Supporting Information

Dipicolylamine based fluorescent probes and their potential for the quantification of Fe^{3+} in aqueous solutions

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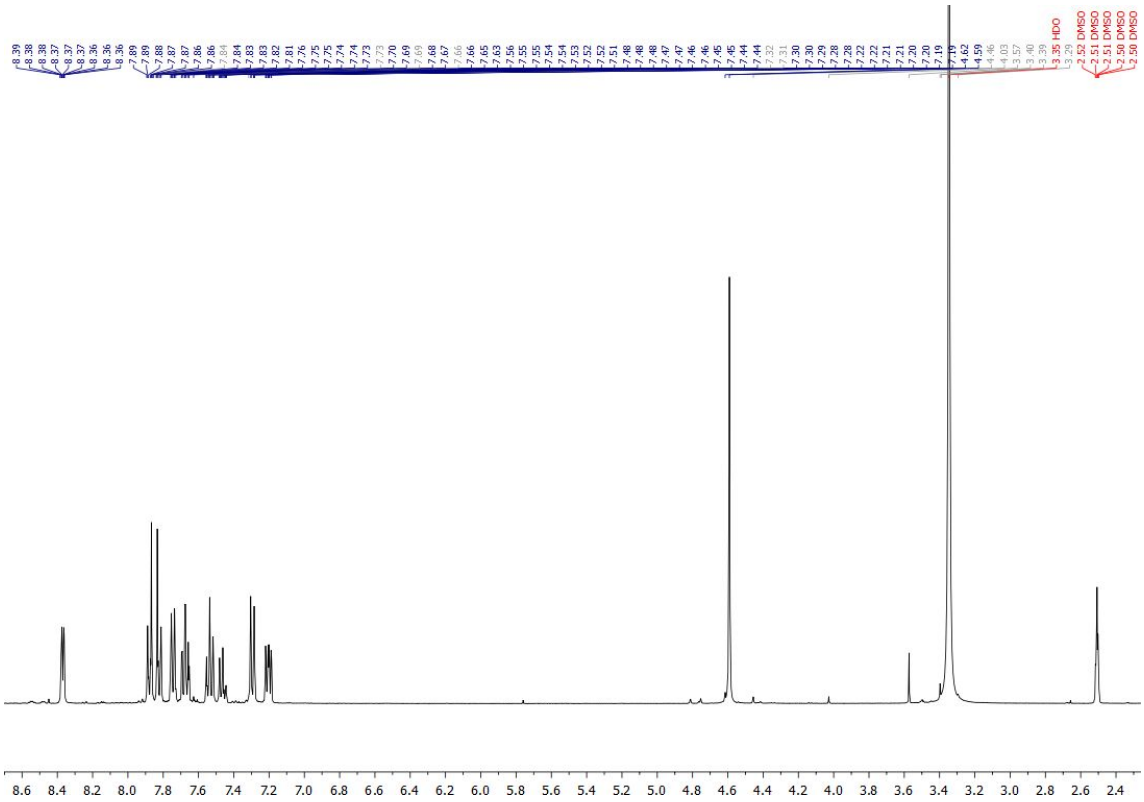
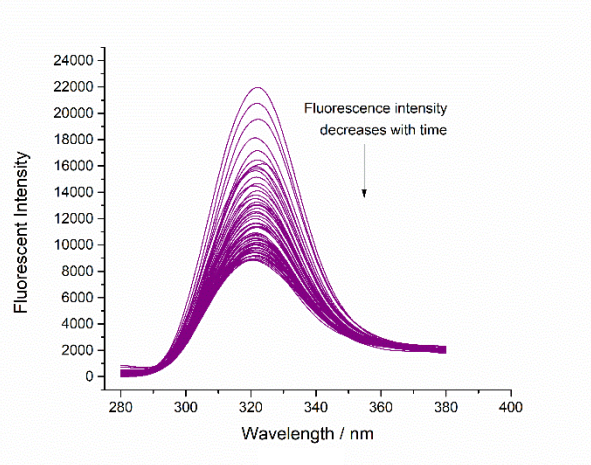


Figure S1: ^{1}H NMR spectrum of L1


Fluorescent Intensity
Wavelength / nm
Fluorescence intensity
decreases with time
24000
22000
20000
18000
16000
14000
12000
10000
8000
6000
4000
2000
0
280
300
320
340
360
380
400

(a)

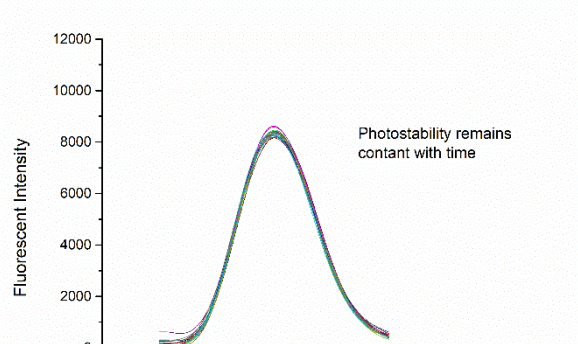
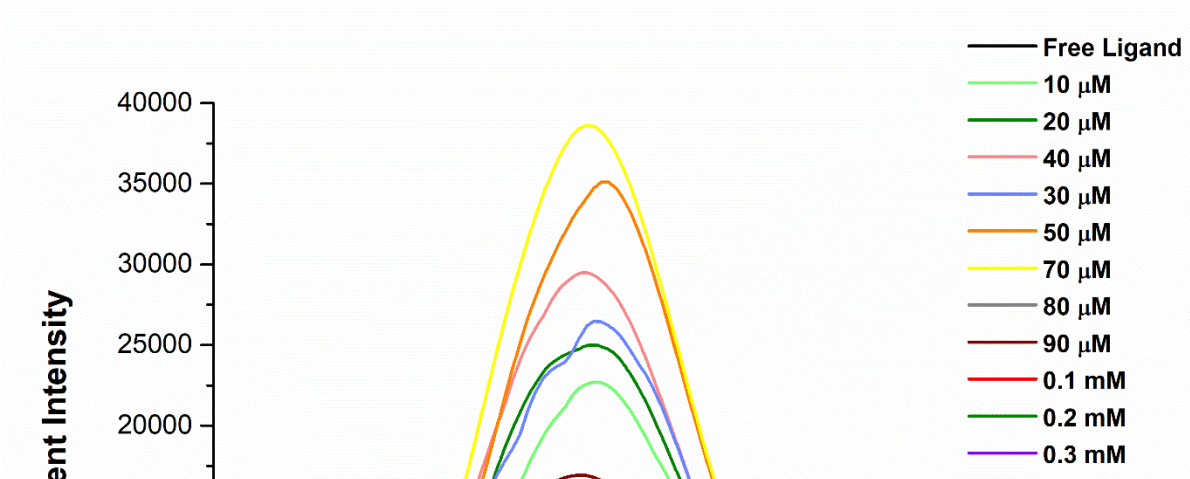
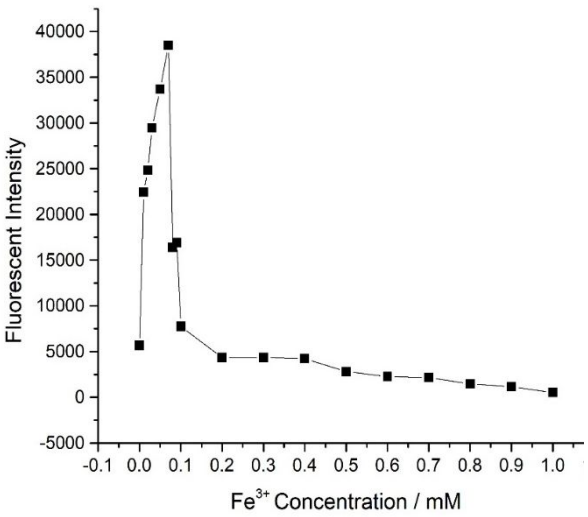
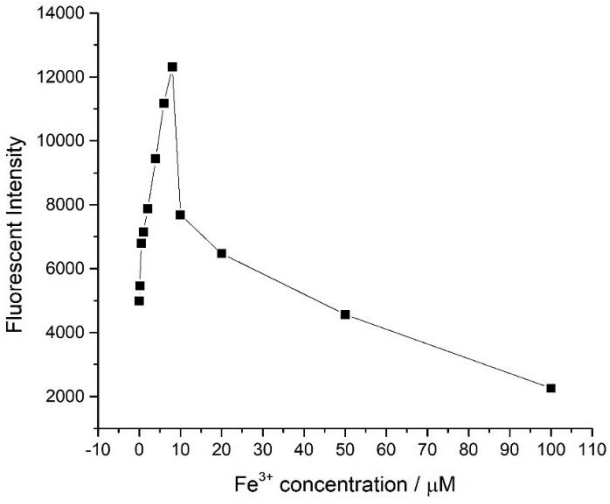

Fluorescent Intensity
Photostability remains
contant with time
12000
10000
8000
6000
4000
2000

Figure S2: Photostability results of (a) L1 ligand and (b) L2 ligand over 2 hours




Fluorescent Intensity
40000
35000
30000
25000
20000
15000
10000
5000
0
-5000
-0.1 0.0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1.0
Fe3+ Concentration / mM

(b)


Fluorescent Intensity
14000
12000
10000
8000
6000
4000
2000
-10 0 10 20 30 40 50 60 70 80 90 100 110
Fe3+ concentration / μM

(c)

Figure S3: Fluorescence intensity change with different Fe^{3+} concentrations; (a) spectral data of 10.00 μM ligand concentration and peak analysis of (b) 10.00 μM (c) 1.00 μM L1 ligand concentrations at pH 7.4

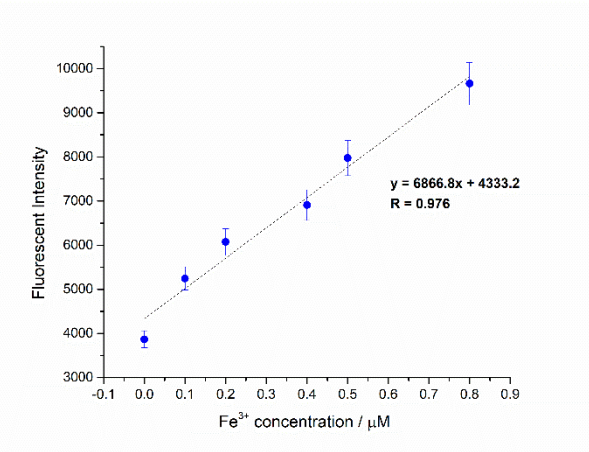
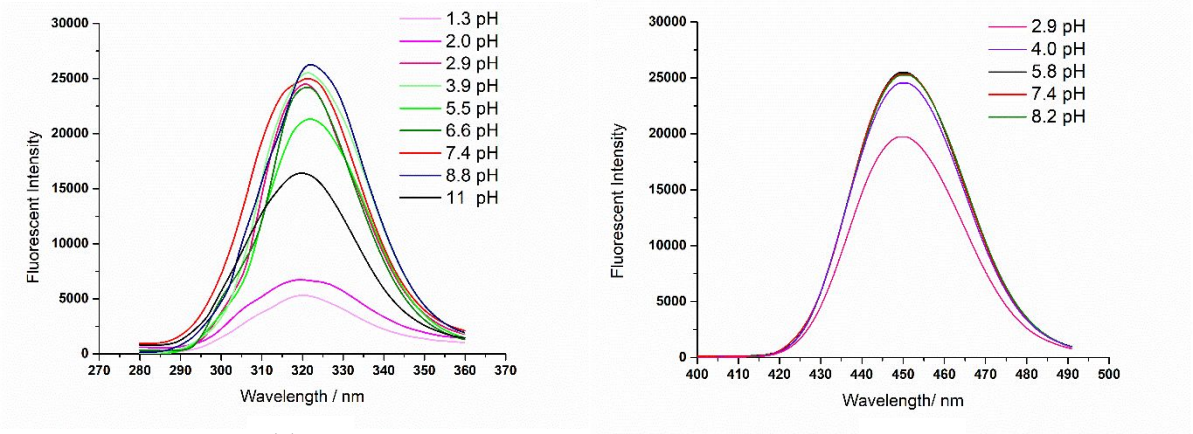
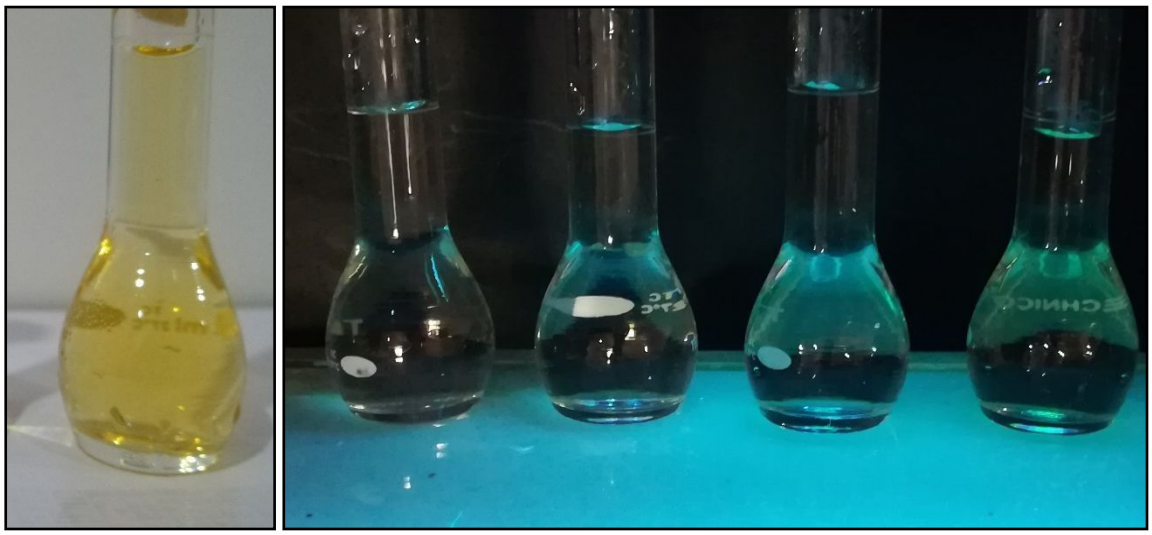


Figure S4: Fluorescence intensity increase with different Fe^{3+} concentrations in L2 ligand (1.00 μM) at pH 7.4



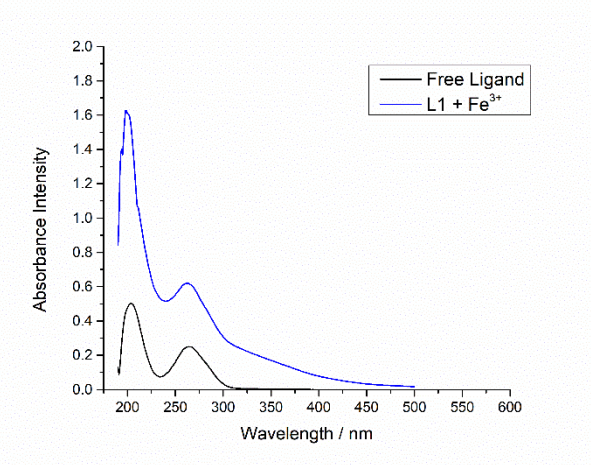
(a) (b)

Figure S5: Fluorescence intensity change of (a) L1-Fe^{3+} and (b) L2-Fe^{3+} system with different pH levels

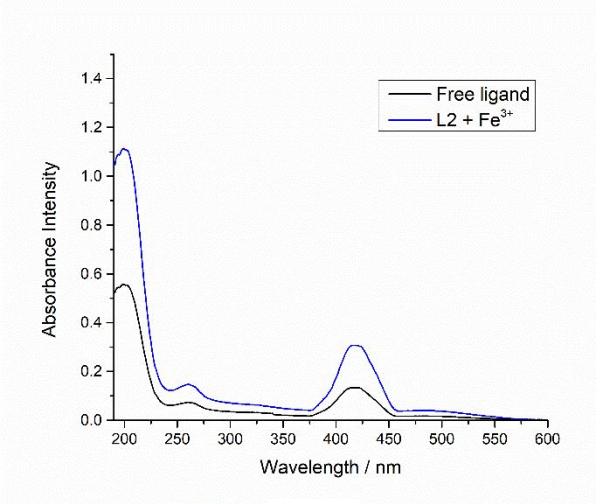


(a) (b)

Figure S6: Colors of the Fe^{3+}-L2 complex under visible light (a) and UV light (b) with ligand concentration of 5.00 μM at 7.4 pH

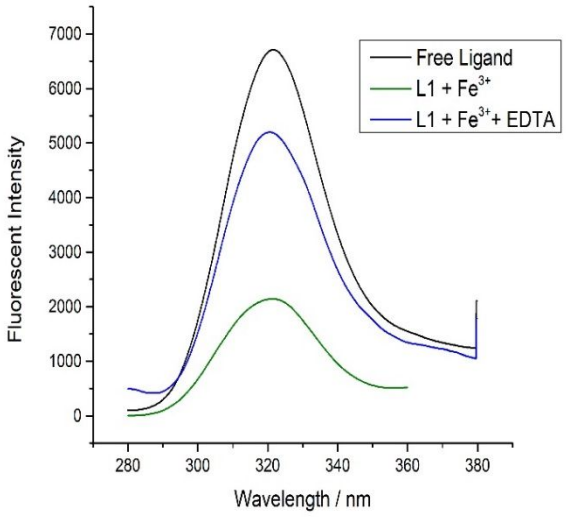

Free Ligand
L1 + Fe3+
Absorbance Intensity
Wavelength / nm
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6
1.8
2.0
200
250
300
350
400
450
500
550
600

(a)

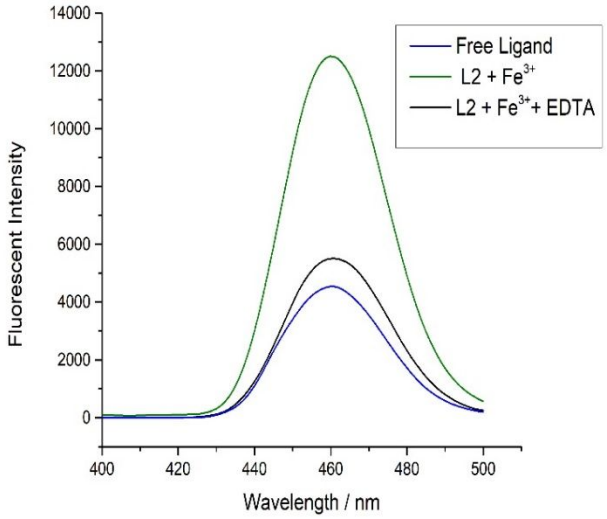

Free ligand
L2 + Fe3+
Absorbance Intensity
Wavelength / nm
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
200
250
300
350
400
450
500
550
600

(b)

Figure S7: UV-Visible absorbance change of (a) L1 ligand (10.00 µM) (b) L2 ligand (0.50 µM) and their respective ligand metal systems in 10 mM HEPES buffer



(a)



(b)

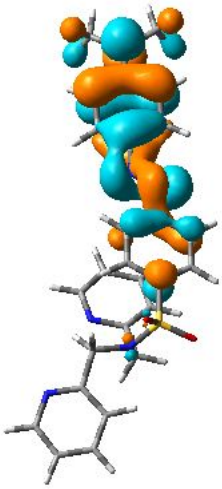
Figure S8: The effect of the addition of EDTA into (a) Fe^{3+}-L1 (b) Fe^{3+}-L2 systems

TDDFT results

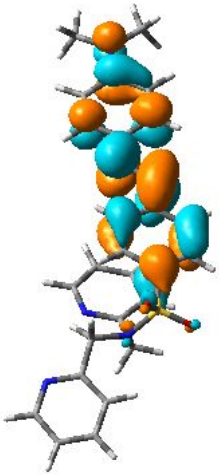
Excitation energies, oscillator strengths, natural transition orbitals the key excitations (HOTO: highest occupied transition orbitals; LUTO: lowest unoccupied natural transition orbitals)

Excited State 1: Singlet 2.6280 eV 471.78 nm f=0.2265 <S**2>=0.000
127 ->129 0.63993
128 ->129 -0.28149

Excited State 2: Singlet 2.7146 eV 456.74 nm f=1.2214 <S**2>=0.000
127 ->129 0.27450
128 ->129 0.64566



HOTO



LUTO

Excited State 3: Singlet 4.0373 eV 307.10 nm f=0.0438 <S**2>=0.000
126 ->129 0.68958

Excited State 4: Singlet 4.2153 eV 294.13 nm f=0.0290 <S**2>=0.000
123 ->129 -0.25969
124 ->129 0.14690
125 ->129 0.58717
128 ->135 -0.12424

Excited State 5: Singlet 4.2329 eV 292.91 nm f=0.0054 <S**2>=0.000

120 ->129 0.10640
123 ->129 0.49525
125 ->129 0.14439
128 ->130 -0.36720
128 ->132 0.12221
128 ->136 -0.18189

Excited State 6: Singlet 4.2563 eV 291.30 nm f=0.0014 <S**2>=0.000
123 ->129 0.32189
125 ->129 0.26426
128 ->130 0.52350
128 ->131 0.13097
128 ->136 -0.10886

Excited State 7: Singlet 4.4132 eV 280.94 nm f=0.0055 <S**2>=0.000
120 ->129 0.42347
121 ->129 0.21269
122 ->129 0.12093
125 ->129 -0.13714
128 ->130 0.20914
128 ->132 0.40675

Excited State 8: Singlet 4.5527 eV 272.33 nm f=0.0459 <S**2>=0.000
120 ->129 -0.23883
121 ->129 0.56393
124 ->129 -0.21304
128 ->131 0.12166
128 ->133 -0.17542
128 ->135 0.14002

Excited State 9: Singlet 4.6154 eV 268.63 nm f=0.1440 <S**2>=0.000
121 ->129 0.24059
123 ->129 0.22076
128 ->131 -0.27319

128 ->132 -0.17553
128 ->133 0.30878
128 ->135 -0.28026
128 ->136 0.30081

Excited State 10: Singlet 4.6583 eV 266.16 nm f=0.0531 <S**2>=0.000
120 ->129 0.12975
124 ->129 0.27128
128 ->130 -0.12110
128 ->131 0.50796
128 ->132 -0.24050
128 ->135 -0.15106
128 ->136 0.13997

Excited State 11: Singlet 4.6752 eV 265.19 nm f=0.0043 <S**2>=0.000
120 ->129 -0.12040
121 ->129 0.17546
124 ->129 0.56666
125 ->129 -0.14199
128 ->131 -0.26019
128 ->135 0.12958

Excited State 12: Singlet 4.7154 eV 262.93 nm f=0.0108 <S**2>=0.000
120 ->129 -0.31541
122 ->129 -0.15328
124 ->129 0.14499
128 ->131 0.19290
128 ->132 0.43538
128 ->133 0.31123

Excited State 13: Singlet 4.7810 eV 259.33 nm f=0.0025 <S**2>=0.000
119 ->129 -0.12228
120 ->129 -0.15886
122 ->129 0.63726

128 ->133 0.15232
128 ->135 0.12153

Excited State 14: Singlet 4.7901 eV 258.83 nm f=0.0018 <S**2>=0.000
120 ->129 0.22013
121 ->129 0.10509
122 ->129 -0.11072
128 ->131 0.10074
128 ->132 -0.14066
128 ->133 0.45583
128 ->135 0.35592
128 ->136 -0.19059

Excited State 15: Singlet 4.8620 eV 255.01 nm f=0.0195 <S**2>=0.000
119 ->130 -0.13479
121 ->130 -0.22021
122 ->130 0.13532
122 ->131 0.10511
124 ->130 0.12896
126 ->130 0.55148
126 ->131 0.14807
126 ->132 0.11476

Excited State 16: Singlet 4.9575 eV 250.09 nm f=0.0252 <S**2>=0.000
127 ->130 0.37837
127 ->131 0.10214
127 ->132 -0.32472
127 ->133 0.13117
128 ->135 0.26806
128 ->136 0.33702

Excited State 17: Singlet 4.9745 eV 249.24 nm f=0.0260 <S**2>=0.000
127 ->130 -0.32549
127 ->132 0.27874

127 ->133 -0.11804
128 ->134 -0.10903
128 ->135 0.28975
128 ->136 0.37066

Excited State 18: Singlet 5.0534 eV 245.35 nm f=0.0031 <S**2>=0.000
117 ->129 0.11802
119 ->129 0.65438

Excited State 19: Singlet 5.0713 eV 244.48 nm f=0.0048 <S**2>=0.000
119 ->129 -0.13114
122 ->130 -0.24207
122 ->131 0.36558
124 ->130 0.12150
124 ->131 -0.24042
126 ->131 -0.27416
128 ->134 -0.31348

Excited State 20: Singlet 5.0748 eV 244.31 nm f=0.0013 <S**2>=0.000
122 ->130 -0.12760
122 ->131 0.20768
124 ->131 -0.13206
126 ->131 -0.14645
128 ->134 0.59972

$[Fe(L2)(H_2O)_3]^{3+}$

S=3/2

Excited State 1: 4.505 0.3623 eV 3421.86 nm f=0.0000 <S**2>=4.824
148B ->150B -0.17874
148B ->151B 0.80075
148B ->153B 0.36555
148B ->154B 0.50727
148B <-151B 0.25655
148B <-153B 0.11602

148B <-154B 0.16973

Excited State 2: 4.509 0.6323 eV 1960.92 nm f=0.0000 <S**2>=4.832
148B ->150B 0.64276
148B ->154B 0.16545
148B ->156B -0.10016
148B ->157B 0.66664
148B ->159B 0.10493
148B ->162B -0.26559
148B ->163B 0.15425
148B <-162B -0.10512

Excited State 3: 4.696 1.1266 eV 1100.56 nm f=0.0003 <S**2>=5.264
151A ->152A 0.90007
151A ->153A 0.32736
151A ->157A -0.10474
146B ->149B -0.22138

Excited State 4: 4.505-?Sym 1.5265 eV 812.20 nm f=0.0000 <S**2>=4.824
148B ->150B -0.10156
148B ->153B 0.13781
148B ->157B -0.25976
148B ->161B 0.19467
148B ->162B -0.67674
148B ->163B 0.61816
148B ->166B -0.10192
148B <-162B -0.13414
148B <-163B 0.11509

Excited State 5: 4.504 1.8098 eV 685.07 nm f=0.0001 <S**2>=4.822
148B ->152B 0.23650
148B ->160B 0.94384
148B ->165B -0.17656

Excited State 6: 4.584 2.0565 eV 602.90 nm f=0.2007 <S**2>=5.003
140A ->152A 0.14737
144A ->152A 0.27257
146A ->152A 0.17706
147A ->152A -0.10756
148A ->152A 0.78117
148A ->153A 0.15277
147B ->149B -0.42812

Excited State 7: 5.051 2.0955 eV 591.67 nm f=0.0018 <S**2>=6.129
145A ->152A 0.18776
151A ->152A 0.35359
151A ->153A -0.32305
146B ->149B 0.81573
146B ->161B -0.17884

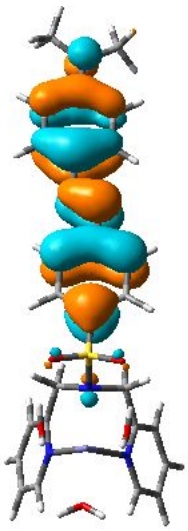
Excited State 8: 4.532 2.1268 eV 582.97 nm f=0.0051 <S**2>=4.886
145A ->152A 0.96198
145A ->153A -0.12015
146B ->149B -0.16574

Excited State 9: 4.488 2.6301 eV 471.41 nm f=0.0107 <S**2>=4.785
146A ->152A -0.44388
147A ->152A -0.59702
147A ->153A -0.14587
150A ->152A 0.61932
143B ->149B -0.11731

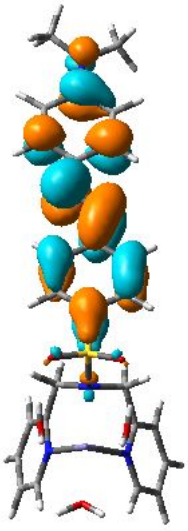
Excited State 10: 4.376 2.6703 eV 464.30 nm f=0.0114 <S**2>=4.537
146A ->152A 0.35232
147A ->152A 0.47218
147A ->153A 0.11214
150A ->152A 0.78296

Excited State 11: 4.510 2.6943 eV 460.18 nm f=0.0003 <S**2>=4.836
149A ->152A 0.99560

Excited State 12: 4.718 2.7351 eV 453.30 nm f=1.0882 <S**2>=5.316
140A ->152A 0.10599
144A ->153A -0.11277
148A ->152A 0.46661
148A ->153A -0.21458
142B ->149B -0.23159
147B ->149B 0.75438



HOTO



LUTO

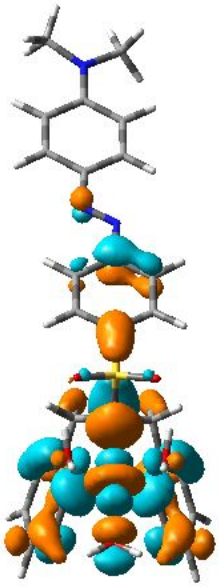
Excited State 13: 4.573 2.8678 eV 432.33 nm f=0.0066 <S**2>=4.978
151A ->152A -0.21983
151A ->153A 0.84525
151A ->163A 0.10258
146B ->149B 0.44576

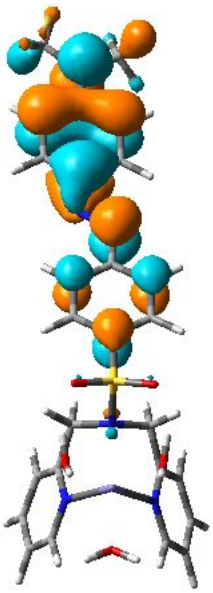
Excited State 14: 4.531 3.0148 eV 411.25 nm f=0.0098 <S**2>=4.882
140A ->152A 0.46736
144A ->152A 0.43543
146A ->152A 0.38209
147A ->152A -0.37035
148A ->152A -0.34938
148A ->153A -0.24688
142B ->149B -0.23502
147B ->149B -0.10043
147B ->153B 0.10821

Excited State 15: 4.584 3.1322 eV 395.83 nm f=0.0599 <S**2>=5.004
140A ->152A -0.35685
144A ->152A -0.23552
146A ->152A 0.67194
147A ->152A -0.44559
148A ->153A 0.19482
142B ->149B 0.19048
147B ->149B 0.19383

Excited State 16: 4.915 3.2680 eV 379.39 nm f=0.0000 <S**2>=5.789
148B ->149B 0.99115

Excited State 17: 4.476 3.2802 eV 377.97 nm f=0.1247 <S**2>=4.758
140A ->152A -0.27836
144A ->152A 0.79330
144A ->153A 0.12052
146A ->152A -0.11888
148A ->152A -0.14371
148A ->153A 0.23669
142B ->149B 0.21281
143B ->155B -0.10496
147B ->149B 0.27065





HOTO			LUTO
Excited State 18:	4.762	3.6481 eV 339.86 nm	f=0.1369 <S**2>=5.418
140A ->152A	0.64668		
144A ->152A	-0.17197		
145A ->159A	0.10195		
147A ->153A	-0.13960		
148A ->153A	0.43875		
141B ->156B	-0.10124		
142B ->149B	0.23854		
143B ->149B	-0.21010		
143B ->155B	-0.13791		
147B ->149B	0.26723		
Excited State 19:	4.513	3.6524 eV 339.46 nm	f=0.0009 <S**2>=4.842
143A ->152A	0.99506		
Excited State 20:	5.304	3.6925 eV 335.77 nm	f=0.0000 <S**2>=6.782
142A ->155A	0.23619		
143A ->154A	0.31014		
146A ->160A	-0.22627		
147A ->160A	0.16476		
149A ->154A	-0.19905		
149A ->156A	0.37224		
149A ->157A	-0.15288		
150A ->154A	0.14165		
139B ->152B	-0.22022		
140B ->150B	0.31842		
140B ->157B	-0.13292		
144B ->158B	0.29631		
145B ->150B	0.20352		
145B ->151B	0.24458		
145B ->153B	0.12273		
145B ->154B	-0.33292		

Cartesian coordinates of the optimized structures

L2

S 2.73270000 2.45660000 10.56230000

O 2.42720000 1.03170000 10.44830000

O 2.71670000 3.09940000 11.87590000

N 2.43240000 4.66150000 7.04480000

N 1.63940000 3.27190000 9.63050000

N -0.73620000 5.99610000 9.91310000

N 7.88730000 3.20870000 7.70840000
N 8.10680000 4.36520000 7.24590000
N 12.71950000 5.27990000 4.25570000
C 3.36890000 5.16560000 6.23960000
H 3.33420000 6.24210000 6.08200000
C 4.34820000 4.39660000 5.61760000
H 5.09250000 4.86470000 4.98160000
C 4.34190000 3.02390000 5.83720000
H 5.08730000 2.38330000 5.37520000
C 3.37070000 2.48580000 6.67360000
H 3.34230000 1.42110000 6.88310000
C 2.44550000 3.34100000 7.27120000
C 1.42360000 2.81710000 8.25320000
H 0.42190000 3.15960000 7.97280000
H 1.40950000 1.72500000 8.25350000
C 1.24350000 4.63170000 9.96720000
H 1.59260000 5.32930000 9.19960000
H 1.71500000 4.89940000 10.91700000
C -0.25540000 4.76360000 10.10980000
C -1.06310000 3.67950000 10.45210000
H -0.61910000 2.69930000 10.59370000
C -2.43000000 3.88720000 10.59800000
H -3.08650000 3.06260000 10.86130000
C -2.93970000 5.16660000 10.40200000
H -3.99960000 5.37640000 10.50300000
C -2.04940000 6.18150000 10.06440000
H -2.41050000 7.19540000 9.90000000
C 4.31680000 2.70890000 9.80940000
C 5.08960000 1.60870000 9.45270000
H 4.73950000 0.60710000 9.67700000
C 6.28700000 1.81840000 8.78170000
H 6.91000000 0.98300000 8.47740000
C 6.69390000 3.11300000 8.44520000
C 5.91710000 4.21440000 8.84220000

H 6.25140000 5.21300000 8.58550000
C 4.73400000 4.01360000 9.52620000
H 4.12410000 4.86370000 9.81690000
C 9.27540000 4.51280000 6.51590000
C 10.22090000 3.49650000 6.27700000
H 10.04230000 2.50870000 6.68900000
C 11.35190000 3.74610000 5.53580000
H 12.05970000 2.94210000 5.37190000
C 11.60170000 5.03560000 4.98760000
C 10.64470000 6.05270000 5.23210000
H 10.79200000 7.04940000 4.83460000
C 9.51570000 5.78670000 5.97800000
H 8.78410000 6.56820000 6.16360000
C 13.68320000 4.22550000 4.01690000
H 14.10480000 3.84490000 4.95550000
H 14.50060000 4.62020000 3.41410000
H 13.23410000 3.38490000 3.47330000
C 12.95380000 6.59970000 3.70840000
H 12.15480000 6.89580000 3.01710000
H 13.89450000 6.59670000 3.15870000
H 13.02310000 7.35640000 4.50000000

$[Fe(L2)(H_2O)_3]^{3+}$

S=1/2

S 3.06640000 2.37450000 11.14410000
O 2.98710000 0.93200000 11.37360000
O 3.04040000 3.30950000 12.26910000
N -0.79400000 1.47290000 9.86390000
N 1.66750000 2.74950000 10.22930000
N -0.73820000 4.06460000 10.77460000
N 7.68210000 3.49890000 7.63620000
N 8.18720000 4.65770000 7.68370000
N 12.52840000 5.69480000 4.41840000

C -2.06550000 1.08670000 9.67780000
H -2.69810000 1.08020000 10.55800000
C -2.55950000 0.73500000 8.43190000
H -3.59380000 0.42760000 8.33040000
C -1.70670000 0.80260000 7.33580000
H -2.06030000 0.54800000 6.34200000
C -0.39150000 1.20930000 7.52840000
H 0.30180000 1.27560000 6.69680000
C 0.03530000 1.53210000 8.80970000
C 1.48140000 1.86370000 9.06380000
H 1.99700000 0.91980000 9.26720000
H 1.93350000 2.30620000 8.17010000
C 1.54600000 4.18790000 9.92330000
H 2.02070000 4.41780000 8.96370000
H 2.07500000 4.74710000 10.70150000
C 0.11690000 4.65870000 9.92670000
C -0.26860000 5.73270000 9.13590000
H 0.44490000 6.18360000 8.45480000
C -1.56980000 6.21240000 9.23480000
H -1.89150000 7.04970000 8.62430000
C -2.44950000 5.59830000 10.11890000
H -3.47450000 5.93370000 10.22630000
C -1.99630000 4.52170000 10.86480000
H -2.65210000 3.99010000 11.54500000
C 4.46750000 2.72550000 10.13910000
C 4.96820000 1.72030000 9.31150000
H 4.54680000 0.72140000 9.32770000
C 6.04180000 2.02550000 8.48840000
H 6.47170000 1.27760000 7.83100000
C 6.59740000 3.31100000 8.50370000
C 6.08330000 4.30590000 9.35200000
H 6.53830000 5.28940000 9.35740000
C 5.01220000 4.01470000 10.17590000
H 4.61770000 4.76270000 10.85490000

C 9.26120000 4.84340000 6.82530000
C 9.75700000 3.86140000 5.93100000
H 9.28360000 2.88720000 5.90510000
C 10.82410000 4.14180000 5.12610000
H 11.20950000 3.37080000 4.47160000
C 11.46480000 5.42320000 5.18980000
C 10.95420000 6.40650000 6.09490000
H 11.39040000 7.39610000 6.13610000
C 9.87240000 6.11410000 6.88250000
H 9.46300000 6.85350000 7.56220000
C 12.96390000 4.80850000 3.34760000
H 13.66340000 4.06490000 3.74560000
H 13.47600000 5.40960000 2.59620000
H 12.11450000 4.31300000 2.88170000
C 13.33400000 6.89520000 4.60220000
H 12.89730000 7.72500000 4.03560000
H 14.33470000 6.69440000 4.21990000
H 13.40580000 7.15650000 5.65670000
Fe -0.23610000 2.29870000 11.61550000
O 0.46950000 3.26110000 13.28190000
H 0.38750000 2.80380000 14.13380000
O 0.40790000 0.47330000 12.29350000
H 0.37390000 0.29680000 13.24720000
H 1.34320000 0.33610000 12.03030000
H 1.42620000 3.44970000 13.16910000
O -2.11670000 1.96680000 12.73440000
H -2.27560000 2.51410000 13.51910000
H -2.32930000 1.06090000 13.00800000

S=3/2

S 3.10480000 2.32980000 11.31970000
O 3.04120000 0.88840000 11.55630000
O 3.07890000 3.26750000 12.44100000

N -0.78450000 1.47510000 9.79090000
N 1.69230000 2.69420000 10.39900000
N -0.72510000 4.11550000 10.76930000
N 7.66020000 3.47080000 7.74070000
N 8.14800000 4.63750000 7.76020000
N 12.36440000 5.69550000 4.34170000
C -2.05400000 1.19290000 9.47030000
H -2.75630000 1.13700000 10.29520000
C -2.46640000 1.00010000 8.16000000
H -3.50390000 0.76910000 7.94770000
C -1.52620000 1.13000000 7.14390000
H -1.81310000 1.00400000 6.10490000
C -0.20970000 1.43460000 7.47440000
H 0.54870000 1.54960000 6.70750000
C 0.12560000 1.59060000 8.81280000
C 1.55930000 1.81050000 9.21750000
H 1.97950000 0.83490000 9.48070000
H 2.13190000 2.21230000 8.37510000
C 1.60830000 4.13580000 10.06860000
H 2.17230000 4.34960000 9.15470000
H 2.06590000 4.69460000 10.89070000
C 0.19000000 4.62190000 9.92970000
C -0.12250000 5.61930000 9.01540000
H 0.63930000 5.99560000 8.34100000
C -1.42020000 6.11950000 8.98560000
H -1.68920000 6.89850000 8.27960000
C -2.36510000 5.60150000 9.86430000
H -3.38870000 5.95790000 9.87250000
C -1.97670000 4.59140000 10.73190000
H -2.68580000 4.13200000 11.41230000
C 4.49140000 2.68770000 10.29700000
C 4.99410000 1.67860000 9.47540000
H 4.58260000 0.67600000 9.50560000
C 6.05460000 1.98700000 8.63660000

H 6.48420000 1.23750000 7.98100000
C 6.59430000 3.27920000 8.63040000
C 6.08120000 4.27680000 9.47590000
H 6.52450000 5.26550000 9.46470000
C 5.02340000 3.98240000 10.31620000
H 4.62810000 4.73360000 10.99130000
C 9.19520000 4.82760000 6.86970000
C 9.67050000 3.84470000 5.96540000
H 9.20600000 2.86580000 5.96100000
C 10.70660000 4.13100000 5.12300000
H 11.07800000 3.36080000 4.45940000
C 11.33490000 5.41960000 5.15660000
C 10.84740000 6.40280000 6.07420000
H 11.27440000 7.39680000 6.09560000
C 9.79560000 6.10420000 6.89960000
H 9.40160000 6.84370000 7.58810000
C 12.75800000 4.80300000 3.25930000
H 13.43940000 4.03510000 3.64190000
H 13.27730000 5.39240000 2.50400000
H 11.88530000 4.33770000 2.80400000
C 13.16630000 6.90350000 4.48170000
H 12.71630000 7.71540000 3.89970000
H 14.16210000 6.69700000 4.08950000
H 13.25340000 7.19360000 5.52710000
Fe -0.23660000 2.24050000 11.73730000
O 0.52380000 3.19040000 13.48350000
H 0.36590000 2.78540000 14.35090000
O 0.46970000 0.33870000 12.39580000
H 0.32080000 0.07480000 13.31740000
H 1.43340000 0.25480000 12.23950000
H 1.49110000 3.32900000 13.41430000
O -2.13410000 1.94580000 12.65490000
H -2.39200000 2.50930000 13.40120000
H -2.42520000 1.04950000 12.88550000

S=5/2

S 3.10290000 2.32380000 11.29920000
O 3.03900000 0.88200000 11.53350000
O 3.08080000 3.26000000 12.42190000
N -0.79420000 1.46620000 9.80300000
N 1.68700000 2.69010000 10.38460000
N -0.72590000 4.11490000 10.76610000
N 7.66200000 3.47070000 7.72500000
N 8.15110000 4.63650000 7.75000000
N 12.38310000 5.70220000 4.35260000
C -2.06600000 1.17980000 9.49510000
H -2.75990000 1.12220000 10.32700000
C -2.49100000 0.98500000 8.18920000
H -3.52990000 0.75030000 7.98760000
C -1.56170000 1.11780000 7.16350000
H -1.85890000 0.99080000 6.12760000
C -0.24290000 1.42620000 7.48090000
H 0.50730000 1.54370000 6.70610000
C 0.10580000 1.58310000 8.81570000
C 1.54330000 1.80520000 9.20560000
H 1.96720000 0.83020000 9.46520000
H 2.10700000 2.20670000 8.35690000
C 1.60360000 4.13110000 10.05310000
H 2.16270000 4.34290000 9.13570000
H 2.06690000 4.69020000 10.87180000
C 0.18530000 4.61940000 9.92130000
C -0.13060000 5.61630000 9.00770000
H 0.62810000 5.99140000 8.32890000
C -1.42770000 6.11840000 8.98440000
H -1.69940000 6.89730000 8.27920000
C -2.36870000 5.60240000 9.86840000
H -3.39170000 5.96040000 9.88190000

C -1.97700000 4.59260000 10.73490000
H -2.68320000 4.13510000 11.41960000
C 4.48790000 2.68340000 10.27440000
C 4.99090000 1.67610000 9.45090000
H 4.57920000 0.67340000 9.47860000
C 6.05280000 1.98590000 8.61420000
H 6.48300000 1.23750000 7.95750000
C 6.59360000 3.27750000 8.61210000
C 6.08000000 4.27340000 9.45930000
H 6.52440000 5.26160000 9.45150000
C 5.02090000 3.97760000 10.29740000
H 4.62570000 4.72710000 10.97460000
C 9.20210000 4.82850000 6.86390000
C 9.68060000 3.84810000 5.95870000
H 9.21560000 2.86950000 5.94950000
C 10.72050000 4.13650000 5.12150000
H 11.09430000 3.36820000 4.45700000
C 11.34950000 5.42450000 5.16210000
C 10.85860000 6.40510000 6.08060000
H 11.28610000 7.39890000 6.10670000
C 9.80300000 6.10460000 6.90040000
H 9.40660000 6.84220000 7.58960000
C 12.77970000 4.81330000 3.26830000
H 13.45660000 4.04150000 3.65100000
H 13.30470000 5.40420000 2.51820000
H 11.90790000 4.35270000 2.80640000
C 13.18680000 6.90800000 4.50150000
H 12.74200000 7.72310000 3.92000000
H 14.18440000 6.70080000 4.11410000
H 13.26870000 7.19410000 5.54850000
Fe -0.23430000 2.24420000 11.74070000
O 0.53350000 3.20160000 13.47930000
H 0.37190000 2.80760000 14.35100000
O 0.47720000 0.34910000 12.41470000

H 0.34800000 0.10100000 13.34350000

H 1.43660000 0.25660000 12.23800000

H 1.50170000 3.33250000 13.40790000

O -2.12410000 1.95300000 12.67530000

H -2.38910000 2.52780000 13.41030000

H -2.41500000 1.05950000 12.91660000

$[Fe(L2)]^{3+}$

S=3/2

S 3.42787200 3.50062200 10.99780200
O 3.85243000 2.35218900 11.78648600
O 3.21170700 4.80495000 11.60694200
N -0.42332400 1.74904500 10.13066800
N 1.91653800 3.06748800 10.31960200
N -0.10022500 4.67767600 11.44517900
N 6.92573500 4.02004500 6.25383800
N 6.99737400 5.15566200 5.69997000
N 9.99413200 5.55899900 1.06998000
C -1.69513000 1.42501400 9.84711800
H -2.45041700 1.84228900 10.50505900
C -2.04047600 0.61393000 8.77686400
H -3.08255100 0.37683200 8.59464400
C -1.02817000 0.13021400 7.95498700
H -1.25740800 -0.51019400 7.10937100
C 0.28378900 0.51011100 8.21178700
H 1.09639900 0.19292500 7.56655800
C 0.54738300 1.32389800 9.30692200
C 1.95074800 1.79710900 9.57732700
H 2.49196800 1.06042600 10.17634900
H 2.48171600 1.90731800 8.62342900
C 1.31790600 4.16761800 9.53690100
H 0.60873800 3.70887800 8.84157500
H 2.06493100 4.67338200 8.91541500
C 0.57625500 5.15409600 10.38893400
C 0.55120700 6.49893700 10.04100200
H 1.12547800 6.84481900 9.18795900
C -0.20702600 7.37965100 10.80241100
H -0.23841100 8.43514800 10.55144000
C -0.91485300 6.88518100 11.89218400
H -1.51918200 7.53161900 12.51846300
C -0.83023400 5.53178900 12.18070000
H -1.36144100 5.10633400 13.02532800
C 4.52563500 3.69640100 9.62474200
C 5.18843200 2.57642700 9.12286200

H 5.09201400 1.61102700 9.60768100
C 5.98898600 2.73180200 8.00074900
H 6.52270900 1.89004400 7.57282700
C 6.11703400 3.98950500 7.39695700
C 5.46371900 5.11183100 7.93274400
H 5.59314200 6.07881200 7.46099000
C 4.66582200 4.96656600 9.05312100
H 4.16891200 5.82317300 9.49641900
C 7.78221500 5.17937000 4.55658200
C 8.46753000 4.05728700 4.02569800
H 8.38557100 3.10371200 4.53358800
C 9.20745700 4.18152800 2.88464900
H 9.70251900 3.30978000 2.47658600
C 9.28522100 5.44060800 2.20286400
C 8.59145700 6.56603200 2.74893800
H 8.66001700 7.53714100 2.27637000
C 7.86675600 6.42740700 3.90277700
H 7.34561500 7.27340500 4.33738300
C 10.85755800 4.49014400 0.58396200
H 11.36624300 3.99816200 1.41184300
H 11.60430200 4.92710200 -0.07779100
H 10.26510100 3.76060900 0.02085300
C 9.94522000 6.76305900 0.25003500
H 8.93822900 7.17760700 0.23196100
H 10.23430200 6.49743200 -0.76614300
H 10.65079000 7.50597500 0.63831800
Fe 0.16610100 2.60506400 12.10027600
S -3.02274200 2.57952700 13.59923700
O -3.49596400 2.54384300 12.22035900
O -2.65670100 3.83704600 14.23876100
N 0.62766700 0.48990800 12.59497900
N -1.56645500 1.65512700 13.59788900
N 0.61244500 3.34310700 14.11039700
N -6.63423300 -0.57018800 17.07851600
N -6.64271000 -0.27720100 18.31231900
N -9.74108600 -3.27742000 21.82478700
C 1.85511600 -0.03726000 12.46383300
H 2.66730700 0.67337100 12.35041900
C 2.08815000 -1.40385700 12.48157100
H 3.09824400 -1.78041700 12.36671100
C 1.00684400 -2.26066500 12.65876700
H 1.14814900 -3.33648900 12.67691600
C -0.25754900 -1.71619800 12.84951900
H -1.11868200 -2.34835600 13.03901900
C -0.40826600 -0.33534200 12.81390300
C -1.75134200 0.29269500 13.07193200
H -2.32905800 0.35416800 12.14602800
H -2.31525000 -0.33359200 13.77472500
C -0.92435600 1.65246600 14.92912700
H -0.28757900 0.76388000 14.97313100

H -1.66297000 1.53487000 15.72974400
C -0.06661500 2.85990800 15.16147600
C 0.05777900 3.40425200 16.43382500
H -0.52027300 2.99367900 17.25506100
C 0.91935800 4.47701000 16.62678000
H 1.02953600 4.92150600 17.61084000
C 1.62785800 4.97430900 15.53817900
H 2.30930900 5.81156700 15.63806800
C 1.44159000 4.38234800 14.29865500
H 1.96627800 4.74254100 13.42022300
C -4.14433800 1.71517400 14.63434700
C -4.90903900 0.67582400 14.09810300
H -4.87205000 0.45251900 13.03688900
C -5.72958700 -0.05027700 14.94590900
H -6.33824900 -0.86485600 14.56704300
C -5.79076300 0.24959800 16.31456900
C -5.03320500 1.31667100 16.82805300
H -5.10562100 1.55138600 17.88366800
C -4.20996300 2.04955900 15.99317300
H -3.63433500 2.88649500 16.37614300
C -7.44188100 -1.06153200 19.11624000
C -8.22719100 -2.14818200 18.67575300
H -8.22304900 -2.40278800 17.62109200
C -8.98269400 -2.87527700 19.56256500
H -9.57384200 -3.70445300 19.19248800
C -8.99762000 -2.55542700 20.95143700
C -8.20797400 -1.45881900 21.38657600
H -8.18938700 -1.17907100 22.43273800
C -7.45463900 -0.74007800 20.48525800
H -6.84887400 0.09717800 20.82017200
C -10.53380800 -4.39900400 21.36176500
H -11.29016100 -4.08254200 20.63320300
H -11.04790300 -4.84584200 22.21206900
H -9.90591900 -5.17001600 20.89872000
C -9.74324200 -2.93666600 23.23310800
H -8.73850800 -3.01668900 23.66627900
H -10.39935400 -3.62440500 23.76557600
H -10.11143900 -1.91652700 23.39698900

S=5/2

S 3.42818400 3.48517900 10.89543400
O 3.87736300 2.35084700 11.69481400
O 3.20655800 4.79295300 11.49954300
N -0.42523400 1.66356600 10.18251400
N 1.87991100 3.02118700 10.29246700
N -0.09335000 4.60823300 11.48781900
N 6.87580800 3.97239700 6.10330700
N 6.90643700 5.10193200 5.52763500

N 10.05790800 5.78019100 0.99442300
C -1.70122800 1.31672400 9.95069400
H -2.43653600 1.72351000 10.63650300
C -2.07522900 0.49765200 8.89651400
H -3.11960400 0.24262900 8.75668300
C -1.08878100 0.03007900 8.03456900
H -1.34097800 -0.61584100 7.19976200
C 0.22536400 0.43395200 8.23700400
H 1.01669200 0.13129200 7.55923200
C 0.51833600 1.25504800 9.31906100
C 1.91924700 1.76020900 9.53401900
H 2.50414800 1.03210500 10.10192700
H 2.40946000 1.89488400 8.56169500
C 1.24674300 4.11338700 9.52442500
H 0.51930700 3.64894000 8.85187600
H 1.97212200 4.62273200 8.88035700
C 0.52426400 5.09305100 10.40019200
C 0.45501900 6.43549100 10.04875000
H 0.98253400 6.78994700 9.16940600
C -0.28643300 7.30237200 10.84189300
H -0.35202600 8.35599500 10.58955600
C -0.93287300 6.79817500 11.96542800
H -1.52070600 7.43531200 12.61648200
C -0.80652500 5.44827300 12.25442800
H -1.28608000 5.01389200 13.12475400
C 4.47174000 3.66684800 9.49733800
C 5.14733100 2.54932600 9.00031700
H 5.07167200 1.59005100 9.50149000
C 5.93607800 2.69821000 7.87147000
H 6.48144500 1.85542200 7.45951200
C 6.05197200 3.94386100 7.23771700
C 5.37682600 5.05890900 7.76433100
H 5.49144200 6.02001200 7.27660500
C 4.58825000 4.92498300 8.89229200
H 4.08448400 5.78505400 9.32225700
C 7.70958400 5.19038400 4.41065900
C 8.49319800 4.14158000 3.88389700
H 8.47776700 3.17724700 4.38077200
C 9.26413100 4.33331700 2.76377000
H 9.85508700 3.50775100 2.38536700
C 9.29551000 5.59383900 2.09932100
C 8.50345000 6.64368300 2.63401000
H 8.49679500 7.61854300 2.16218700
C 7.73692400 6.43636100 3.75920000
H 7.13296000 7.24145000 4.16806800
C 10.86926200 4.69881600 0.47188500
H 11.60508700 4.35698200 1.20994400
H 11.40877800 5.05170700 -0.40636700
H 10.25273300 3.84237700 0.17271100
C 10.07403800 7.06799000 0.33050800

H 9.07326400 7.34977000 -0.01912400
H 10.73379600 7.01503400 -0.53490200
H 10.44427200 7.85767200 0.99605900
Fe 0.27159900 2.54019500 12.09886300
S -2.87338800 2.46879300 13.75195200
O -3.39443700 2.44198000 12.39167100
O -2.50434800 3.71940700 14.39938500
N 0.73975200 0.42477000 12.59727300
N -1.43707700 1.54208600 13.71575300
N 0.74524300 3.27471100 14.11266700
N -6.55192900 -0.56981200 17.25317500
N -6.57977800 -0.26884800 18.48182200
N -10.05691800 -3.09525500 21.72353900
C 1.96815600 -0.08574600 12.41625900
H 2.76367100 0.63610600 12.26353800
C 2.22374100 -1.44853300 12.43215300
H 3.23394400 -1.80927500 12.27517500
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C 0.12070300 2.78120800 15.19314400
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C 1.78751300 4.92851200 15.49818100
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H -6.86419300 0.05173900 20.98861300
C -11.09394100 -3.97512400 21.20009700
H -11.51915200 -3.56993600 20.28301900
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