Supporting Information

Synthesis, Crystal Structure, Magnetic Property and DFT Calculations of an Unusual Dinuclear μ_2-Alkoxido Bridged Iron(III) Complex

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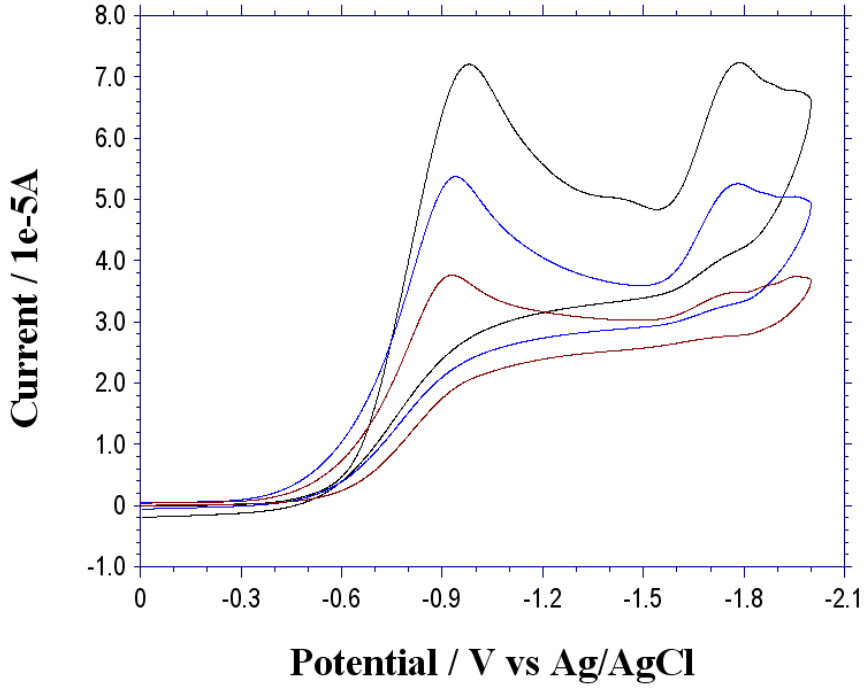

Figure S1. Cyclic voltammograms at 298 K in CH_3CN solvent (0.1 mol dm^{-3}, Ag–AgCl reference electrode) at a platinum working electrode of complex **1** at a scan rate of 20, 50 and100 mV s^{-1}.

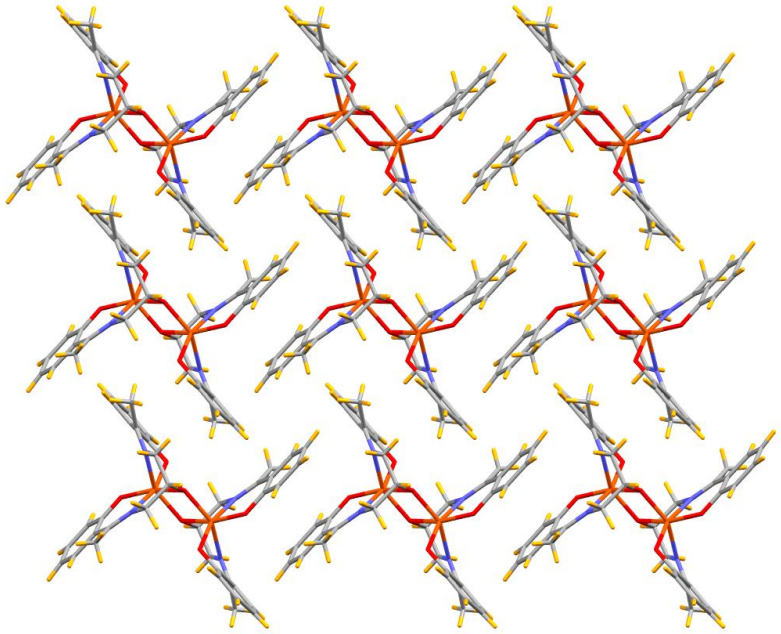

Figure S2. Packing of the complex **1** along crystallographic *b* axis.

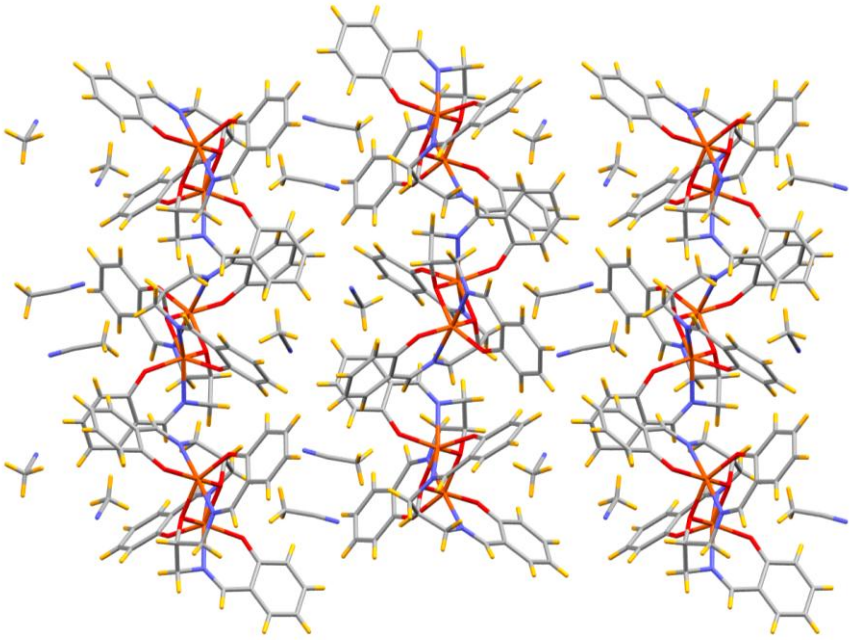

Figure S3. Packing of the complex **3** along crystallographic *a* axis.

Table S1. Crystal data and structure refinement of complex **3.**

	2
Formula	$C_{34}H_{30}Fe_2N_4O_6$, $2(C_2H_3N)$
M	784.43
Crystal System	Monoclinic
Space Group	P21/n (No. 14)
a/Å	11.139(5)
b/Å	14.648(5)
c/Å	22.488(5)
β/°	95.343(5)
V/Å^3	3653(2)
Z	4
D_c/g cm^{-3}	1.426
μ/mm^{-1}	0.849
F (000)	1624
R(int)	0.039
Total Reflections	26607
Unique reflections	7096
$I>2\sigma(I)$	5365
R1, *w*R2	0.0370, 0.1083
Temp (K)	293

Table S2 Comparison of experimental and theoretical dimensions in the metal coordination sphere, distances, Å, angles (°) of complexes 1 and **3**.

atom labels	dist./angle exp.	dist./angle theor.
	Complex 1	
Fe(1) – O(1)	2.058(2)	2.097
Fe(1) – O(2)	1.902(2)	1.934
Fe(1) – O(3)	1.927(2)	1.972
Fe(1) – N(1)	2.127(2)	2.163
Fe(1) – N(2)	2.188(2)	2.222
Fe(1) – O(1)′	1.981(2)	2.019
O(1)-Fe(1)-O(2)	160.62(8)	159.18
O(1)-Fe(1)-O(3)	109.76(7)	111.32
O(1)-Fe(1)-N(1)	75.59(7)	74.95
O(1)-Fe(1)-N(2)	77.78(7)	77.50
O(1)-Fe(1)-O(1)′	76.51(7)	76.63
O(2)-Fe(1)-O(3)	89.53(8)	89.47
O(2)-Fe(1)-N(1)	105.97(8)	108.61
O(2)-Fe(1)-N(2)	83.12(8)	82.39
O(1)′-Fe(1)-O(2)	103.73(8)	101.87
O(3)-Fe(1)-N(1)	83.23(7)	81.49
O(3)-Fe(1)-N(2)	163.36(7)	160.59
O(1)′ -Fe(1)-O(3)	96.86(7)	98.90
N(1)-Fe(1)-N(2)	84.47(7)	84.44
O(1)′-Fe(1)-N(1)	150.30(8)	149.51
O(1)′-Fe(1)-N(2)	99.38(7)	100.00
Fe(1)-O(1)-Fe(1)′	103.49(7)	103.37
	Complex 3	
Fe(1) – O(1)	2.015(2)	2.055
Fe(1) – O(2)	2.021(2)	2.050
Fe(1) – O(3)	1.923(2)	1.965
Fe(1) – N(1)	2.134(2)	2.169
Fe(1) – N(3)	2.139(2)	2.170
Fe(1) – O(5)	1.934(2)	1.966
Fe(2) – O(1)	2.052(2)	2.087
Fe(2) – O(2)	2.019(2)	2.091
Fe(2) – O(4)	1.932(2)	1.970
Fe(2) – O(6)	1.919(2)	1.971
Fe(2) – N(2)	2.151(2)	2.198
Fe(2) – N(4)	2.167(2)	2.203
O(2)-Fe(1)-O(3)	93.18(8)	96.86
O(2)-Fe(1)-N(1)	107.05(7)	107.31
O(2)-Fe(1)-N(3)	77.08(8)	77.10
O(2)-Fe(1)-O(5)	158.35(8)	156.61
O(3)-Fe(1)-N(1)	85.42(8)	84.04
O(3)-Fe(1)-N(3)	95.01(8)	92.56
O(3) -Fe(1)-O(5)	100.67(8)	97.45

N(1)-Fe(1)-N(3)	175.83(8)	174.17
N(2)-Fe(2)-N(4)	152.79(8)	152.16
O(1)-Fe(1)-O(2)	73.93(7)	75.62
O(1)-Fe(1)-O(3)	153.64(8)	156.61
O(1)-Fe(1)-O(5)	98.99(7)	96.86
O(1)-Fe(1)-N(1)	76.93(7)	77.10
O(1)-Fe(1)-N(3)	104.02(8)	107.31
Fe(1)-O(1)-Fe(2)	105.93(7)	105.16
Fe(1)-O(2)-Fe(2)	106.98(8)	105.03

Cartesian coordinates of BP86-D3/def2-TZVP optimized complexes.

1 (with Methyl group)

Fe	-0.7955546	0.6509077	-1.2420433
O	-1.9336730	2.1236021	-0.5897227
O	-0.8148447	-0.9735945	0.0850841
O	-0.3771126	1.6954844	-2.8157413
N	-2.7253198	-0.2851977	-1.5278557
N	-0.0420755	-1.0131181	-2.5078904
C	-3.8742797	1.7677828	-2.0009221
C	0.9267217	0.2895048	-4.3054555
C	0.3475204	1.5404479	-3.8913325
C	-5.1077826	-0.4897774	-2.0124711
C	0.7115883	-0.9610789	-3.5724904
C	-2.9304336	2.6019125	-1.2966489
C	-1.2757407	-2.0573976	-0.6828506
C	-3.8339687	0.3119914	-1.8580970
C	-3.1211330	4.0091270	-1.3480887
C	-2.6989517	-1.6981329	-1.1641329
C	-0.2899247	-2.2922438	-1.8339327
C	1.3925513	-2.2070727	-4.1088060
C	1.7001614	0.2845139	-5.4926807
C	0.5696820	2.6915226	-4.6985988
C	-5.0189453	3.7708076	-2.8341529
C	1.3321654	2.6377285	-5.8512074
C	-4.8917905	2.3916465	-2.7577987
C	1.9085549	1.4223377	-6.2575875
C	-4.1301266	4.5798858	-2.1060710
H	-1.3265369	-2.9817108	-0.0785636
H	-2.4161069	4.6270753	-0.7907288
H	-4.2272000	5.6669251	-2.1436411

H	0.1099159	3.6215344	-4.3625718
H	-5.5863894	1.7706688	-3.3251807
H	2.1467789	-0.6483085	-5.8337235
H	1.4833043	3.5416753	-6.4447986
H	-5.8012454	4.2176257	-3.4477736
H	2.5103335	1.3681050	-7.1650814
H	-5.0171476	-1.2218054	-2.8298375
H	-5.9822748	0.1399799	-2.1950123
H	-5.2934690	-1.0652803	-1.0921151
H	2.4562646	-2.0127780	-4.2975927
H	1.3247850	-3.0446576	-3.4106017
H	0.9429463	-2.5183615	-5.0637177
H	-3.4057916	-1.8799790	-0.3356927
H	-3.0044066	-2.3485061	-2.0040525
H	-0.6858899	-3.0523264	-2.5305371
H	0.6428316	-2.6763215	-1.3872414
Fe	0.8069213	-0.6493271	1.2438440
O	1.9460434	-2.1231619	0.5948879
O	0.8279975	0.9742916	-0.0845154
O	0.3853839	-1.6927349	2.8172839
N	2.7356488	0.2856828	1.5332806
N	0.0501600	1.0153858	2.5064975
C	3.8806105	-1.7674539	2.0143278
C	-0.9354680	-0.2888310	4.2938008
C	-0.3540100	-1.5398296	3.8831116
C	5.1163040	0.4887892	2.0276164
C	-0.7100480	0.9633501	3.5664189
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C	1.2895168	2.0579427	0.6835315
C	3.8423233	-0.3119306	1.8693265
C	3.1308038	-4.0087601	1.3577488
C	2.7118992	1.6977138	1.1661685
C	0.3032904	2.2945292	1.8341823
C	-1.3899965	2.2097611	4.1029426
C	-1.7248073	-0.2861856	5.4704980
C	-0.5902251	-2.6933604	4.6828358
C	5.0203178	-3.7703009	2.8544670
C	-1.3686597	-2.6419137	5.8248260
C	4.8938748	-2.3911664	2.7769914
C	-1.9470824	-1.4263826	6.2279190
C	4.1357305	-4.5793972	2.1212154
H	1.3417315	2.9819779	0.0789216
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H	5.5857242	-1.7699905	3.3475335
H	-2.1740888	0.6464761	5.8085024

H	-1.5308964	-3.5477602	6.4125667
H	5.7989021	-4.2171451	3.4727789
H	-2.5615237	-1.3739850	7.1270015
H	5.0236611	1.2210476	2.8445689
H	5.9895573	-0.1418085	2.2132454
H	5.3054821	1.0639396	1.1077636
H	-2.4598059	2.0238152	4.2651148
H	-1.2982136	3.0558023	3.4180181
H	-0.9593032	2.5032931	5.0719998
H	3.4195082	1.8762492	0.3376219
H	3.0177864	2.3498472	2.0045505
H	0.7014062	3.0522778	2.5321262
H	-0.6278377	2.6821977	1.3873642

1 (with Methyl group)

Fe	-0.6869895	0.6914513	-1.3091276
O	-1.8451307	2.2036047	-0.7820846
O	-0.8081452	-1.0029311	0.0211953
O	-0.1505236	1.7655372	-2.8715974
N	-2.5884236	-0.2716047	-1.6615224
N	0.0827674	-0.9624609	-2.5134932
C	-3.8405958	1.7588901	-2.0652800
C	1.0027922	0.2852910	-4.3886197
C	0.5453248	1.5787836	-3.9590732
C	0.7183822	-0.9066207	-3.6400182
C	-2.9117449	2.6391081	-1.4025011
C	-1.1991670	-2.0802526	-0.7983113
C	-3.6781233	0.3294421	-2.0126864
C	-3.2178520	4.0265933	-1.3947433
C	-2.5800934	-1.7101815	-1.3915964
C	-0.1224795	-2.2633482	-1.8748365
C	1.7442662	0.1675685	-5.5865767
C	0.8660575	2.6945113	-4.7810054
C	-5.2582593	3.6553745	-2.6671870
C	1.5989819	2.5418378	-5.9471867
C	-5.0015849	2.2939940	-2.6674746
C	2.0482235	1.2731707	-6.3636052
C	-4.3520640	4.5184838	-2.0215295
H	-1.2882902	-3.0147174	-0.2164413
H	-2.5187102	4.6938172	-0.8893668
H	-4.5458657	5.5930943	-2.0094425
H	0.5124913	3.6741451	-4.4575369
H	-5.7025863	1.6046590	-3.1455482
H	2.0802693	-0.8271451	-5.8920720
H	1.8287764	3.4206908	-6.5533452
H	-6.1511241	4.0518601	-3.1502787
H	2.6235569	1.1643377	-7.2828848

H	-3.3620324	-1.9452811	-0.6524209
H	-2.7885083	-2.2936500	-2.3061298
H	-0.3998206	-3.0384348	-2.6112731
H	0.8047156	-2.5722926	-1.3643793
Fe	0.6830389	-0.6919274	1.3042656
O	1.8384442	-2.2079295	0.7815826
O	0.8052893	1.0012026	-0.0270020
O	0.1429404	-1.7641132	2.8669150
N	2.5876481	0.2679316	1.6529642
N	-0.0789873	0.9647219	2.5102252
C	3.8346664	-1.7641540	2.0638452
C	-0.9928843	-0.2783427	4.3916122
C	-0.5460715	-1.5742038	3.9580749
C	-0.7066467	0.9120891	3.6414346
C	2.9031587	-2.6442574	1.4046923
C	1.2007185	2.0784647	0.7904019
C	3.6759185	-0.3345054	2.0061964
C	3.2041502	-4.0328731	1.4040208
C	2.5825113	1.7058754	1.3796803
C	0.1273462	2.2644911	1.8697723
C	-1.7266828	-0.1573170	5.5939963
C	-0.8696222	-2.6889614	4.7802437
C	5.2456309	-3.6626534	2.6750555
C	-1.5948274	-2.5329902	5.9507784
C	4.9938079	-2.3003701	2.6686222
C	-2.0333487	-1.2619191	6.3713733
C	4.3364268	-4.5257065	2.0335747
H	1.2899946	3.0123343	0.2075674
H	2.5027794	-4.7000536	0.9016943
H	4.5262285	-5.6010808	2.0271270
H	-0.5241906	-3.6704354	4.4535894
H	5.6970779	-1.6111971	3.1435956
H	-2.0546456	0.8391368	5.9025492
H	-1.8269832	-3.4111061	6.5571084
H	6.1369932	-4.0599417	3.1602601
H	-2.6027677	-1.1505442	7.2940218
H	3.3622157	1.9367229	0.6367927
H	2.7963352	2.2910584	2.2918953
H	0.4078702	3.0399929	2.6046108
H	-0.8006721	2.5743626	1.3613282
H	1.0876389	-1.8473845	-4.0873244
H	-1.0681739	1.8547408	4.0910643
H	-4.5778555	-0.2694082	-2.2435012
H	4.5770390	0.2629252	2.2352760
Fe	-0.6869895	0.6914513	-1.3091276
O	-1.8451307	2.2036047	-0.7820846
O	-0.8081452	-1.0029311	0.0211953

O	-0.1505236	1.7655372	-2.8715974
N	-2.5884236	-0.2716047	-1.6615224
N	0.0827674	-0.9624609	-2.5134932
C	-3.8405958	1.7588901	-2.0652800
C	1.0027922	0.2852910	-4.3886197
C	0.5453248	1.5787836	-3.9590732
C	0.7183822	-0.9066207	-3.6400182
C	-2.9117449	2.6391081	-1.4025011
C	-1.1991670	-2.0802526	-0.7983113
C	-3.6781233	0.3294421	-2.0126864
C	-3.2178520	4.0265933	-1.3947433
C	-2.5800934	-1.7101815	-1.3915964
C	-0.1224795	-2.2633482	-1.8748365
C	1.7442662	0.1675685	-5.5865767
C	0.8660575	2.6945113	-4.7810054
C	-5.2582593	3.6553745	-2.6671870
C	1.5989819	2.5418378	-5.9471867
C	-5.0015849	2.2939940	-2.6674746
C	2.0482235	1.2731707	-6.3636052
C	-4.3520640	4.5184838	-2.0215295
H	-1.2882902	-3.0147174	-0.2164413
H	-2.5187102	4.6938172	-0.8893668
H	-4.5458657	5.5930943	-2.0094425
H	0.5124913	3.6741451	-4.4575369
H	-5.7025863	1.6046590	-3.1455482
H	2.0802693	-0.8271451	-5.8920720
H	1.8287764	3.4206908	-6.5533452
H	-6.1511241	4.0518601	-3.1502787
H	2.6235569	1.1643377	-7.2828848
H	-3.3620324	-1.9452811	-0.6524209
H	-2.7885083	-2.2936500	-2.3061298
H	-0.3998206	-3.0384348	-2.6112731
H	0.8047156	-2.5722926	-1.3643793
Fe	0.6830389	-0.6919274	1.3042656
O	1.8384442	-2.2079295	0.7815826
O	0.8052893	1.0012026	-0.0270020
O	0.1429404	-1.7641132	2.8669150
N	2.5876481	0.2679316	1.6529642
N	-0.0789873	0.9647219	2.5102252
C	3.8346664	-1.7641540	2.0638452
C	-0.9928843	-0.2783427	4.3916122
C	-0.5460715	-1.5742038	3.9580749
C	-0.7066467	0.9120891	3.6414346
C	2.9031587	-2.6442574	1.4046923
C	1.2007185	2.0784647	0.7904019
C	3.6759185	-0.3345054	2.0061964
C	3.2041502	-4.0328731	1.4040208

C	2.5825113	1.7058754	1.3796803
C	0.1273462	2.2644911	1.8697723
C	-1.7266828	-0.1573170	5.5939963
C	-0.8696222	-2.6889614	4.7802437
C	5.2456309	-3.6626534	2.6750555
C	-1.5948274	-2.5329902	5.9507784
C	4.9938079	-2.3003701	2.6686222
C	-2.0333487	-1.2619191	6.3713733
C	4.3364268	-4.5257065	2.0335747
H	1.2899946	3.0123343	0.2075674
H	2.5027794	-4.7000536	0.9016943
H	4.5262285	-5.6010808	2.0271270
H	-0.5241906	-3.6704354	4.4535894
H	5.6970779	-1.6111971	3.1435956
H	-2.0546456	0.8391368	5.9025492
H	-1.8269832	-3.4111061	6.5571084
H	6.1369932	-4.0599417	3.1602601
H	-2.6027677	-1.1505442	7.2940218
H	3.3622157	1.9367229	0.6367927
H	2.7963352	2.2910584	2.2918953
H	0.4078702	3.0399929	2.6046108
H	-0.8006721	2.5743626	1.3613282
H	1.0876389	-1.8473845	-4.0873244
H	-1.0681739	1.8547408	4.0910643
H	-4.5778555	-0.2694082	-2.2435012
H	4.5770390	0.2629252	2.2352760

3 (with Methyl group)

Fe	-1.5127953	1.2091950	0.2325197
Fe	1.0402140	-0.8076743	-0.1168477
O	-0.7295571	-0.5612979	0.9079718
O	0.2573123	0.9799177	-0.7749029
O	2.0853379	-1.3069004	1.4508521
O	-2.3088302	2.4094616	-1.0581764
O	1.4481337	-1.4637265	-1.9053563
O	-2.6430388	1.5321072	1.7700288
N	2.8538521	0.4930365	-0.4058096
N	0.2215649	-2.8978320	0.0246233
N	-0.2239704	2.7423649	1.1773465
N	-2.8620137	-0.2809144	-0.6801013
C	-1.8283719	3.5669128	2.7980902
C	-4.2503619	1.2614857	-1.9388372
C	-0.7961538	-2.9343158	1.0692748
C	4.3913445	-0.9207523	0.7894862
C	3.3665861	-1.5535126	1.5794820
C	1.6322003	-3.8752140	-1.6623450
C	1.8939688	-2.6227263	-2.3240084

C	0.7293372	-3.9709568	-0.5118618
C	-3.4531697	2.4340875	-1.6876290
C	-1.6191677	-1.6455222	0.9439185
C	4.0875060	0.1604263	-0.1519222
C	3.7646017	-2.4893888	2.5739383
H	2.9735288	-2.9329798	3.1797388
C	-2.4729068	-1.6481872	-0.3374203
C	-3.9220977	3.6858548	-2.1734324
H	-3.2865416	4.5538651	-1.9945637
C	-2.8289459	2.5608771	2.5538691
C	-3.8115959	-0.0830277	-1.5557912
C	2.6709156	-2.6403860	-3.5150885
H	2.8344708	-1.6833324	-4.0119672
C	-5.1398404	3.8062380	-2.8186310
H	-5.4755219	4.7867709	-3.1623186
C	-4.0782637	2.6766124	3.2235200
H	-4.8105366	1.8889875	3.0429051
C	1.1291835	2.7276466	0.6227450
C	-0.4878618	3.4954529	2.2113902
C	1.1008165	2.1010777	-0.7832758
C	2.4940687	1.6435184	-1.2277035
C	5.7337839	-1.3141178	1.0073583
H	6.5243854	-0.8630885	0.4089344
C	2.2072851	-5.0472888	-2.2105362
H	2.0336948	-6.0045223	-1.7207129
C	-2.1683674	4.6493196	3.6458964
H	-1.4420796	5.4449458	3.8094007
C	6.0917154	-2.2563339	1.9600242
H	7.1375276	-2.5349611	2.0896572
C	5.0917149	-2.8375866	2.7576456
H	5.3580206	-3.5704793	3.5220420
C	-4.3664845	3.7524911	4.0447415
H	-5.3440356	3.8179018	4.5269160
C	-5.9464400	2.6737661	-3.0237685
H	-6.9167175	2.7631240	-3.5124569
C	-5.4910738	1.4345836	-2.6001179
H	-6.1330963	0.5689976	-2.7615060
C	3.2084234	-3.8123600	-4.0180730
H	3.8103241	-3.7846616	-4.9287479
C	-3.4106438	4.7618737	4.2513092
H	-3.6379236	5.6228068	4.8800304
C	2.9868640	-5.0321423	-3.3572096
H	3.4151844	-5.9581733	-3.7409805
H	-2.2809680	-1.5441511	1.8255849
H	-1.4574661	-3.8143368	1.0052870
H	0.7092068	2.8449050	-1.5036759
H	-0.3081182	-2.9343143	2.0578044

H	-1.8591152	-2.0661795	-1.1578652
H	2.4325780	1.3336487	-2.2840725
H	1.5693528	3.7379344	0.5716782
H	3.2116137	2.4769991	-1.1498515
H	1.7806339	2.1059732	1.2659588
H	-3.3468232	-2.3074843	-0.2000825
C	5.2630159	0.8733834	-0.7932313
H	5.9139980	1.3310999	-0.0351605
H	5.8743355	0.1507440	-1.3520784
H	4.9470887	1.6478167	-1.4963840
C	0.6199198	4.3120545	2.8509918
H	0.8520670	5.2075217	2.2519690
H	0.3639458	4.6343654	3.8634075
H	1.5396196	3.7152098	2.9088292
C	-4.4762430	-1.2699735	-2.2285080
H	-5.2170298	-1.7416863	-1.5628001
H	-4.9805575	-0.9889680	-3.1564757
H	-3.7268497	-2.0343917	-2.4706328
C	0.4021764	-5.3598002	0.0036531
H	-0.1088894	-5.9606034	-0.7625087
H	1.3298090	-5.8880868	0.2647670
H	-0.2227633	-5.3330234	0.8998394

3 (without Methyl group)

Fe	-1.2886016	1.0264882	0.1691353
Fe	1.2894249	-0.9927518	-0.1514486
O	-0.5234005	-0.7540085	0.8548569
O	0.4939506	0.8183309	-0.8314084
O	2.2790528	-1.6720928	1.4114679
O	-2.1606411	2.2443101	-1.1030857
O	1.9256894	-1.5918677	-1.9191384
O	-2.4534753	1.3907317	1.7104571
N	3.0182626	0.3607194	-0.2573890
N	0.3844104	-3.0020506	-0.1552722
N	-0.0757182	2.6169494	1.0099414
N	-2.6764725	-0.4366574	-0.6300111
C	-1.7488493	3.5527706	2.5106810
C	-4.1938656	1.1132021	-1.7357577
C	-0.5608706	-3.1271088	0.9422110
C	4.5058392	-0.7455201	1.3036975
C	3.5197293	-1.6538787	1.8220906
C	1.4776296	-3.9586960	-2.0949864
C	2.0751950	-2.7304776	-2.5430232
C	0.6243862	-4.0006695	-0.9398883
C	-3.3356377	2.2666843	-1.6701024
C	-1.4116102	-1.8481291	0.9220906
C	4.1685988	0.2475110	0.3209945

C	3.9304628	-2.5540484	2.8425530
H	3.1810912	-3.2363410	3.2453953
C	-2.3461519	-1.8161954	-0.3050166
C	-3.8050450	3.4686659	-2.2671172
H	-3.1507315	4.3400909	-2.2251779
C	-2.6667354	2.4459929	2.4469378
C	-3.7863251	-0.1736092	-1.2442039
C	2.8484989	-2.7760062	-3.7350692
H	3.2946373	-1.8436752	-4.0831483
C	-5.0523722	3.5355603	-2.8667723
H	-5.3838340	4.4784412	-3.3067594
C	-3.8431289	2.5210513	3.2419417
H	-4.5332679	1.6776935	3.1999391
C	1.2819592	2.6731638	0.4878232
C	-0.4894202	3.5404484	1.8192361
C	1.3375667	1.9486051	-0.8730804
C	2.7555785	1.4489556	-1.1851438
C	5.8262687	-0.7844143	1.8061885
H	6.5565355	-0.0805131	1.3977733
C	1.6817078	-5.1474109	-2.8319300
H	1.2121624	-6.0666628	-2.4717436
C	-2.0533569	4.6628793	3.3331690
H	-1.3394562	5.4902819	3.3695762
C	6.2028751	-1.6847960	2.7890664
H	7.2271896	-1.7055226	3.1604303
C	5.2367631	-2.5693382	3.3061080
H	5.5181521	-3.2797149	4.0861970
C	-4.1096191	3.6285141	4.0304771
H	-5.0277414	3.6554539	4.6211701
C	-5.8974187	2.4093315	-2.9172394
H	-6.8763813	2.4726668	-3.3919647
C	-5.4582905	1.2196895	-2.3612897
H	-6.0912469	0.3290740	-2.4016633
C	3.0335034	-3.9616752	-4.4287248
H	3.6393629	-3.9596487	-5.3372088
C	-3.2164938	4.7169324	4.0821411
H	-3.4351051	5.5828282	4.7067204
C	2.4535759	-5.1647118	-3.9818264
H	2.6059139	-6.0912795	-4.5348433
H	-2.0089012	-1.7736653	1.8498601
H	-1.1756299	-4.0431511	0.8672296
H	0.9912586	2.6302509	-1.6722007
H	0.0031451	-3.1489509	1.8880890
H	4.9664596	0.9706001	0.0717416
H	-1.7970886	-2.2403976	-1.1639078
H	0.1303715	-4.9691963	-0.7390702
H	2.7588199	1.0444845	-2.2096512

H	0.1782152	4.3937866	2.0366549
H	1.6539333	3.7109236	0.4086316
H	-4.4915003	-1.0008546	-1.4443155
H	3.5110723	2.2533853	-1.1143778
H	1.9354571	2.1291762	1.1923213
H	-3.2503217	-2.4309371	-0.1400379