486.2582	496.6958
Frequencies --	501.8114	516.5672	522.3946
Frequencies --	539.1631	573.7555	577.5547
Frequencies --	596.8300	608.5725	618.9865
Frequencies --	629.4021	640.1684	644.5482
Frequencies --	657.7685	660.4057	671.3680
Frequencies --	674.7013	676.6619	678.4005
Frequencies --	682.9560	687.5917	698.8144
Frequencies --	715.4055	716.3642	729.4405
Frequencies --	749.6251	763.3112	784.4271
Frequencies --	806.9223	862.5985	955.0913
Frequencies --	994.4231	1039.2153	1052.4480
Frequencies --	1095.3638	1142.3390	1201.8892
Frequencies --	1264.1462	1288.4293	1358.7160
Frequencies --	3643.8324	3656.9951	3667.4601
Frequencies --	3676.8389	3682.5828	3683.1354
Frequencies --	3686.3765	3694.4810	3700.9669
Frequencies --	3706.4581	3715.7511	3733.7148

Zero-point vibrational energy 526418.3 (Joules/Mol)
125.81699 (Kcal/Mol) 5.456 eV

Atom No	Natural Electron Configuration

Fe	1	[core]4S(0.20)3d(6.59)4p(0.49)4d(0.03)
Fe	2	[core]4S(0.23)3d(6.84)4p(0.66)4d(0.04)5p(0.01)
Fe	3	[core]4S(0.21)3d(6.56)4p(0.50)4d(0.03)
Fe	4	[core]4S(0.25)3d(6.92)4p(0.73)4d(0.04)5p(0.01)
Fe	5	[core]4S(0.23)3d(6.78)4p(0.58)4d(0.03)5p(0.01)
Fe	6	[core]4S(0.22)3d(6.64)4p(0.50)4d(0.03)5p(0.01)
Fe	7	[core]4S(0.24)3d(6.73)4p(0.60)4d(0.04)5p(0.01)
Fe	8	[core]4S(0.21)3d(6.52)4p(0.41)4d(0.02)
H	9	1S(0.84)2S(0.01)
H	10	1S(0.85)2S(0.01)
H	11	1S(0.85)2S(0.01)
H	12	1S(0.88)2S(0.01)
H	13	1S(0.87)2S(0.01)
O	14	[core]2S(1.70)2p(5.12)3S(0.01)3p(0.02)
O	15	[core]2S(1.70)2p(5.13)3S(0.01)3p(0.01)
O	16	[core]2S(1.70)2p(5.10)3p(0.02)
O	17	[core]2S(1.70)2p(5.18)3S(0.01)3p(0.01)
H	18	1S(0.54)
H	19	1S(0.53)
H	20	1S(0.53)
H	21	1S(0.52)
O	22	[core]2S(1.71)2p(5.14)3S(0.01)3p(0.02)
O	23	[core]2S(1.71)2p(5.14)3p(0.01)
O	24	[core]2S(1.70)2p(5.14)3p(0.02)
O	25	[core]2S(1.70)2p(5.15)3S(0.01)3p(0.02)
H	26	1S(0.53)
H	27	1S(0.53)
H	28	1S(0.53)
H	29	1S(0.52)
O	30	[core]2S(1.69)2p(5.20)3S(0.01)3p(0.02)
O	31	[core]2S(1.69)2p(5.09)3p(0.02)
O	32	[core]2S(1.68)2p(5.04)3p(0.02)
O	33	[core]2S(1.70)2p(5.19)3S(0.01)3p(0.01)
H	34	1S(0.51)
H	35	1S(0.53)
H	36	1S(0.52)
H	37	1S(0.51)

****

******* Alpha spin orbitals *******

****

Atom	No	Natural Electron Configuration
Fe	1	[core]3d(4.81)4p(0.27)4d(0.02)6S(0.12)
Fe	2	[core]3d(4.63)4p(0.36)4d(0.02)6S(0.13)5d(0.01)

Fe	3	[core]3d(4.83)4p(0.27)4d(0.02)6S(0.12)
Fe	4	[core]3d(4.55)4p(0.39)4d(0.03)6S(0.13)5d(0.01)
Fe	5	[core]3d(4.68)4p(0.31)4d(0.02)6S(0.13)
Fe	6	[core]3d(4.79)4p(0.27)4d(0.02)6S(0.13)
Fe	7	[core]3d(4.72)4p(0.20)4d(0.02)5p(0.12)6S(0.13)5d(0.01)
Fe	8	[core]3d(4.86)4p(0.23)4d(0.01)6S(0.12)
H	9	1S(0.39)
H	10	1S(0.39)2S(0.01)
H	11	1S(0.39)2S(0.01)
H	12	1S(0.41)
H	13	1S(0.42)
O	14	[core]2S(0.86)2p(2.65)3p(0.01)
O	15	[core]2S(0.86)2p(2.64)4p(0.01)
O	16	[core]2S(0.86)2p(2.63)3p(0.01)
O	17	[core]2S(0.86)2p(2.67)3p(0.01)
H	18	1S(0.27)
H	19	1S(0.27)
H	20	1S(0.26)
H	21	1S(0.26)
O	22	[core]2S(0.86)2p(2.65)3p(0.01)
O	23	[core]2S(0.87)2p(2.66)3p(0.01)
O	24	[core]2S(0.86)2p(2.64)3p(0.01)
O	25	[core]2S(0.86)2p(2.65)3p(0.01)
H	26	1S(0.27)
H	27	1S(0.27)
H	28	1S(0.27)
H	29	1S(0.26)
O	30	[core]2S(0.86)2p(2.70)4S(0.01)4p(0.01)
O	31	[core]2S(0.85)2p(2.63)4p(0.01)
O	32	[core]2S(0.85)2p(2.59)3p(0.01)
O	33	[core]2S(0.86)2p(2.69)4p(0.01)
H	34	1S(0.26)
H	35	1S(0.26)
H	36	1S(0.26)
H	37	1S(0.26)

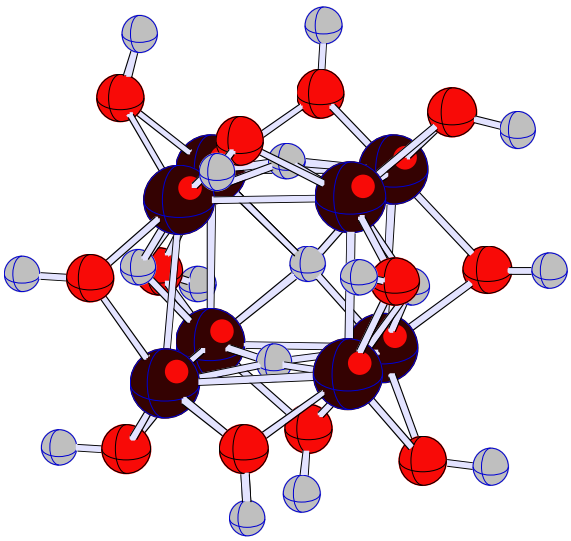
NBO analysis skipped by request.

****
******* Beta spin orbitals *******
****

Atom	No	Natural Electron Configuration
Fe	1	[core]3d(1.78)4p(0.22)4d(0.01)6S(0.09)

Fe 2 [core]3d(2.21)4p(0.30)4d(0.01)6S(0.10)
Fe 3 [core]3d(1.73)4p(0.23)4d(0.01)6S(0.09)
Fe 4 [core]3d(2.38)4p(0.34)4d(0.01)6S(0.11)
Fe 5 [core]3d(2.10)4p(0.27)4d(0.01)6S(0.10)
Fe 6 [core]3d(1.85)4p(0.23)4d(0.01)6S(0.09)
Fe 7 [core]3d(2.01)4p(0.18)4d(0.01)5p(0.11)6S(0.11)
Fe 8 [core]3d(1.66)4p(0.19)4d(0.01)6S(0.09)
H 9 1S(0.45)
H 10 1S(0.46)
H 11 1S(0.46)
H 12 1S(0.48)
H 13 1S(0.46)
O 14 [core]2S(0.84)2p(2.47)
O 15 [core]2S(0.84)2p(2.49)
O 16 [core]2S(0.84)2p(2.47)
O 17 [core]2S(0.84)2p(2.51)
H 18 1S(0.27)
H 19 1S(0.26)
H 20 1S(0.26)
H 21 1S(0.26)
O 22 [core]2S(0.84)2p(2.48)
O 23 [core]2S(0.84)2p(2.48)
O 24 [core]2S(0.84)2p(2.50)
O 25 [core]2S(0.84)2p(2.50)
H 26 1S(0.27)
H 27 1S(0.26)
H 28 1S(0.26)
H 29 1S(0.26)
O 30 [core]2S(0.83)2p(2.50)
O 31 [core]2S(0.84)2p(2.46)
O 32 [core]2S(0.84)2p(2.44)3p(0.01)
O 33 [core]2S(0.84)2p(2.50)
H 34 1S(0.25)
H 35 1S(0.26)
H 36 1S(0.26)
H 37 1S(0.25)

HF=-11024.2663138\S2=168.988769\S2-1=0.\S2A=168.754166



TITLE

Fe	2.3429305061,0.5679181487,-0.3881006096
Fe	1.1532866381,-1.5632943843,0.1668985514
Fe	0.5018449905,1.026393516,-2.1931030609
Fe	-0.5957235824,-1.0497478152,-1.4830009246
Fe	0.6746372402,1.2024419237,1.4640591445
Fe	-0.3961880313,-0.960250127,2.0370104697
Fe	-1.0565865014,1.5794071931,-0.2826513454
Fe	-2.3591067917,-0.5778823114,0.3250869144
H	1.0605439379,-0.4903883657,-1.1861628096
H	1.2311174796,-0.425702919,1.4171287083
H	-1.3285078682,0.4220147955,-1.5473590886
H	0.7187027783,1.4297547675,-0.2435498757
H	-0.5906239617,-1.0310228504,0.2486858268
O	3.1353531046,-1.2491125622,0.0207864705
O	0.0832111992,0.5008185875,3.2780914497
O	-0.1360903808,-0.4893409481,-3.3713544647
O	-2.9865062668,1.2981819905,0.2483852551
H	3.6586923592,-1.3285505246,0.8356849076
H	-0.6540611954,0.9630931775,3.712315922
H	0.5669115373,-1.0603555296,-3.7297342019
H	-3.6832378133,1.5504091102,-0.3792090766
O	2.6458238876,1.6346448095,1.2922180081
O	-0.6495692256,2.6562967293,-1.9980792528
O	0.5093669037,-2.742660235,1.719646428
O	-2.4522323868,-1.835686423,-1.2189367803
H	3.2170547372,1.246410432,1.9760875952
H	-0.1934752656,3.4908208553,-1.7932579254
H	1.1718713031,-3.003438934,2.3809407572
H	-3.1036393064,-1.6687991253,-1.9198623247
O	2.4720384448,1.3442505978,-2.2031223684

O -0.6906661992,2.6327579242,1.3389276561
O 0.3882231649,-2.7533767298,-1.2449257733
O -2.3702255077,-1.2421981245,2.1816304341
H 2.9471051733,2.1502434565,-2.4548302656
H -1.4638837364,2.5996707297,1.929979116
H -0.1777445629,-3.4418169813,-0.8485947588
H -2.7348488813,-2.1098044369,2.4182461476
END

$Fe_8O_{12}H_{18}$

$$$$$$$$$$$$$ Fe_8O_12H_18 NEUTRAL S = 27 head fe8o12h18_27_GF.out

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UBPW91/6-311+G* scf=(VSHIFT=5,NoIncFock,MAXCYC=77,Tight,NoVarAcc) NO SYMM OPT=RFO IOP(5/13=1,5/36=1,8/11=1) INT=UltraFine GUESS=READ GEOM=CHECKPOINT

Charge = 0 Multiplicity = 27

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	2.235808	0.430039	-0.216149
2	26	0	1.103353	-1.728326	0.108543
3	26	0	0.342438	0.962580	-2.024089
4	26	0	-0.652739	-1.526235	-1.708315
5	26	0	0.639616	1.600128	1.693359
6	26	0	-0.362258	-0.950900	1.978987
7	26	0	-1.118269	1.661820	-0.123359
8	26	0	-2.279817	-0.457480	0.201664
9	1	0	1.191780	-0.796887	-1.208832
10	1	0	-1.215983	0.772288	1.213597
11	1	0	1.161754	-0.451608	1.081380
12	1	0	-1.222575	0.417844	-1.130926
13	1	0	0.452235	1.219786	-0.125794
14	1	0	-0.459156	-1.252245	0.136132
15	8	0	3.091982	-1.429460	0.119145
16	8	0	0.317783	0.418789	3.280954
17	8	0	-0.278457	-0.422113	-3.324006
18	8	0	-3.113393	1.433830	-0.027108

19	1	0	3.511874	-1.555115	0.988353
20	1	0	-0.249701	0.702404	4.015658
21	1	0	0.322821	-0.738871	-4.017206
22	1	0	-3.493653	1.622358	-0.904419
23	8	0	2.574450	1.753192	1.264063
24	8	0	-0.742874	2.681848	-1.781064
25	8	0	0.592533	-2.773171	1.770389
26	8	0	-2.595602	-1.759064	-1.290222
27	1	0	3.278446	1.710579	1.929737
28	1	0	-0.300974	3.508884	-1.515727
29	1	0	1.327355	-2.934733	2.387403
30	1	0	-3.288379	-1.685262	-1.965169
31	8	0	2.310313	1.355658	-1.983619
32	8	0	-0.492622	3.157403	1.092811
33	8	0	0.449362	-3.116356	-1.157973
34	8	0	-2.320766	-1.378561	1.981383
35	1	0	2.671257	2.254668	-2.044560
36	1	0	-1.182951	3.498233	1.686539
37	1	0	0.019541	-3.848842	-0.680918
38	1	0	-2.584717	-2.312714	2.018927

Distance matrix (angstroms):

		1	2	3	4	5
1	Fe	0.000000				
2	Fe	2.458946	0.000000			
3	Fe	2.671534	3.516829	0.000000		
4	Fe	3.794373	2.534891	2.698943	0.000000	
5	Fe	2.750119	3.715548	3.783411	4.797469	0.000000
6	Fe	3.670907	2.500194	4.492507	3.743205	2.755554
7	Fe	3.574315	4.059862	2.497074	3.590613	2.528721
8	Fe	4.620944	3.615185	3.721124	2.727204	3.870658
9	H	1.892290	1.615821	2.117014	2.045405	3.804376
10	H	3.751822	3.585182	3.598263	3.760056	2.087759
11	H	1.901176	1.606185	3.509293	3.497085	2.203807
12	H	3.577341	3.398863	1.882483	2.106546	3.583592
13	H	1.952689	3.028239	1.918785	3.356482	1.867910
14	H	3.196406	1.633662	3.196022	1.874708	3.430493
15	O	2.074415	2.010989	4.227919	4.167962	4.203647
16	O	3.988568	3.910423	5.332897	5.442226	2.004893
17	O	4.087354	3.924027	1.998167	1.992394	5.486918
18	O	5.445850	5.272436	4.019052	4.200388	4.131917
19	H	2.649530	2.570027	5.045683	4.961537	4.324633
20	H	4.915295	4.796326	6.074279	6.155740	2.643836
21	H	4.412925	4.313938	2.620656	2.627287	6.179144
22	H	5.892543	5.778031	4.050254	4.316327	4.881891
23	O	2.014060	3.952255	4.052023	5.477629	1.987789

24	O	4.048721	5.140895	2.047644	4.209677	3.892687
25	O	4.111841	2.028391	5.330707	3.899606	4.374230
26	O	5.411869	3.954714	4.071608	2.000932	5.536476
27	H	2.707712	4.458008	4.981203	6.258322	2.651696
28	H	4.195646	5.660279	2.675083	5.051064	3.850493
29	H	4.350341	2.588204	5.968281	4.762304	4.638927
30	H	6.168486	4.856898	4.494149	2.652898	6.293470
31	O	1.996564	3.917250	2.007158	4.142557	4.046129
32	O	4.073845	5.233189	3.902516	5.459707	2.016861
33	O	4.081095	1.989572	4.171248	2.011464	5.514663
34	O	5.372387	3.918476	5.349523	4.051911	4.209442
35	H	2.619537	4.791494	2.663327	5.045517	4.304419
36	H	4.972117	5.918968	4.746062	6.086989	2.631464
37	H	4.841144	2.508882	5.005812	2.627167	5.976032
38	H	5.979609	4.194394	5.970073	4.271232	5.080616

		6	7	8	9	10
6	Fe	0.000000				
7	Fe	3.437690	0.000000			
8	Fe	2.660709	2.438497	0.000000		
9	H	3.549781	3.543983	3.762536	0.000000	
10	H	2.069793	1.608809	1.915223	3.758695	0.000000
11	H	1.837827	3.334138	3.552231	2.316288	2.677506
12	H	3.505019	1.604228	1.913047	2.703839	2.371173
13	H	3.131354	1.631528	3.222509	2.405591	2.185675
14	H	1.869843	2.998923	1.987649	2.177584	2.415046
15	O	3.952190	5.228866	5.459650	2.403007	4.960250
16	O	2.008387	3.898296	4.122790	4.732855	2.598338
17	O	5.329951	3.910525	4.054262	2.603077	4.784913
18	O	4.156933	2.010413	2.079480	4.990699	2.361599
19	H	4.044172	5.746547	5.947047	3.284109	5.274483
20	H	2.625664	4.336629	4.473618	5.623258	2.964816
21	H	6.038925	4.796051	4.965054	2.940309	5.657987
22	H	4.974064	2.500812	2.650008	5.281921	3.224344
23	O	4.055550	3.945816	5.438720	3.811809	3.915623
24	O	5.242109	1.982263	4.018555	4.021434	3.583050
25	O	2.067803	5.116861	4.009203	3.624990	4.018833
26	O	4.040876	3.904681	2.004885	3.908538	3.818403
27	H	4.510058	4.852698	6.211360	4.526828	4.646841
28	H	5.666256	2.453224	4.753661	4.567511	3.971827
29	H	2.637649	5.780424	4.891414	4.185890	4.646331
30	H	4.965666	4.393701	2.686971	4.629588	4.520944
31	O	5.307079	3.912733	5.397427	2.546539	4.795547
32	O	4.204813	2.026640	4.129841	4.875569	2.495318
33	O	3.897235	5.134088	4.045572	2.435921	4.849667
34	O	2.004657	3.888425	2.004361	4.780564	2.536964
35	H	5.972170	4.289871	6.075723	3.492747	5.284286

36	H	4.533635	2.579211	4.365276	5.698296	2.766866
37	H	3.952080	5.654457	4.191340	3.311687	5.144953
38	H	2.606810	4.747292	2.614824	5.194044	3.469759

		11	12	13	14	15
11	H	0.000000				
12	H	3.366789	0.000000			
13	H	2.180422	2.111490	0.000000		
14	H	2.040065	2.231018	2.647674	0.000000	
15	O	2.368094	4.857016	3.747901	3.555598	0.000000
16	O	2.511574	4.673048	3.502228	3.644981	4.594479
17	O	4.634922	2.531104	3.668557	3.562910	4.922387
18	O	4.802135	2.413677	3.573410	3.779764	6.835678
19	H	2.597969	5.549677	4.278176	4.072725	0.973459
20	H	3.454553	5.245454	4.232260	4.349166	5.558282
21	H	5.175124	3.472298	4.358460	4.257377	5.025392
22	H	5.469693	2.580689	4.042073	4.307465	7.330202
23	O	2.624924	4.683644	2.592300	4.416746	3.421688
24	O	4.651853	2.403853	2.511141	4.385570	5.934625
25	O	2.487650	4.679189	4.422544	2.467804	3.283201
26	O	4.631594	2.578664	4.418004	2.618349	5.868864
27	H	3.142474	5.594462	3.528958	5.095587	3.629444
28	H	4.956816	3.248376	2.781943	5.042024	6.210652
29	H	2.810522	5.488220	4.933764	3.330257	3.244187
30	H	5.532364	3.063751	5.080828	3.550701	6.717053
31	O	3.738932	3.753382	2.631051	4.354821	3.576242
32	O	3.970144	3.603195	2.476310	4.512355	5.902264
33	O	3.552898	3.909818	4.457301	2.444386	3.385275
34	O	3.714457	3.757600	4.345243	2.624213	5.724365
35	H	4.401593	4.401202	3.110740	5.182022	4.293185
36	H	4.633045	4.174743	3.339117	5.049226	6.709243
37	H	3.993939	4.466539	5.117263	2.763881	3.991667
38	H	4.287046	4.385539	5.128496	3.031092	6.050968

		16	17	18	19	20
16	O	0.000000				
17	O	6.684917	0.000000			
18	O	4.873042	4.727677	0.000000		
19	H	4.399378	5.852072	7.338877	0.000000	
20	H	0.970704	7.425365	5.007961	5.330141	0.000000
21	H	7.389407	0.970771	5.696409	5.990988	8.181195
22	H	5.787311	4.513508	0.974585	7.921889	5.964621
23	O	3.307723	5.824209	5.841291	3.449590	4.080596
24	O	5.645392	3.497275	3.202074	6.612443	6.145194
25	O	3.542019	5.677936	5.887591	3.258495	4.222583
26	O	5.841789	3.360488	3.472483	6.521868	6.301940
27	H	3.501433	6.693411	6.690398	3.406677	4.220817
28	H	5.739312	4.327022	3.798887	6.815593	6.202837

29	H	3.614385	6.442988	6.680902	2.938164	4.285683
30	H	6.704718	3.535763	3.676335	7.415098	7.120731
31	O	5.706455	3.414504	5.766336	4.330007	6.555283
32	O	3.597879	5.689207	3.330670	6.185040	3.824796
33	O	5.676145	3.532756	5.888656	4.052551	6.468236
34	O	3.446924	5.764804	3.545678	5.919203	3.571834
35	H	6.104948	4.183653	6.181106	4.941624	6.904184
36	H	3.778536	6.425947	3.305292	6.932905	3.756650
37	H	5.830784	4.337879	6.176517	4.499338	6.545545
38	H	4.180709	6.118835	4.301436	6.229323	4.304669

		21	22	23	24	25
21	H	0.000000				
22	H	5.461714	0.000000			
23	O	6.258755	6.445255	0.000000		
24	O	4.223429	3.075356	4.597808	0.000000	
25	O	6.140633	6.570554	4.967124	6.644799	0.000000
26	O	4.122430	3.519852	6.752019	4.836862	4.534308
27	H	7.078252	7.341767	0.969818	5.557375	5.229104
28	H	4.968897	3.758441	4.367808	0.974509	7.145706
29	H	6.844700	7.405761	4.979335	7.294378	0.973023
30	H	4.259962	3.479609	7.524871	5.058176	5.495399
31	O	3.531664	5.909469	3.282565	3.334930	5.838713
32	O	6.477512	3.918096	3.377583	2.923685	6.066990
33	O	3.720707	6.169851	5.839071	5.952213	2.951876
34	O	6.586411	4.325393	5.855388	5.756098	3.236783
35	H	4.285763	6.301258	3.347810	3.450826	6.644855
36	H	7.263133	3.946051	4.164339	3.589488	6.518426
37	H	4.571074	6.505883	6.457035	6.666447	2.737571
38	H	6.882271	4.985670	6.611991	6.540487	3.220048

		26	27	28	29	30
26	O	0.000000				
27	H	7.543938	0.000000			
28	H	5.750430	5.283689	0.000000		
29	H	5.504246	5.059163	7.707534	0.000000	
30	H	0.970021	8.356149	6.008806	6.466148	0.000000
31	O	5.852375	4.046925	3.416742	6.203184	6.371255
32	O	5.854316	4.124887	2.639079	6.488636	6.373296
33	O	3.336396	6.390381	6.677185	3.656987	4.082929
34	O	3.305104	6.395046	6.340067	3.986892	4.074999
35	H	6.664749	4.057061	3.269079	6.955448	7.144692
36	H	6.204504	4.812370	3.321522	6.940886	6.681050
37	H	3.402557	6.952923	7.411867	3.458406	4.156045
38	H	3.355162	7.111366	7.183333	3.978316	4.094125

		31	32	33	34	35
31	O	0.000000				
32	O	4.535102	0.000000			

```
   33  O    4.913628   6.731523   0.000000
   34  O    6.681622   4.970577   4.533111   0.000000
   35  H    0.970677   4.546224   5.879690   7.370811   0.000000
   36  H    5.501234   0.972231   7.382986   5.016441   5.506584
   37  H    5.833651   7.245405   0.974096   4.320552   6.792935
   38  H    7.310174   5.929311   4.465889   0.971454   8.062145
             36         37         38
   36  H    0.000000
   37  H    7.812193   0.000000
   38  H    5.986864   4.053518   0.000000
Alpha  occ. eigenvalues --   -0.19574  -0.19301  -0.19083  -0.18733  -0.18392
 Alpha  occ. eigenvalues --   -0.18212  -0.17884  -0.17813  -0.15536
 Alpha virt. eigenvalues --   -0.11242  -0.11072  -0.07920  -0.06992  -0.04682
1.16 eV
  Beta  occ. eigenvalues --   -0.18095  -0.17746  -0.17633  -0.16489  -0.15948
  Beta  occ. eigenvalues --   -0.15887  -0.15708  -0.15540
  Beta virt. eigenvalues --   -0.13612  -0.13251  -0.12562  -0.12390  -0.12296
0.52 eV
Mulliken atomic spin densities:
             1
    1  Fe   3.381663
    2  Fe   1.937751
    3  Fe   3.406159
    4  Fe   3.438395
    5  Fe   3.469170
    6  Fe   3.400906
    7  Fe   1.852742
    8  Fe   3.413617
    9  H   -0.036670
   10  H   -0.024401
   11  H   -0.043116
   12  H   -0.040798
   13  H   -0.062252
   14  H   -0.061606
   15  O    0.159434
   16  O    0.164282
   17  O    0.179729
   18  O    0.141686
   19  H    0.006508
   20  H    0.012408
   21  H    0.011129
   22  H    0.007903
   23  O    0.176634
   24  O    0.137282
   25  O    0.105420
   26  O    0.181881
```

27	H	0.008749
28	H	0.003690
29	H	0.004594
30	H	0.008439
31	O	0.177776
32	O	0.106116
33	O	0.168468
34	O	0.171446
35	H	0.010258
36	H	0.010325
37	H	0.003729
38	H	0.010558

Sum of Mulliken atomic spin densities = 26.00000

Dipole moment (field-independent basis, Debye):

X= 0.3342 Y= 0.4528 Z= 2.0203 Tot= 2.0972

Isotropic polarizability for W= 0.000000 318.82 Bohr**3. 1.24 A**3

Frequencies --	48.1301	60.6778	68.5784
Frequencies --	83.4831	99.0625	101.2418
Frequencies --	104.1917	107.8370	114.2473
Frequencies --	115.8776	117.3912	120.1410
Frequencies --	126.0898	128.4239	128.8711
Frequencies --	133.8467	136.7205	138.6343
Frequencies --	146.7755	153.1630	157.4926
Frequencies --	160.6093	170.6782	176.6618
Frequencies --	194.8080	204.5042	210.5977
Frequencies --	213.3721	224.3975	229.1730
Frequencies --	256.2873	259.4617	275.2734
Frequencies --	286.4025	305.6597	307.1417
Frequencies --	325.3027	333.9177	341.8860
Frequencies --	343.5785	345.8318	354.1620
Frequencies --	358.5410	362.9788	389.2132
Frequencies --	406.4446	408.6530	426.6475
Frequencies --	429.8468	437.8261	439.8218
Frequencies --	444.9790	468.1147	478.8493
Frequencies --	483.0247	489.5055	502.1609
Frequencies --	510.9883	523.6908	538.7485
Frequencies --	561.6933	569.9226	592.6301
Frequencies --	622.4916	635.8348	646.8153
Frequencies --	652.2907	654.3925	657.1090
Frequencies --	673.8159	676.4935	691.2770

```
Frequencies --   704.6388            705.2086            710.4500
Frequencies --   714.9996            722.3575            725.5646
Frequencies --   726.1417            732.6398            746.1422
Frequencies --   752.3390            783.4357            853.7451
Frequencies --   937.2107            975.3866           1054.3068
Frequencies --  1102.5873           1120.9408           1184.2008
Frequencies --  1411.1113           1471.3311           1516.8926
Frequencies --  1525.2195           1548.4053           1565.6035
Frequencies --  3650.8590           3651.1919           3658.4310
Frequencies --  3660.8265           3669.5279           3688.6689
Frequencies --  3704.3020           3709.6018           3712.0798
Frequencies --  3713.5133           3716.3028           3717.0543
[headnode:~/feon] ggutsev% grep "Inten" fe8o12h18_27_GF.out
IR Inten    --     4.0916              2.1585              0.9692
IR Inten    --     0.9894              3.5337              3.6245
IR Inten    --     5.9895              4.6009              4.1688
IR Inten    --     4.4911              1.0305              4.9262
IR Inten    --     0.3320              1.8084              4.2522
IR Inten    --     4.1291              1.2670              2.7209
IR Inten    --     1.1914              0.0668              6.3141
IR Inten    --     2.3141              2.5615              4.7785
IR Inten    --    13.1279              4.6849              7.5619
IR Inten    --    11.5973              0.6178             24.3001
IR Inten    --     0.5579              1.1997              1.7693
IR Inten    --     1.1962              1.2251              1.2179
IR Inten    --   100.4007              0.6826             11.8113
IR Inten    --     3.3150              2.4886              5.0936
IR Inten    --     1.8431            127.0496            183.4211
IR Inten    --   123.3496            255.8432            144.0109
IR Inten    --    74.3429             25.6378             39.8455
IR Inten    --    44.2331            180.4056             90.4091
IR Inten    --    22.5419             64.3963              8.5135
IR Inten    --    30.5000             11.6480             32.0782
IR Inten    --     1.7673             35.9594             19.5370
IR Inten    --    19.8496             92.4602             48.9276
IR Inten    --    10.3883             21.4869             31.8948
IR Inten    --    92.4956            101.1080             21.8926
IR Inten    --    41.4637             11.3348              8.4137
IR Inten    --    76.3457             89.4031             52.5879
IR Inten    --    32.4551             50.2047             73.9823
IR Inten    --     8.3344             14.3353              1.5149
IR Inten    --     3.2525              2.7927              2.2308
IR Inten    --     0.4981              1.1494              0.5859
IR Inten    --     1.8653              7.9889             10.4978
IR Inten    --    14.8717             28.3097             66.6254
IR Inten    --    23.8425             21.6900             13.1240
```

IR Inten -- 27.1900 8.0386 35.2167
IR Inten -- 44.7047 34.5920 55.1925
IR Inten -- 57.6078 38.3056 23.8440
Zero-point vibrational energy 551410.3 (Joules/Mol)
131.79022 (Kcal/Mol) 5.714 eV

Atom	No	Natural Electron Configuration
Fe	1	[core]4S(0.21)3d(6.55)4p(0.50)4d(0.03)5p(0.01)
Fe	2	[core]4S(0.28)3d(7.05)4p(0.78)4d(0.05)5p(0.01)
Fe	3	[core]4S(0.20)3d(6.53)4p(0.48)4d(0.03)5p(0.01)
Fe	4	[core]4S(0.20)3d(6.51)4p(0.46)4d(0.03)5p(0.01)
Fe	5	[core]4S(0.20)3d(6.50)4p(0.43)4d(0.03)5p(0.01)
Fe	6	[core]4S(0.21)3d(6.54)4p(0.50)4d(0.03)5p(0.01)
Fe	7	[core]4S(0.29)3d(7.08)4p(0.81)4d(0.05)5p(0.01)
Fe	8	[core]4S(0.21)3d(6.54)4p(0.49)4d(0.03)5p(0.01)
H	9	1S(0.89)2S(0.01)
H	10	1S(0.90)2S(0.01)
H	11	1S(0.90)2S(0.01)
H	12	1S(0.89)2S(0.01)
H	13	1S(0.91)2S(0.01)
H	14	1S(0.89)2S(0.01)
O	15	[core]2S(1.71)2p(5.08)3p(0.02)
O	16	[core]2S(1.70)2p(5.20)3S(0.01)3p(0.01)
O	17	[core]2S(1.70)2p(5.19)3S(0.01)3p(0.01)
O	18	[core]2S(1.71)2p(5.08)3p(0.02)
H	19	1S(0.54)
H	20	1S(0.52)
H	21	1S(0.51)
H	22	1S(0.54)
O	23	[core]2S(1.70)2p(5.21)3S(0.01)3p(0.01)
O	24	[core]2S(1.70)2p(5.09)3p(0.02)
O	25	[core]2S(1.71)2p(5.12)3p(0.02)
O	26	[core]2S(1.70)2p(5.20)3S(0.01)3p(0.01)
H	27	1S(0.52)
H	28	1S(0.53)
H	29	1S(0.54)
H	30	1S(0.52)
O	31	[core]2S(1.70)2p(5.18)3S(0.01)3p(0.01)
O	32	[core]2S(1.70)2p(5.13)3p(0.02)
O	33	[core]2S(1.70)2p(5.09)3p(0.02)
O	34	[core]2S(1.70)2p(5.18)3S(0.01)3p(0.01)
H	35	1S(0.52)
H	36	1S(0.52)
H	37	1S(0.52)
H	38	1S(0.52)

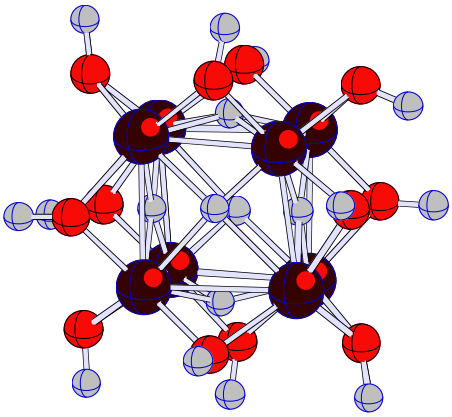
****
******* Alpha spin orbitals *******
****

Atom	No	Natural Electron Configuration
Fe	1	[core]3d(4.85)4p(0.27)4d(0.02)6S(0.12)
Fe	2	[core]3d(4.38)4p(0.42)4d(0.03)6S(0.16)5d(0.01)
Fe	3	[core]3d(4.86)4p(0.26)4d(0.02)6S(0.12)
Fe	4	[core]3d(4.87)4p(0.25)4d(0.02)6S(0.12)
Fe	5	[core]3d(4.87)4p(0.24)4d(0.01)6S(0.12)
Fe	6	[core]3d(4.86)4p(0.27)4d(0.02)6S(0.12)
Fe	7	[core]3d(4.36)4p(0.44)4d(0.03)6S(0.16)5d(0.01)
Fe	8	[core]3d(4.86)4p(0.27)4d(0.02)6S(0.12)
H	9	1S(0.44)2S(0.01)
H	10	1S(0.45)2S(0.01)
H	11	1S(0.45)2S(0.01)
H	12	1S(0.44)2S(0.01)
H	13	1S(0.46)
H	14	1S(0.45)
O	15	[core]2S(0.86)2p(2.64)3p(0.01)
O	16	[core]2S(0.87)2p(2.69)3p(0.01)4S(0.01)4p(0.01)
O	17	[core]2S(0.86)2p(2.69)4S(0.01)4p(0.01)
O	18	[core]2S(0.87)2p(2.63)3p(0.01)
H	19	1S(0.27)
H	20	1S(0.26)
H	21	1S(0.26)
H	22	1S(0.27)
O	23	[core]2S(0.86)2p(2.70)3S(0.01)4p(0.01)
O	24	[core]2S(0.86)2p(2.63)3p(0.01)
O	25	[core]2S(0.86)2p(2.62)3p(0.01)
O	26	[core]2S(0.86)2p(2.70)3S(0.01)4p(0.01)
H	27	1S(0.26)
H	28	1S(0.26)
H	29	1S(0.27)
H	30	1S(0.26)
O	31	[core]2S(0.86)2p(2.69)4S(0.01)4p(0.01)
O	32	[core]2S(0.86)2p(2.63)3p(0.01)
O	33	[core]2S(0.86)2p(2.65)3p(0.01)
O	34	[core]2S(0.87)2p(2.69)4S(0.01)4p(0.01)
H	35	1S(0.26)
H	36	1S(0.27)
H	37	1S(0.26)
H	38	1S(0.26)

****
******* Beta spin orbitals *******
****

Atom	No	Natural Electron Configuration
Fe	1	[core]3d(1.70)4p(0.23)4d(0.01)6S(0.09)
Fe	2	[core]3d(2.67)4p(0.36)4d(0.01)6S(0.12)
Fe	3	[core]3d(1.67)4p(0.22)4d(0.01)6S(0.08)
Fe	4	[core]3d(1.64)4p(0.21)4d(0.01)6S(0.08)
Fe	5	[core]3d(1.62)4p(0.19)4d(0.01)6S(0.08)
Fe	6	[core]3d(1.68)4p(0.23)4d(0.01)6S(0.09)
Fe	7	[core]3d(2.71)4p(0.37)4d(0.01)6S(0.12)
Fe	8	[core]3d(1.68)4p(0.22)4d(0.01)6S(0.09)
H	9	1S(0.45)
H	10	1S(0.45)
H	11	1S(0.45)
H	12	1S(0.45)
H	13	1S(0.45)
H	14	1S(0.45)
O	15	[core]2S(0.84)2p(2.44)3p(0.01)
O	16	[core]2S(0.84)2p(2.51)
O	17	[core]2S(0.84)2p(2.50)
O	18	[core]2S(0.85)2p(2.45)3p(0.01)
H	19	1S(0.27)
H	20	1S(0.26)
H	21	1S(0.25)
H	22	1S(0.27)
O	23	[core]2S(0.83)2p(2.50)
O	24	[core]2S(0.84)2p(2.46)
O	25	[core]2S(0.85)2p(2.50)3p(0.01)
O	26	[core]2S(0.83)2p(2.50)
H	27	1S(0.26)
H	28	1S(0.26)
H	29	1S(0.27)
H	30	1S(0.26)
O	31	[core]2S(0.84)2p(2.49)
O	32	[core]2S(0.84)2p(2.50)
O	33	[core]2S(0.84)2p(2.44)
O	34	[core]2S(0.84)2p(2.49)
H	35	1S(0.26)
H	36	1S(0.26)
H	37	1S(0.26)
H	38	1S(0.26)

HF= -11024.837878 5\S2=182.182501\S2-1=0.\S2A=182.002274



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Fe -2.2798169716,-0.4574800938,0.2016639249
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