

Supporting information for the paper

“X-ray absorption and emission spectroscopies of X-bridged diiron phthalocyanine complexes (FePc)₂X (X = C, N, O) combined with DFT study of (FePc)₂X and their high valent diiron oxo complexes”.

By C. Colombar, E. V. Kudrik, V. Briois, J. C. Shwarbrick, A. B. Sorokin, P. Afanasiev

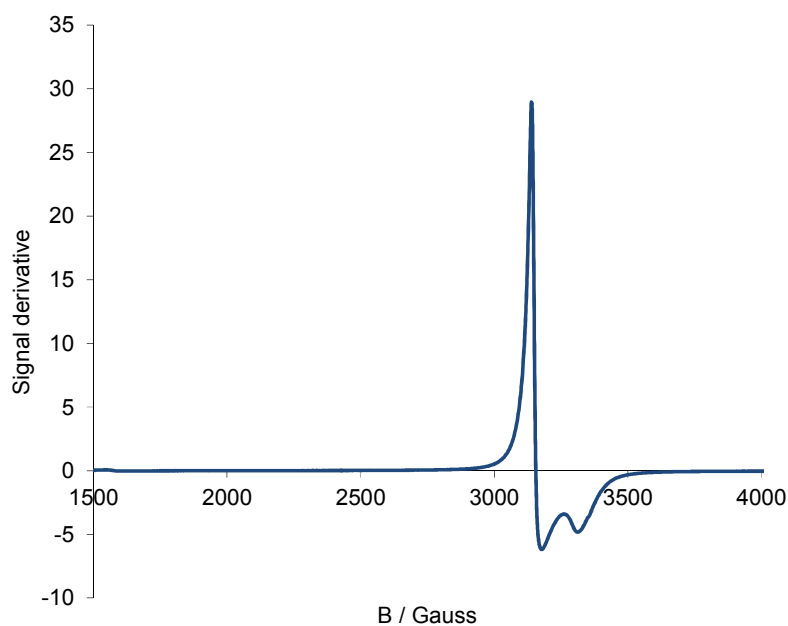


Fig. S1 EPR signal of the solid complex **2** the solids 1 and 3 are EPR-silent.

Table S1. Results of DFT optimization and broken symmetry calculations for complex **1** (carbido-dimer)

Functional	-Etotal, Ha	Multiplicity	J cm ⁻¹	(Fe1-C) ^c	(Fe2-C)	Q/S(Fe1) ^e	Q/S(Fe2)	Q/S(C)
BP86	5901.6027	1	-	1.674	1.674	0.10	0.10	0.17
						0.00	0.00	0.00
BP86	5901.3979	11	-	1.837	1.691	0.33	0.18	0.12
						3.14	1.26	-0.39
BP86	5901.6027 ^a	11BS ^b	-7174	1.674	1.674	0.11	0.11	0.17
						0.00	0.00	-0.00
BP86 ^a	5901.6027 ^a	5BS	-6645	1.674	1.674	0.10	0.10	0.15
						0.00	0.00	-0.00
BP86 ^a	5901.6027 ^a	3BS	-8910	1.674	1.674	0.11	0.10	0.171
						-0.00	0.00	-0.00
B3LYP	5898.8677	1	-	1.672	1.672	0.15	0.15	0.22
						0.0	0.0	0.0
OLYP	5900.5134	1	-	1.678	1.678	0.12	0.12	0.17
						0.00	0.00	0.00
OLYP	5900.2968 ^a	11	-	1.679	1.679	0.31	0.31	0.11
						2.89	2.89	-0.62
OLYP	5900.5134 ^a	11BS	-1900	1.679	1.679	0.15	0.15	0.16
						0.0	0.0	0.0
OLYP	5900.4694 ^a	3	-	1.678	1.678	0.05	0.05	0.12
						0.52	0.52	-0.05
OLYP	5900.4994	3BS	-9647	1.678	1.678	0.12	0.12	0.17
						0.00	0.00	0.00
OLYP	5900.4812	3	-	1.733	1.732	0.16	0.17	0.14
						1.10	1.11	-0.29
[(py)PcFe-C-FePc(py)]py ^d				1.69	1.69	Ref.[S2]		
XRD structure ; Fe-C-Fe angle 177.5 °								
[(Meim)FePc] ₂ C ^c				1.69	1.69	Ref. [S1]		
XRD structure; Fe-C-Fe angle 178 °								

^a single point calculation; ^bBS – broken symmetry solution; ^cinteratomic distance, Å; ^dMeim= 1-methylimidazole ; ^eQ-Loewdin charge; S – Loewdin spin density

[S1] G. Rossi, L. Goedken, C. Ercolani, J. Chem. Soc. Chem. Commun. (1988) 46.

[S2] A. Kienast, C. Bruhn, H. Homborg Z. anorg. Allg. Chem. 1997, 623, 967.

Table S2 Results of DFT optimization and broken symmetry calculations for complex **2** (nitrido-dimer)

Functional	-E _{total} , Ha	Mult.	J cm ⁻¹	^c Fe1-N	Fe2-N	Q/S(Fe1)	Q/S(Fe2)	^d Q/S(N)
BP86	5918.28975	2	-	1.654	1.654	0.18	0.18	0.08
						0.49	0.49	-0.05
BP86	5918.24589	4	-	1.661	1.644	0.17	0.18	0.08
						0.56	0.42	-0.03
BP86 ^a	5918.27858	4 BS ^b	-3458	1.661	1.644	0.19	0.19	0.08
						0.66	0.59	-0.05
BP86 ^a	5918.27543	8 BS	-2546	1.654	1.654	0.18	0.19	0.07
						0.62	0.62	-0.05
B3LYP	5915.5422	2	-	1.766	1.643	0.35	0.27	-0.05
						2.06	-0.64	-0.43
OLYP	5917.19482	2	-	1.655	1.654	0.20	0.20	0.08
						0.52	0.53	-0.09
OLYP ^a	5917.14670	4 BS	-3449	1.655	1.654	0.19	0.21	0.09
						0.58	0.61	-0.11
XR structure (BrFePc) ₂ N; Fe-N-Fe 180 °				1.639	1.639	Ref. [S3]		

^a single point calculation; ^bBS – broken symmetry solution. ^cinteratomic distance, Å;^dQ-Loewdin charge; S – Loewdin spin density

[S3] P. Boujemma, D. Benlian, A. Baldy, M. Pierrot, Acta Crystallogr. Sect. C 45 (1989) 393.

Table S3 Results of DFT optimization and broken symmetry calculations for complex **3** (oxo-dimer).

Functional	-E _{total} , Ha	Mult.	J cm ⁻¹	Fe1-O ^c	Fe2-O	Q/S(Fe1)	Q/S(Fe2)	Q/S(O) ^e
BP86	5938.77525	1	-	1.773	1.775	0.34	0.34	-0.20
						-2.00	2.00	-0.01
BP86	5938.63451	3	-	1.812	1.834	0.41	0.38	-0.33
						2.80	-2.71	0.51
BP86	5938.61794	11	-	1.825	1.890	0.66	0.44	-0.41
						3.98	2.50	0.71
BP86	5938.75480 ^a	11BS	-572	1.773	1.775	0.45	0.39	-0.31
						-2.21	2.18	0.06
OLYP	5937.68709	1	-	1.792	1.792	0.39	0.39	-0.25
						-2.17	2.17	0.00
OLYP	5937.62222	11	-	1.830	1.905	0.71	0.49	-0.43
						4.00	2.56	0.80
OLYP	5937.66847	11BS ^b	-417	1.792	1.792	0.49	0.43	-0.34
						-2.32	2.28	0.04
B3LYP	5936.07997	1	-	1.805	1.805	0.50	0.50	-0.39
						-2.46	2.46	0.00
B3LYP	5936.05663	11BS	-262	1.826	1.890	0.58	0.53	-0.46
						-2.52	2.53	0.03
B3LYP	5935.95690	7BS	2111	1.809	1.799	0.53	0.49	-0.45
						0.90	2.40	0.44
B3LYP	5935.98039	5BS	3722	1.815	1.772	0.54	0.50	-0.45
						2.33	-1.42	0.21
B3LYP	5936.01182	3BS	4012	1.811	1.775	0.55	0.49	-0.39
						0.93	1.06	0.13
XRD : Meim-PcFe-O-FePc-Meim				1.749	1.749	Ref. [S4]		
Fe-N-Fe 176°								

^a single point calculation; ^bBS – broken symmetry calculation. ^cinteratomic distance, Å;^d Meim= 1-methylimidazole; ^eQ-Loewdin charge; S – Loewdin spin density[S4] C. Ercolani, F. Monacelli, S. Dzugan, V.L. Goedken, G. Pennesi, G. Rossi, J. Chem. Soc. Dalton Trans. **1991**, 1309

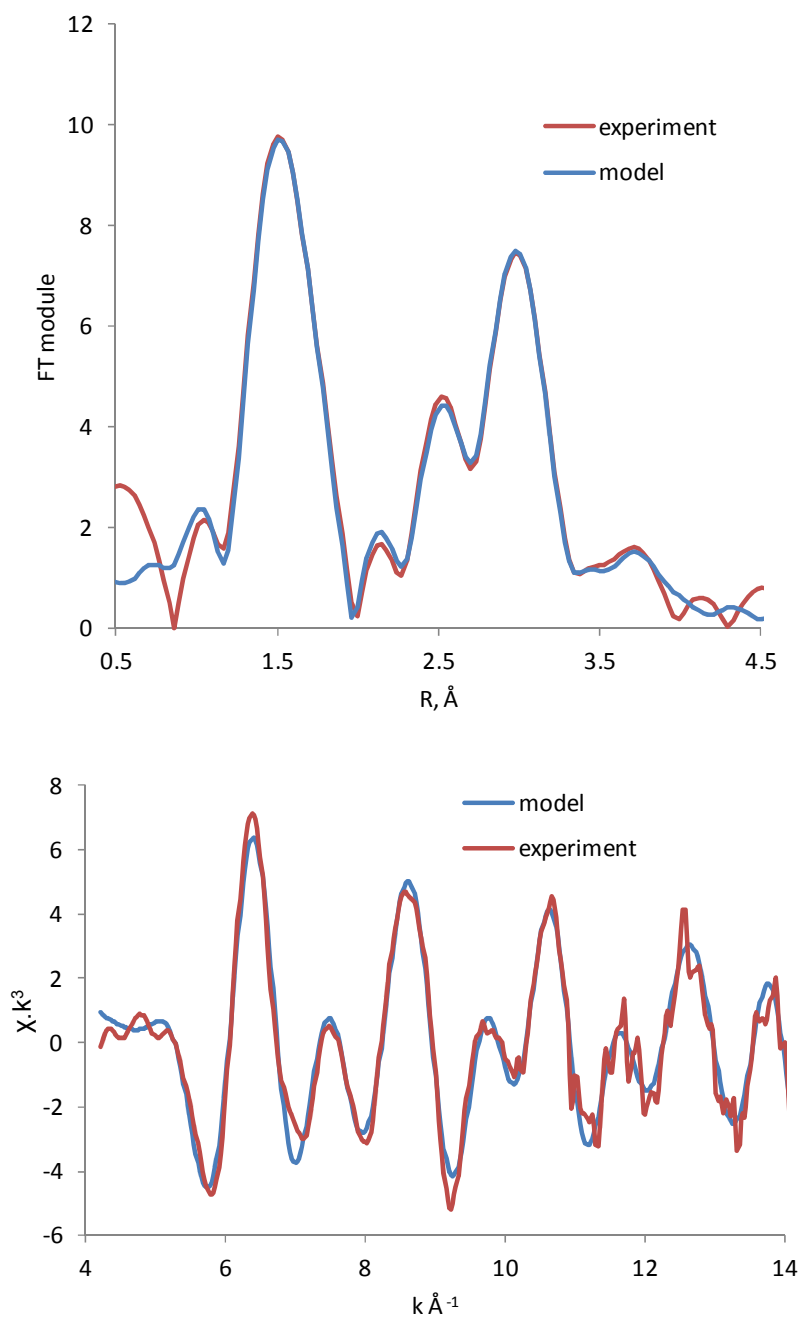


Fig. S 2 EXAFS fitting in R- (top) and k- space (bottom) for nitrido dimer 2

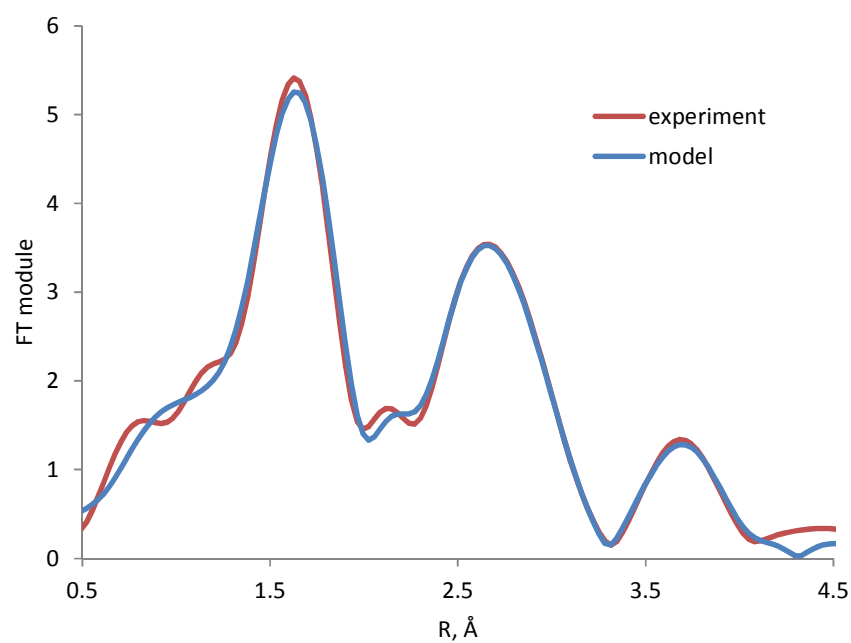
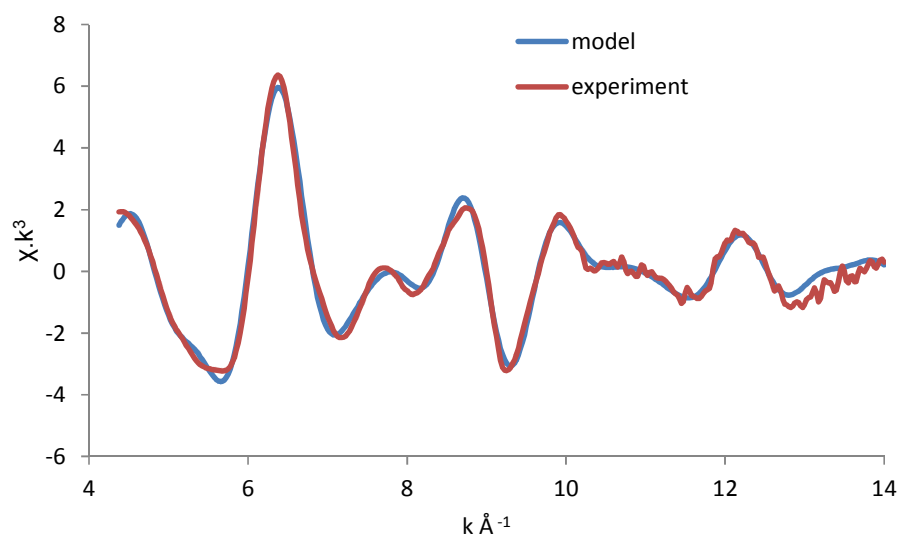


Fig. S3 EXAFS fitting in R- (top) and k- space (bottom) for oxo- dimer **3**

Table S4. Parameters of fitting for the EXAFS spectra of complexes **1-3**.

Shell	R (Å)	N	σ^2 (Å ²)	ΔE (eV)
1 carbido dimer R=6.1%				
C1 (axial)	1.66(2)	1	0.0051(5)	-0.5
N1	1.96(2)	4	0.0072(8)	-0.9
Fe	3.31(1)	1	0.0032(6)	1.1
C2	2.89(4)	8	0.012(3)	1.3
N2	3.44(5)	4	0.013(5)	1.5
C3	4.21(7)	8	0.017(6)	-0.2
2 nitrido dimer R=7.5%				
N1 (axial)	1.64(2)	1	0.0043(5)	-0.2
N2	1.97(3)	4	0.0065(5)	-0.1
Fe	3.28(1)	1	0.0031(5)	0.7
C1	2.91(5)	8	0.0091(5)	2.3
N3	3.45(5)	4	0.014(2)	0.9
C2	4.30(8)	8	0.018(6)	-0.8
3 oxo dimer R=7.0%				
O1 (axial)	1.76(2)	1	0.0061(7)	-0.4
N1	1.97(3)	4	0.0075(8)	0.6
Fe	3.51(2)	1	0.0066(6)	0.1
C1	2.92(6)	8	0.018(8)	0.8
N2	3.44(7)	4	0.020(8)	0.5
C2	4.31(9)	8	0.020(8)	-0.8

Complex 1 orbitals

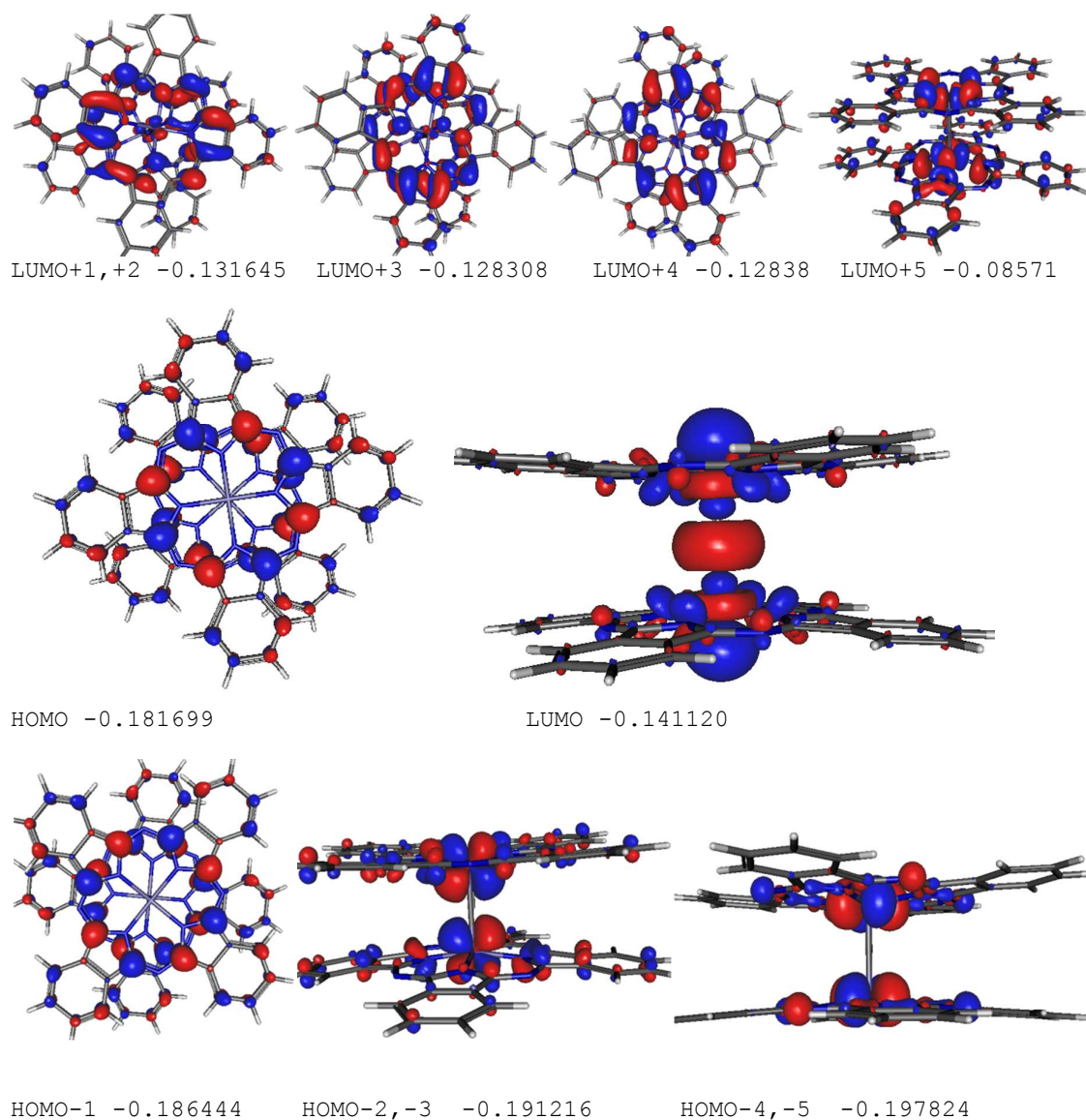
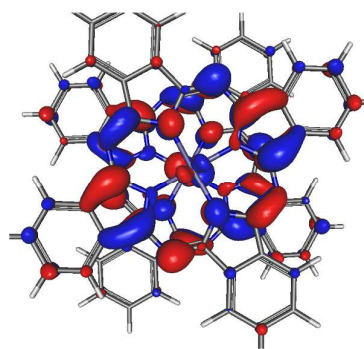
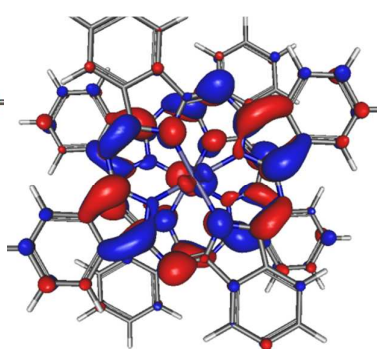


Fig. S4 Isosurfaces (0.025; $\alpha=\beta$) of canonic orbitals for the complex 1 ground state ($S=0$) calculated using UKS DFT with BP86 functional. Energies in Ha are indicated below isosurfaces.

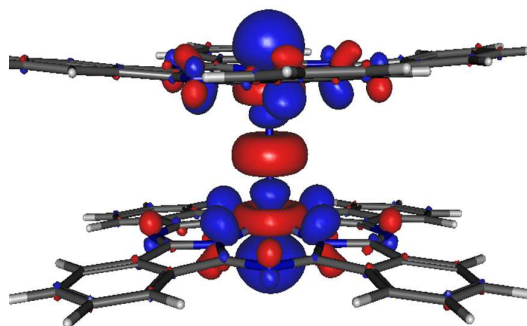
Complex 2 alfa orbitals



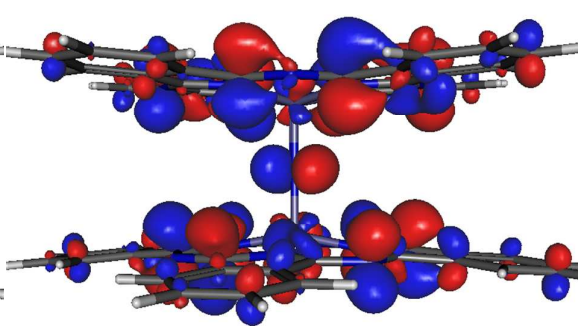
LUMO+1, +2 -0.131521



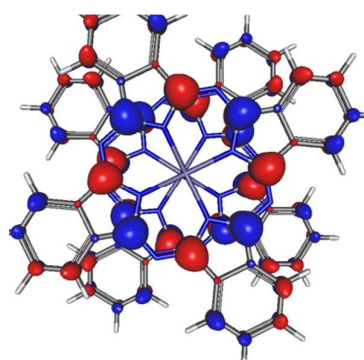
LUMO+2, +3 -0.131521



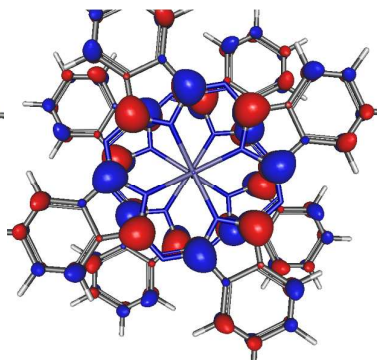
HOMO -0.174056



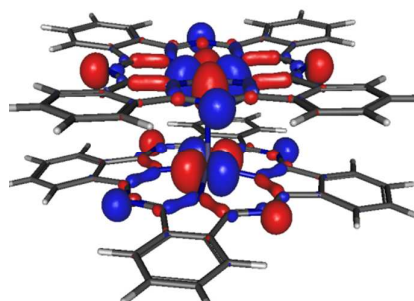
LUMO, LUMO+1 -0.133675



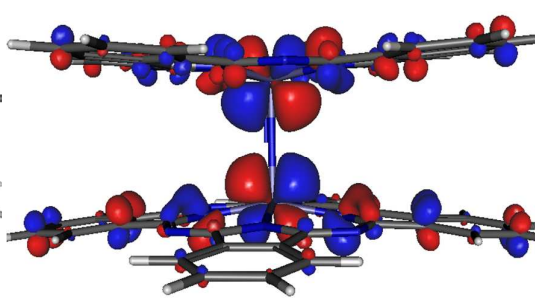
HOMO-1 -0.183041



HOMO-2 -0.186446

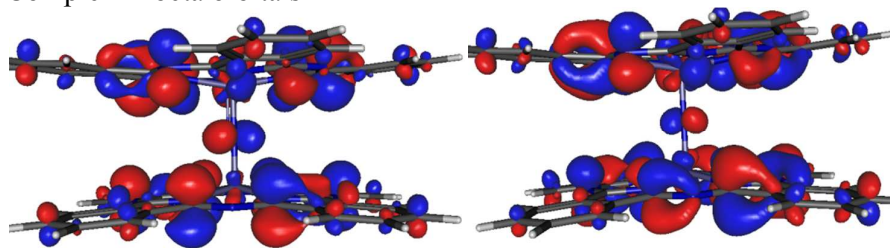


HOMO-3, -4 -0.203399



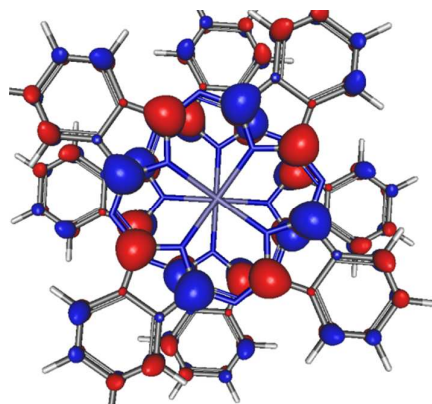
HOMO-5, -6 -0.204399

Complex **2** beta orbitals

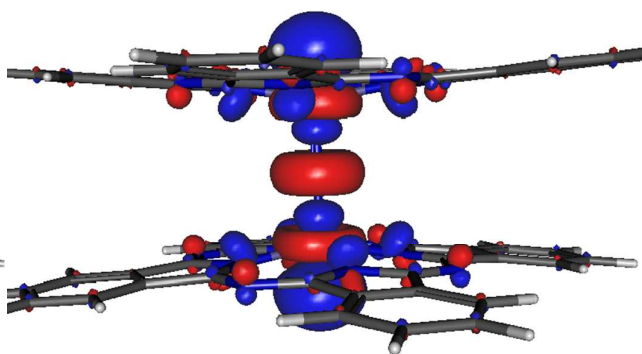


LUMO+1, +2 -0.130249

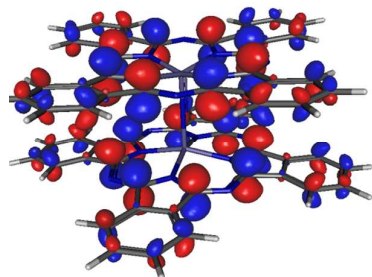
LUMO+3, +4 -0.130924



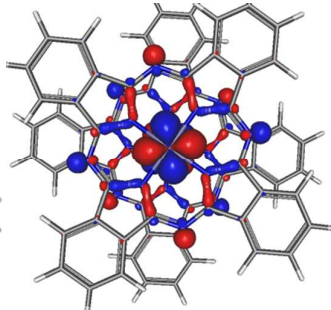
HOMO -0.183141



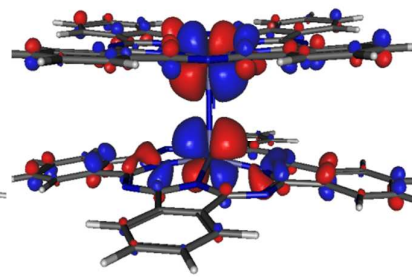
LUMO -0.139909



HOMO-1 -0.186527



HOMO-2, -3 -0.186446



HOMO-4, -5 -0.197945

Fig. S5 Isosurfaces (0.025) of canonic orbitals for the complex **2** ground state ($S=1/2$) calculated using UKS DFT with BP86 functional. Energies in Ha are indicated below isosurfaces.

Complex **3** orbitals (alfa = beta)

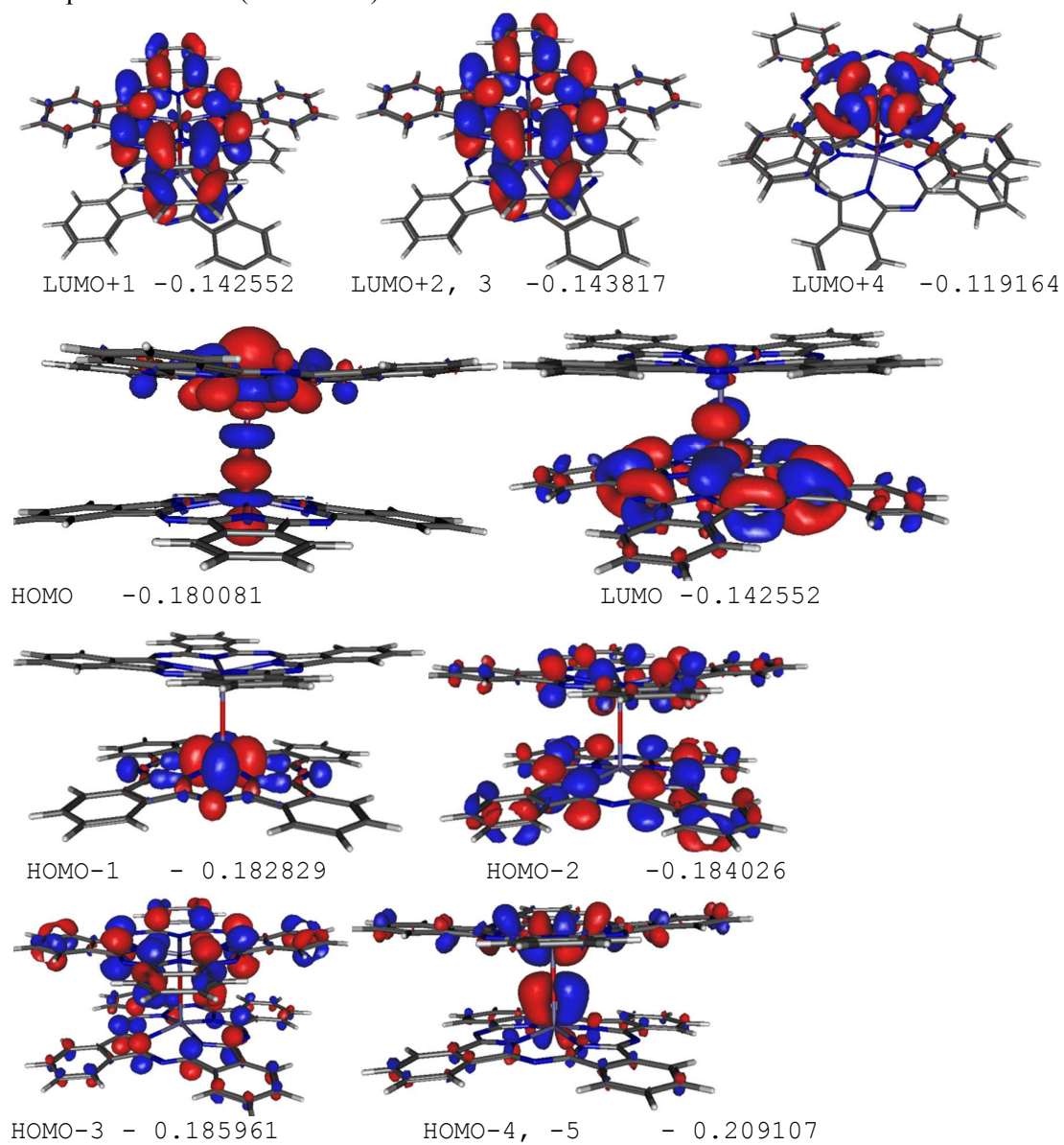
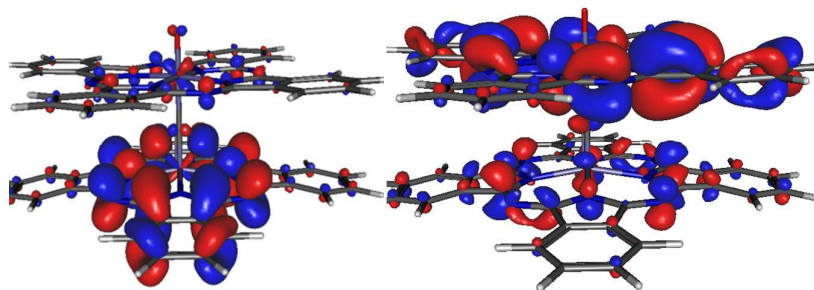
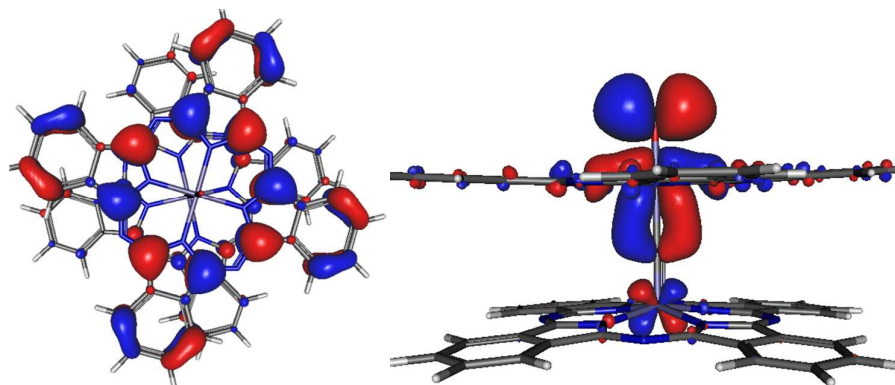


Fig. S6 Isosurfaces of canonic valence zone orbitals for the ground state ($S=0$) complex **3**, calculated using UKS DFT with BP86 functional.

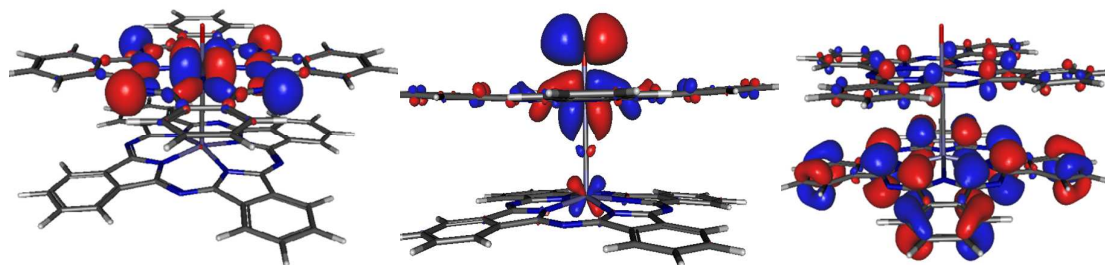
1-O orbitals (alfa=beta)



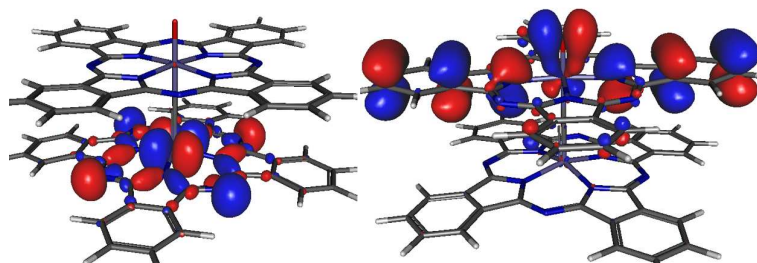
LUMO+1, +2 -0.137743 LUMO+3, 4 -0.133414



HOMO -0.185885 LUMO -0.164982



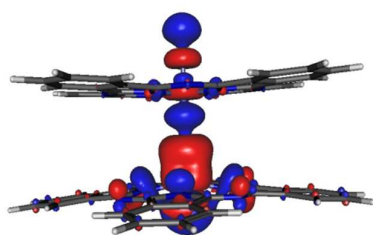
HOMO-3 -0.211162 HOMO-2 -0.19869 HOMO-1 -0.190203



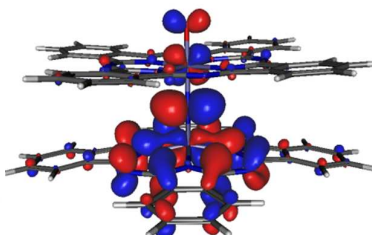
HOMO-4 -0.213138 HOMO-5 -0.227544

Fig. S7 Isosurfaces (0.025) of canonic orbitals for the complex **1-O** ground state ($S=0$) calculated using UKS DFT with BP86 functional. Energies in Ha indicated below isosurfaces.

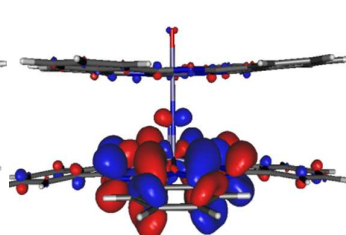
2-O complex alpha orbitals



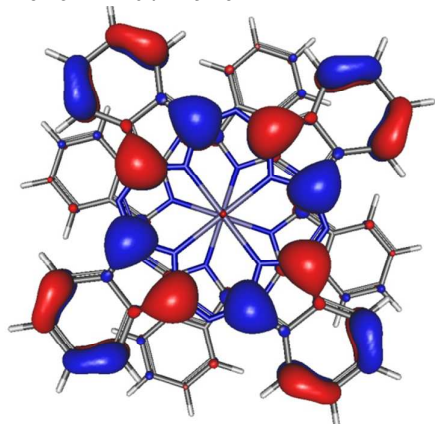
LUMO+1 -0.149787



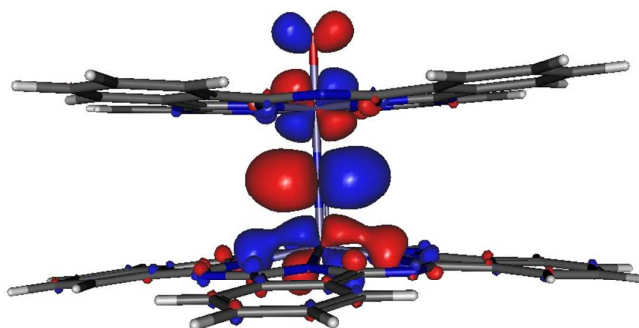
LUMO+2 -0.143817



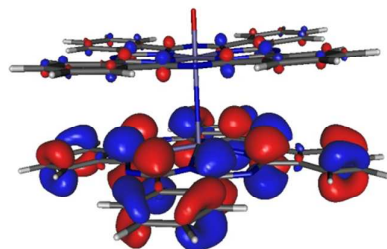
LUMO+3 -0.14051



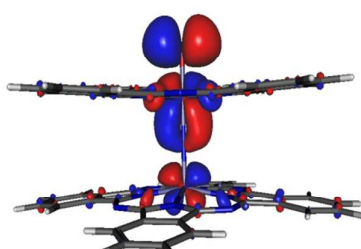
HOMO -0.183431



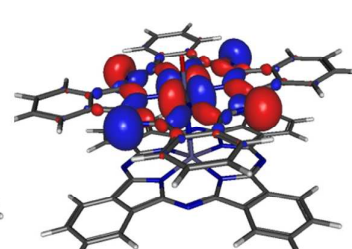
LUMO -0.151877 (dxz)



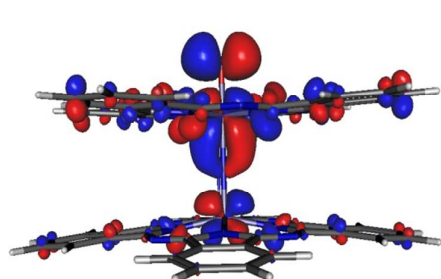
HOMO-1 - 0.192716



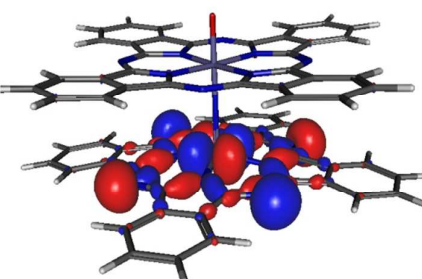
HOMO-2 -0.201944 (dxz)



HOMO-3 -0.213369 (dx2-y2)



HOMO-4 - 0.215614 (dyz)



HOMO-5 -0.22337 (dxy)

2-O complex beta orbitals

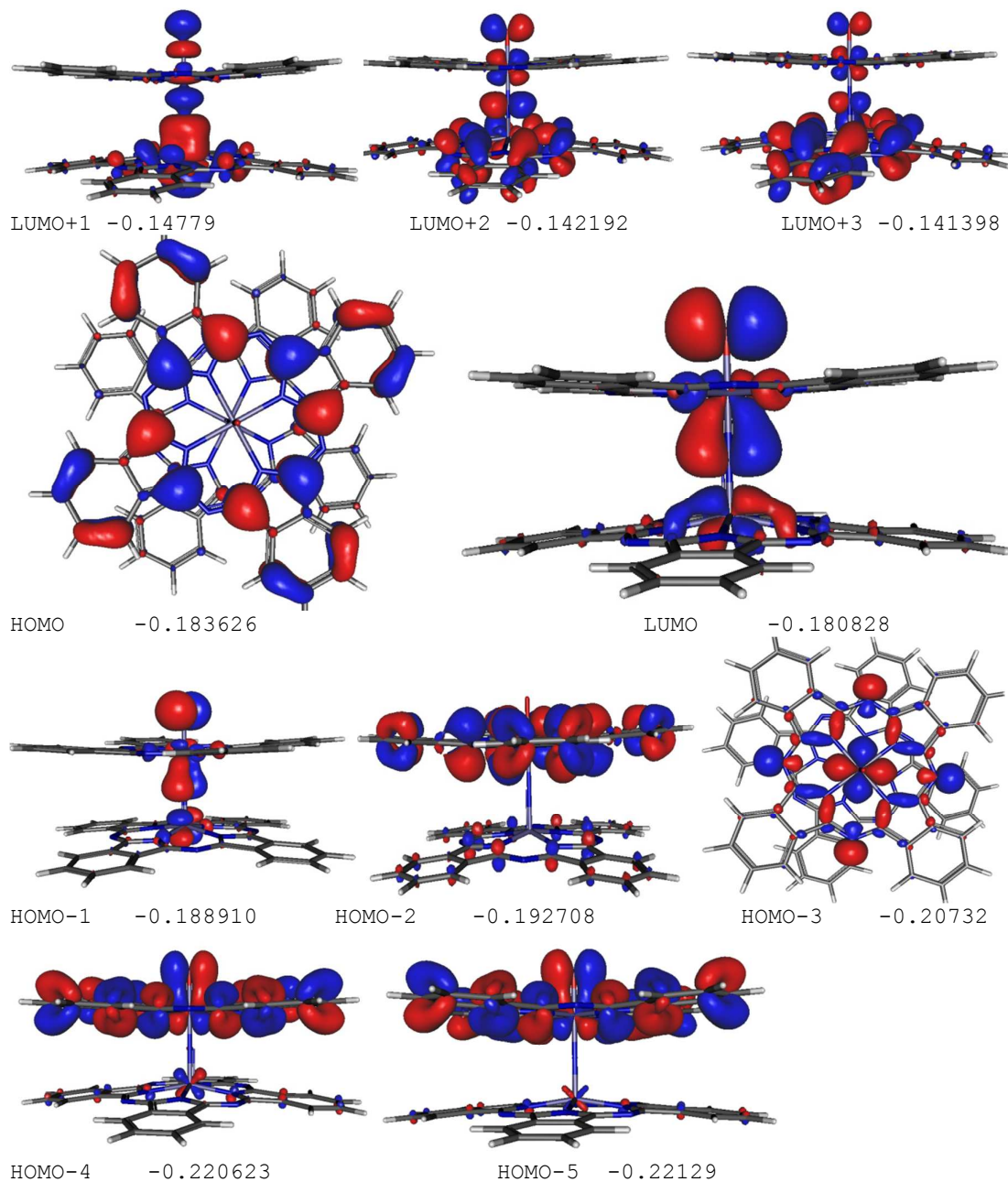
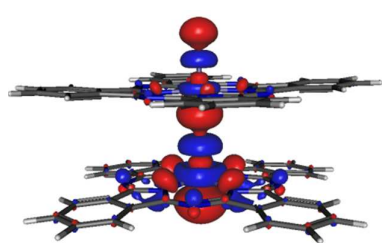
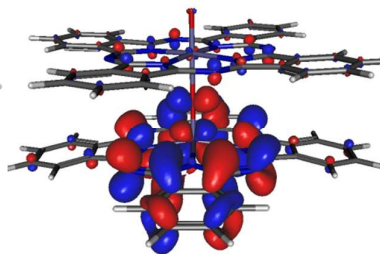


Fig. S8 Isosurfaces of canonic valence zone orbitals for the **2-O** complex ground state ($S=1/2$) calculated using UKS DFT with BP86 functional.

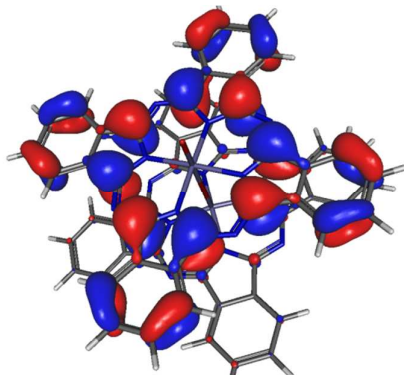
3-O complex, alpha orbitals



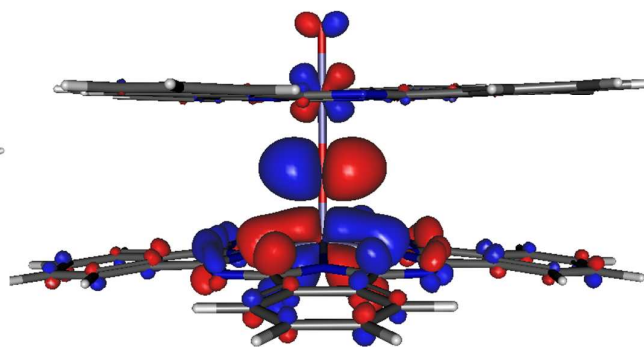
LUMO+2 -0.151625



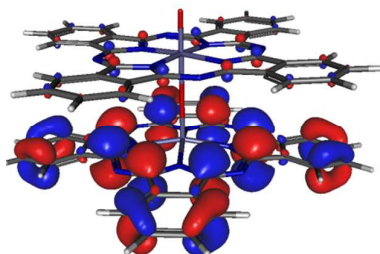
LUMO+3, +4 -0.135196



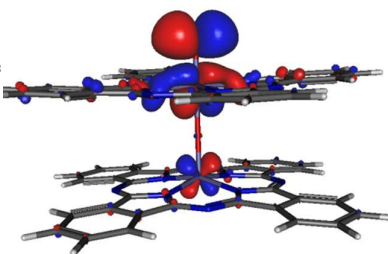
HOMO -0.183731



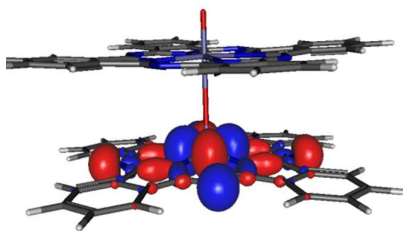
LUMO , LUMO+1 -0.156653 (dxz, dyz)



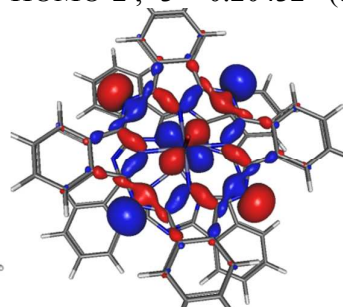
HOMO-1 - 0.191141 Ha



HOMO-2 , -3 -0.20432 (dxz)



HOMO-4 - 0.210354 (dyz)



HOMO-5 -0.22337 (dxy)

3-O complex, beta orbitals

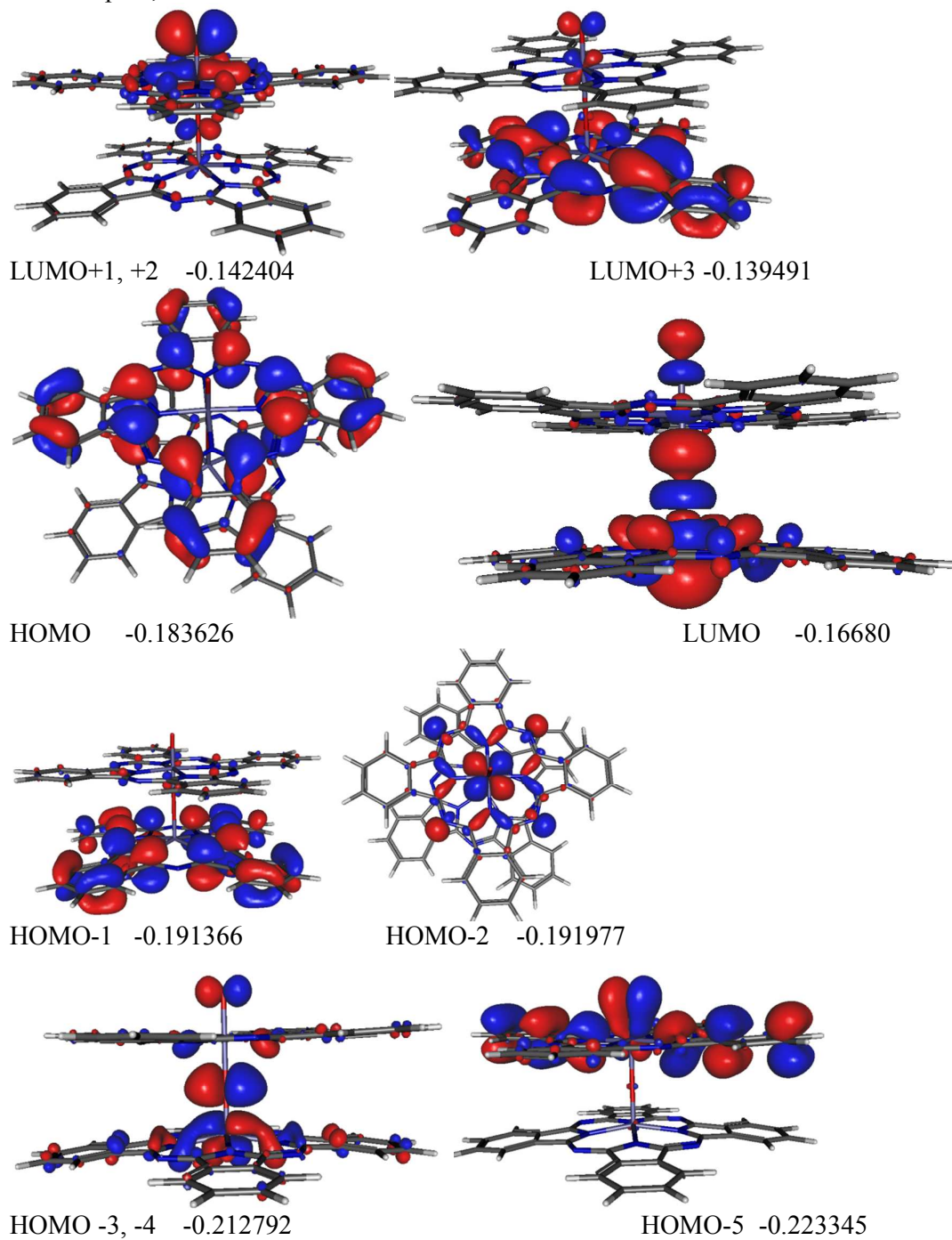


Fig. S 9 Isosurfaces of canonic valence zone orbitals for the **3-O** complex (S=0) calculated using UKS DFT with BP86 functional.

Table S5 Mayer bond orders for the complexes 1-3 calculated with different functionals and 1-O – 3-O, calculated with BP86

Filename	Functional	Multiplicity	Fe1-X ^a	Fe2-X ^b	Fe1-Fe2	Fe2-Ot ^c
1	BP86	1	1.47	1.47	0.45	-
1	B3LYP	1	1.51	1.52	0.27	-
1	OLYP	1	1.49	1.49	0.35	-
1-O	BP86	1	2.13	0.67	0.13	1.87
2	BP86	2	1.64	1.64	0.67	-
2	B3LYP	2	1.78	1.39	0.29	-
2	OLYP	2	1.74	1.55	0.62	-
2-O	BP86	2	1.57	1.68	0.43	1.36
3	BP86	1	1.23	1.23	0.39	-
3	B3LYP	1	1.16	1.16	0.12	-
3	OLYP	1	1.21	1.21	0.28	-
3-O	BP86	1	1.69	0.53	0.12	1.92

^a non-oxygen-bearing atom (for oxo-complexes) ^b oxygen-bearing atom (for oxo-complexes); ^c Ot - terminal oxygen

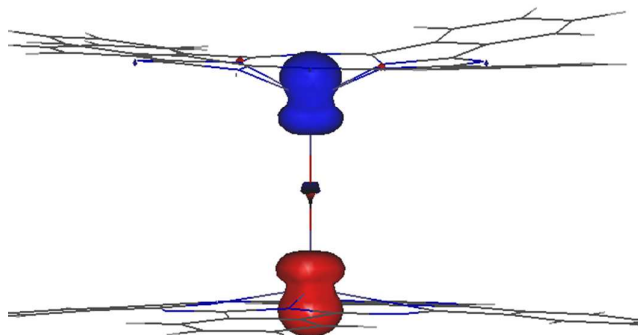


Fig. S10 Spin density in the oxo-dimer 3 calculated from the broken symmetry solution with $S=5/2$ on each site and total $M_s = 0$.

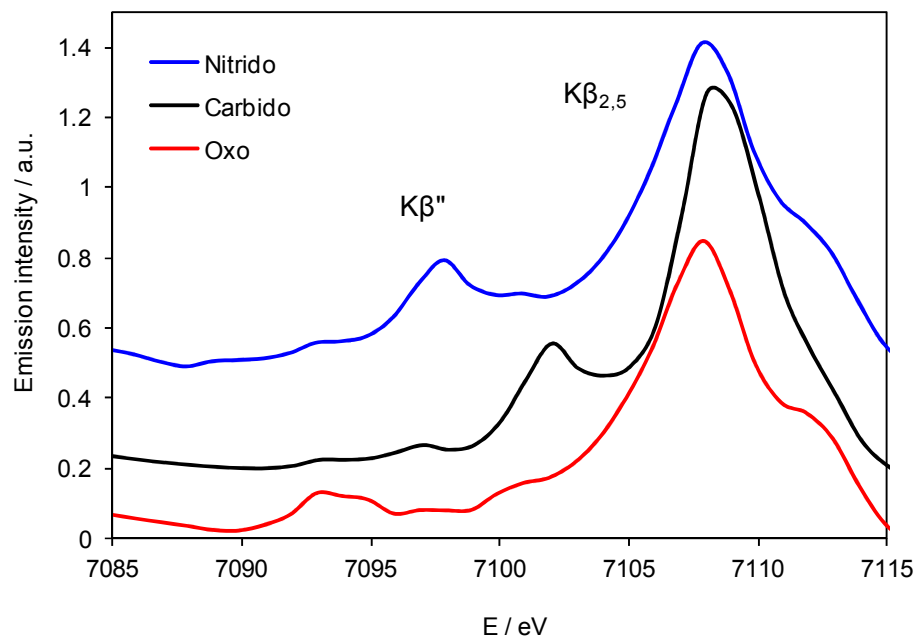


Fig. S11 Valence to core spectra of complexes **1-3** calculated by FEFF8 code

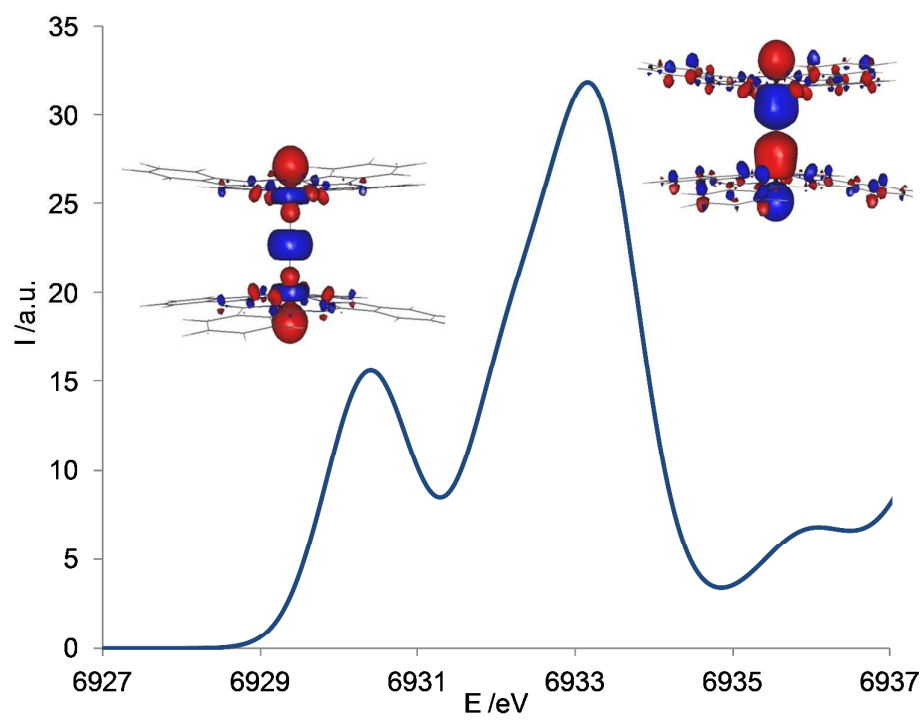


Fig. S12 DFT-calculated XAS pre-edge for the carbido dimer **1** and molecular orbitals providing the strongest contributions to the pre-edge intensity.

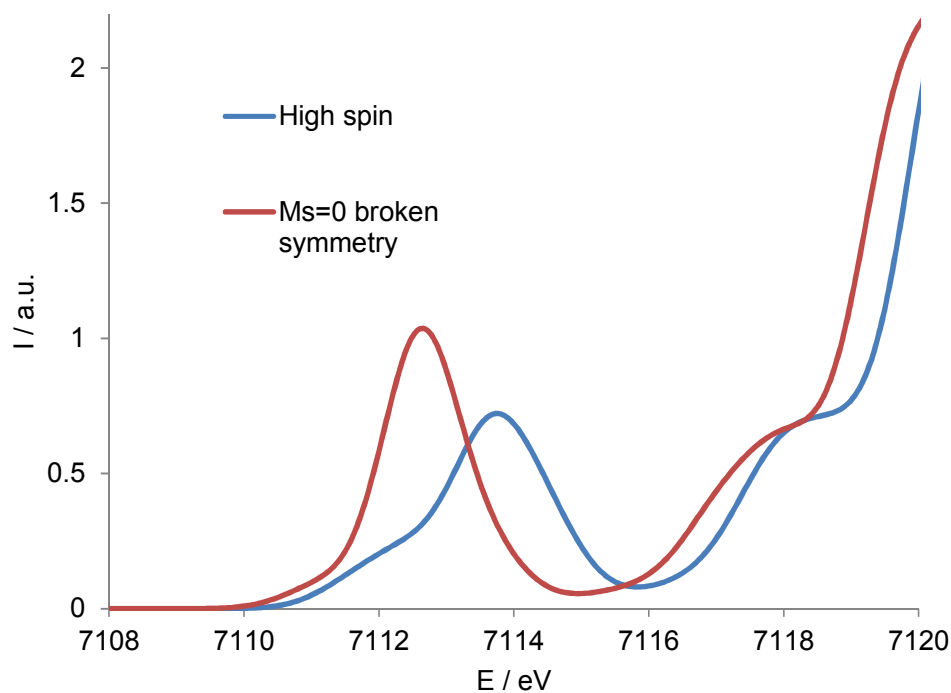


Fig. S13 DFT B3LYP calculated pre-edge XAS feature for the complex (3) multiplicity 11, in the high spin state and for the broken symmetry solution.

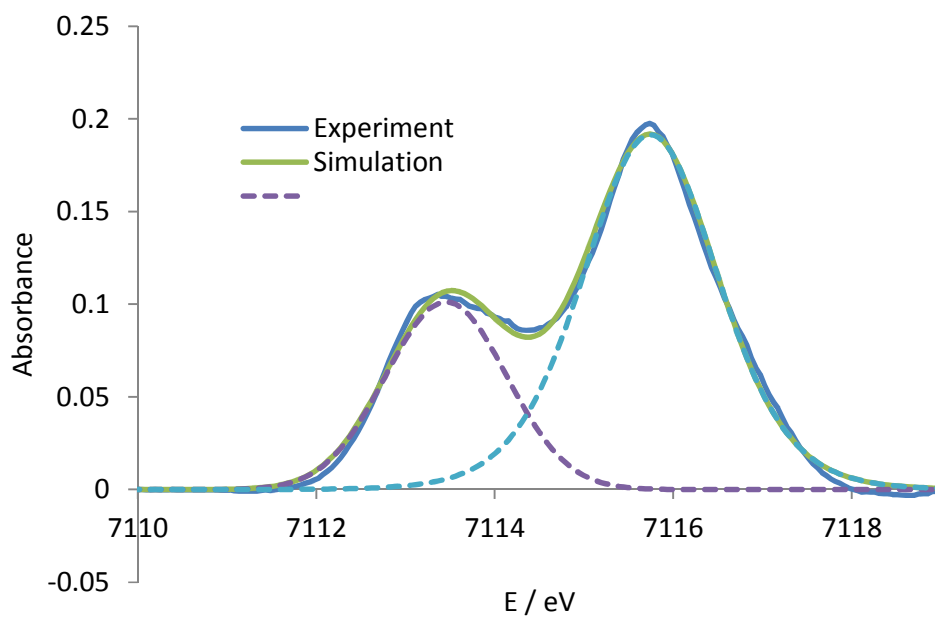


Fig. S14 Example of representation of Fe K XANES pre-edge of (3) acquired at main K β _{1,3} emission energy as a superposition of Pearson VII amplitude functions.

Table S6 Results of DFT BP86 UKS optimizations for the oxo-complexes **1-O** – **3-O**

complex	-E _{total} , Ha	Mult	Fe ₁ -X ^b	Fe ₂ -X	Fe ₂ -O _t	Q/S _{Fe1} ^c	Q/S _{Fe2}	Q/S _X	Q/S _{Ot}
1-O	5976.77432	1	1.589	2.055	1.681	0.11	0.15	0.14	-0.28
						0.00	0.00	0.00	0.00
1-O	5976.69581	3	1.591	2.098	1.721	0.24	0.17	0.15	-0.31
						-0.38	0.29	-0.17	0.77
2-O	5993.46466	2	1.607	1.771	1.730	0.23	0.14	-0.08	-0.31
						0.03	0.37	-0.14	0.75
2-O	5993.43653	4	1.605	2.130	1.662	0.22	0.23	-0.01	-0.28
						0.40	1.20	0.56	0.72
2-O	5993.42587	6	1.642	2.022	1.713	0.23	0.24	-0.05	-0.29
						2.14	-1.23	0.71	0.70
3-O	6013.98015	1	1.665	2.006	1.662	0.35	0.26	-0.15	-0.28
						-1.25	1.14	-0.57	0.734
3-O	6013.96590 ^a	3 ^a	1.665	2.006	1.662	0.34	0.25	-0.15	-0.28
						0.07	1.17	0.02	0.74
3-O	6013.89904	11	1.777	1.962	1.697	0.44	0.24	-0.29	-0.36
						3.67	1.35	0.67	0.80

^a single point calculation; ^b interatomic distance, Å; ^c Q-Loewdin charge, S – Loewdin spin density.

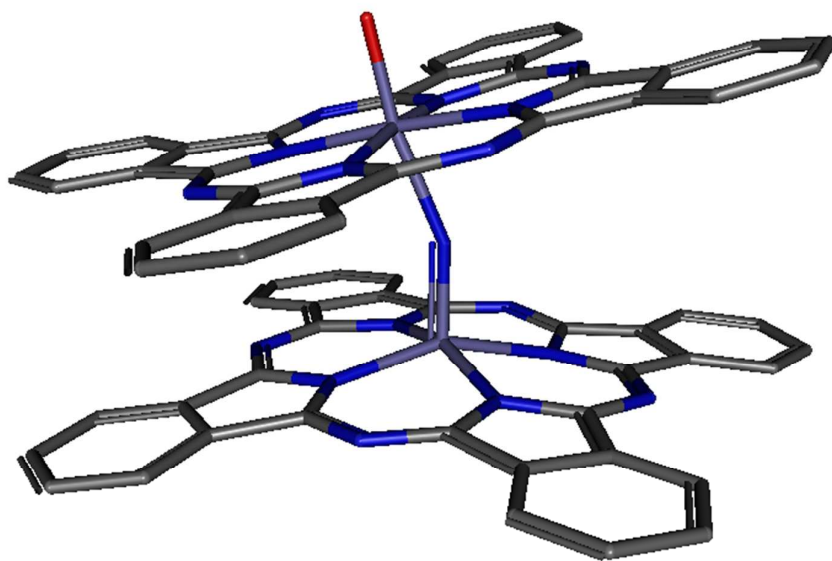
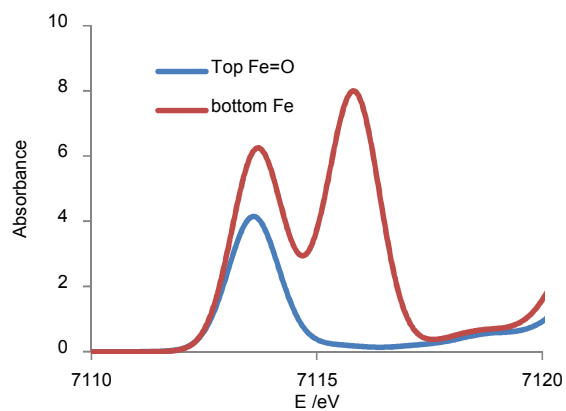
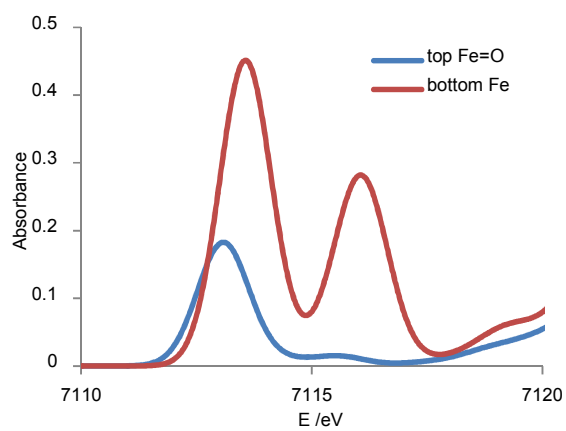


Fig.S15 Distorted geometry obtained from BP86 DFT optimization of **2-O** with multiplicity 6.

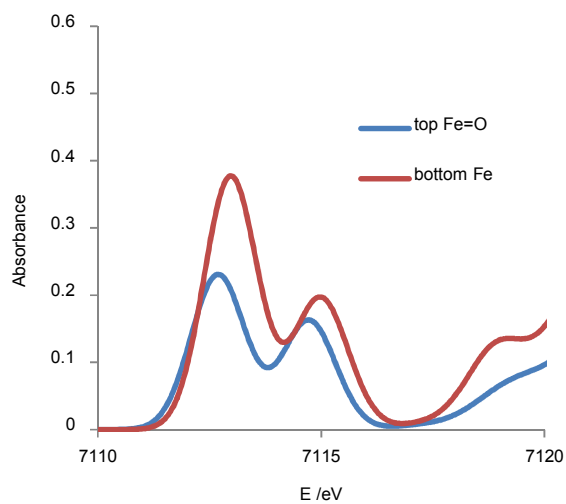
7



1

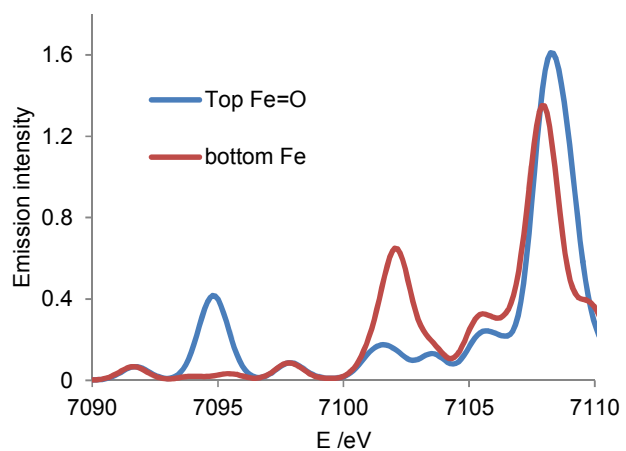


2

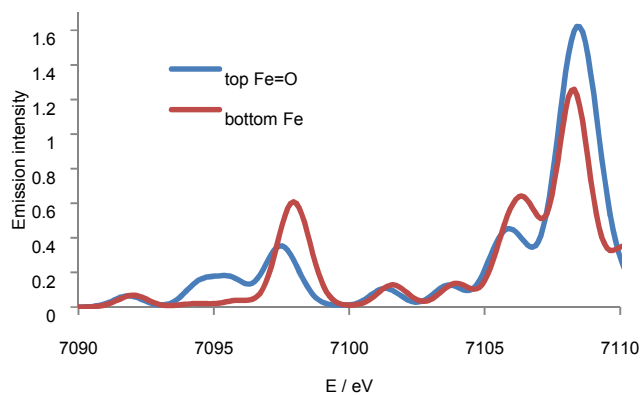


3

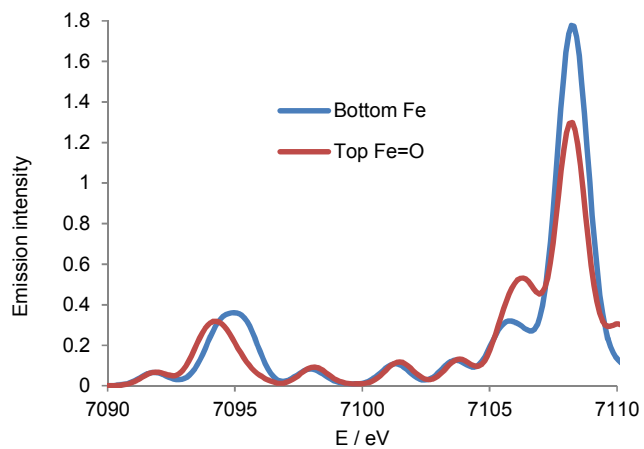
Fig. S16 Separately calculated contributions of two iron atoms to the XAS pre-edge feature of the oxo-complexes of **1-3**.



1



2



3

Fig. S17 XES spectra calculated for two different iron atoms of the oxo-species of **1-3**.

FEFF input file header for the calculation of emission spectra

```
XES -100 0 1.0
FMS 6.5 1
SCF 6.0 1
LDOS -80 0 0.05

HOLE 1 1.0

CONTROL 1 1 1 1 1 1
PRINT 1 0 0 0 0 0

EXCHANGE 0 2.0 0.6
```

POTENTIALS

*	ipot	Z	element
	0	26	Fe
	1	6	C
	2	7	N
	3	1	H
	4	26	Fe

Orca input file header for geometry optimization and calculation of core hole spectra

```
#
! UKS BP86 TZVP def2-TZV/J TightSCF SlowConv SCFConv7 COSMO
! Grid4 NoFinalGrid Normalprint
! PAL16
! OPT
%scf
MaxIter 1500
End
# Finer grid and larger basis for Iron
%method
    SpecialGridAtoms 26
    SpecialGridIntAcc 7.0
end
%basis
    NewGTO 26 "CP(PPP)"
end end
# XAS and XES spectra calculation
%maxcore 1024
%xes CoreOrb 0,0
OrbOp 0,1
DoXAS True
end
```

Optimized geometry of complexes 1, 2 and 3 (xyz files)

115

Coordinates from ORCA-job /home/pavelafanasiev/Bureau/orca28/Fe-CD-XAS-OPT-

f - **complex 1**

C	1.347431	6.433303	-2.277666
C	-0.056889	6.572455	-2.278136
C	0.057147	-6.572894	-2.277019
C	-1.347174	-6.433741	-2.276549
C	6.572738	0.056866	-2.278673
C	-6.433365	1.347025	-2.277684
C	6.433592	-1.347457	-2.278216
C	-6.572508	-0.057298	-2.277858
C	1.950345	5.175684	-2.178426
C	-0.895224	5.457695	-2.179360
C	0.895484	-5.458121	-2.178438
C	-1.950087	-5.176108	-2.177499
C	5.457981	0.895178	-2.179646
C	-5.175750	1.949967	-2.178583
C	5.175995	-1.950386	-2.178775
C	-5.457741	-0.895604	-2.178925
C	1.111067	4.061576	-2.075875
C	-0.291074	4.200563	-2.075737
C	0.291337	-4.200974	-2.074989
C	-1.110810	-4.061982	-2.075124
C	4.200868	0.291016	-2.075839
C	-4.061634	1.110721	-2.075868
C	4.061890	-1.111129	-2.076021
C	-4.200619	-0.291420	-2.075441
C	1.384318	2.634118	-1.975688
C	-0.839553	2.854807	-1.976050
C	0.839813	-2.855183	-1.975561
C	-1.384062	-2.634492	-1.975174
C	2.855116	0.839490	-1.975972
C	-2.634176	1.384013	-1.975746
C	2.634436	-1.384382	-1.975648
C	-2.854849	-0.839860	-1.975662
N	0.191698	1.928079	-1.923047
N	-0.191442	-1.928430	-1.922699
N	2.613045	2.140879	-1.991097
N	-2.140946	2.612740	-1.991267
N	2.141199	-2.613111	-1.990895
N	-2.612787	-2.141255	-1.990645
N	1.928389	-0.191757	-1.922965
N	-1.928113	0.191413	-1.922902
H	1.971395	7.325644	-2.355476
H	-0.493455	7.569928	-2.356876
H	0.493710	-7.570383	-2.355595
H	-1.971140	-7.326090	-2.354236
H	7.570191	0.493446	-2.357579
H	-7.325708	1.970965	-2.355631
H	7.325921	-1.971415	-2.356215
H	-7.569984	-0.493885	-2.356480
H	3.035332	5.063572	-2.177225
H	-1.981168	5.561146	-2.179501
H	1.981429	-5.561571	-2.178583
H	-3.035074	-5.063996	-2.176314
H	5.561410	1.981124	-2.179774
H	-5.063635	3.034953	-2.177612
H	5.063891	-3.035374	-2.177617
H	-5.561174	-1.981549	-2.178831

Fe	0.000137	-0.000163	-1.669576
C	-4.609709	4.687756	2.268869
C	-5.503898	3.596047	2.269330
C	5.503559	-3.595558	2.273024
C	4.609377	-4.687282	2.272625
C	3.595613	5.503909	2.271771
C	-4.687608	-4.609283	2.271749
C	4.687334	4.609723	2.271761
C	-3.595892	-5.503476	2.272227
C	-3.228316	4.492380	2.174942
C	-5.040303	2.280248	2.176019
C	5.040002	-2.279806	2.178829
C	3.228029	-4.491925	2.177895
C	2.279872	5.040330	2.177528
C	-4.492224	-3.227933	2.177120
C	4.491985	3.228351	2.177374
C	-2.280123	-5.039929	2.178219
C	-2.765892	3.176022	2.077429
C	-3.658736	2.085918	2.078201
C	3.658483	-2.085512	2.080207
C	2.765648	-3.175614	2.079513
C	2.085586	3.658787	2.079257
C	-3.175896	-2.765560	2.078927
C	3.175690	2.765949	2.078936
C	-2.085803	-3.658407	2.079703
C	-1.426087	2.612414	1.981914
C	-2.842021	0.883296	1.982235
C	2.841807	-0.882943	1.983397
C	1.425885	-2.612064	1.983248
C	0.883018	2.842081	1.982503
C	-2.612331	-1.425802	1.982729
C	2.612138	1.426153	1.982982
C	-0.883216	-2.841734	1.983122
N	-1.499578	1.227788	1.931926
N	1.499398	-1.227477	1.932654
N	-0.334850	3.361674	1.996531
N	-3.361610	-0.334566	1.996911
N	3.361401	0.334923	1.997758
N	0.334645	-3.361321	1.997661
N	1.227543	1.499645	1.932252
N	-1.227733	-1.499321	1.932384
H	-5.006891	5.701930	2.342545
H	-6.576396	3.785747	2.342913
H	6.576022	-3.785212	2.347264
H	5.006511	-5.701421	2.347037
H	3.785260	6.576391	2.345746
H	-5.701761	-5.006411	2.346010
H	5.701465	5.006875	2.346207
H	-3.785567	-6.575941	2.346379
H	-2.533865	5.333626	2.173961
H	-5.728107	1.433679	2.174986
H	5.727814	-1.433240	2.177755
H	2.533567	-5.333166	2.177007
H	1.433305	5.728136	2.176131
H	-5.333451	-2.533457	2.176159
H	5.333218	2.533880	2.176785
H	-1.433558	-5.727744	2.177176
C	0.000139	-0.000039	0.005086
Fe	-0.000058	0.000124	1.679660

Complex 2

C	1.425301	6.414397	-2.373776
C	0.022716	6.570737	-2.374691
C	-0.022515	-6.571741	-2.368821
C	-1.425105	-6.415452	-2.368135
C	6.571258	-0.023023	-2.371910
C	-6.414781	1.424582	-2.373326
C	6.414977	-1.425615	-2.370671
C	-6.571096	0.021993	-2.373164
C	2.013108	5.150420	-2.265172
C	-0.829347	5.467201	-2.266871
C	0.829493	-5.468089	-2.261828
C	-2.012976	-5.151414	-2.260587
C	5.467643	0.829009	-2.264704
C	-5.150802	2.012498	-2.265347
C	5.150990	-2.013454	-2.262347
C	-5.467527	-0.829963	-2.264872
C	1.160228	4.047591	-2.153099
C	-0.240506	4.203674	-2.153281
C	0.240595	-4.204491	-2.149300
C	-1.160142	-4.048464	-2.149326
C	4.204102	0.240139	-2.151410
C	-4.047934	1.159723	-2.152784
C	4.048076	-1.160599	-2.150892
C	-4.203993	-0.241013	-2.151916
C	1.415745	2.617289	-2.042898
C	-0.804731	2.864827	-2.043580
C	0.804799	-2.865546	-2.040671
C	-1.415705	-2.618084	-2.040335
C	2.865189	0.804357	-2.042355
C	-2.617634	1.415362	-2.042921
C	2.617749	-1.416133	-2.041140
C	-2.865127	-0.805139	-2.041954
N	0.215069	1.929883	-1.979951
N	-0.215051	-1.930570	-1.977858
N	2.639495	2.109777	-2.059247
N	-2.110151	2.639105	-2.060039
N	2.110219	-2.639874	-2.057241
N	-2.639446	-2.110576	-2.057406
N	1.930270	-0.215458	-1.978796
N	-1.930184	0.214725	-1.979196
H	2.059925	7.298434	-2.459319
H	-0.401548	7.572802	-2.461440
H	0.401766	-7.573870	-2.454735
H	-2.059706	-7.299570	-2.453020
H	7.573345	0.401239	-2.458413
H	-7.298838	2.059130	-2.459232
H	7.299054	-2.060248	-2.455744
H	-7.573177	-0.402334	-2.459432
H	3.096676	5.025401	-2.264690
H	-1.913916	5.584289	-2.268445
H	1.914072	-5.585095	-2.263249
H	-3.096546	-5.026430	-2.260259
H	5.584635	1.913589	-2.266523
H	-5.025800	3.096068	-2.265688
H	5.026046	-3.097030	-2.261612
H	-5.584552	-1.914542	-2.265617
Fe	-0.000096	-0.000262	-1.647758
C	-4.665210	4.630639	2.365692

C	-5.546042	3.528019	2.365142
C	5.545861	-3.527195	2.365646
C	4.665000	-4.629791	2.365800
C	3.527760	5.546647	2.362489
C	-4.630504	-4.664969	2.360708
C	4.630373	4.665814	2.362719
C	-3.527887	-5.545800	2.360396
C	-3.281949	4.452799	2.263931
C	-5.067197	2.218332	2.263107
C	5.067082	-2.217474	2.263692
C	3.281772	-4.451902	2.263700
C	2.218008	5.067777	2.261364
C	-4.452595	-3.281663	2.259648
C	4.452478	3.282519	2.261523
C	-2.218139	-5.066909	2.259326
C	-2.804126	3.142651	2.157085
C	-3.683860	2.041457	2.157129
C	3.683781	-2.040557	2.157320
C	2.804006	-3.141723	2.156993
C	2.041079	3.684412	2.155875
C	-3.142387	-2.803800	2.153761
C	3.142274	2.804667	2.155535
C	-2.041202	-3.683532	2.154000
C	-1.457980	2.595075	2.052067
C	-2.852509	0.849374	2.051639
C	2.852479	-0.848440	2.051860
C	1.457907	-2.594104	2.051686
C	0.848947	2.853017	2.051340
C	-2.594728	-1.457586	2.049970
C	2.594628	1.458493	2.051279
C	-0.849034	-2.852116	2.049908
N	-1.517495	1.212693	1.991799
N	1.517468	-1.211706	1.991626
N	-0.375551	3.358878	2.067196
N	-3.358434	-0.375104	2.066263
N	3.358394	0.376040	2.067020
N	0.375472	-3.357912	2.066274
N	1.212227	1.518006	1.991439
N	-1.212325	-1.517089	1.990300
H	-5.074395	5.639423	2.446842
H	-6.620295	3.704424	2.445377
H	6.620089	-3.703630	2.446143
H	5.074148	-5.638597	2.446888
H	3.704212	6.620928	2.442254
H	-5.639341	-5.074168	2.441141
H	5.639207	5.075020	2.443159
H	-3.704331	-6.620086	2.440097
H	-2.597950	5.302585	2.264582
H	-5.745041	1.363776	2.262281
H	5.744964	-1.362947	2.263076
H	2.597732	-5.301655	2.264117
H	1.363456	5.745629	2.260767
H	-5.302354	-2.597629	2.260246
H	5.302253	2.598508	2.261988
H	-1.363590	-5.744758	2.258694
N	-0.000167	0.000574	0.006468
Fe	-0.000056	0.000503	1.660613

Coordinates from ORCA-job- **Complex 3**

/home/pavelafanasiev/Desktop/orca28/Fe-OD-XAS-OPT-n

C	1.527504	6.395445	-2.483851
C	0.127402	6.574024	-2.484318
C	-0.127572	-6.574761	-2.476905
C	-1.527670	-6.396179	-2.476083
C	6.574866	-0.127929	-2.474953
C	-6.396425	1.527287	-2.472732
C	6.396279	-1.528020	-2.473566
C	-6.575015	0.127196	-2.472448
C	2.095284	5.121821	-2.383273
C	-0.742216	5.483639	-2.384006
C	0.742090	-5.484272	-2.378130
C	-2.095406	-5.122445	-2.376674
C	5.484302	0.741809	-2.377420
C	-5.122566	2.095108	-2.375128
C	5.122462	-2.095733	-2.374797
C	-5.484414	-0.742432	-2.374368
C	1.225274	4.031525	-2.279852
C	-0.173849	4.209865	-2.279672
C	0.173769	-4.210383	-2.274973
C	-1.225353	-4.032040	-2.274795
C	4.210369	0.173489	-2.274869
C	-4.032097	1.225066	-2.273895
C	4.032032	-1.225579	-2.274109
C	-4.210437	-0.174000	-2.272992
C	1.457930	2.596726	-2.177063
C	-0.759294	2.879496	-2.176930
C	0.759261	-2.879898	-2.173935
C	-1.457966	-2.597129	-2.173485
C	2.879766	0.759103	-2.175268
C	-2.597010	1.457786	-2.174498
C	2.596984	-1.458184	-2.173855
C	-2.879798	-0.759501	-2.173274
N	0.246300	1.931365	-2.112864
N	-0.246311	-1.931696	-2.110510
N	2.674336	2.069052	-2.194689
N	-2.069287	2.674131	-2.194126
N	2.069247	-2.674550	-2.191916
N	-2.674377	-2.069469	-2.191264
N	1.931645	-0.246479	-2.112028
N	-1.931641	0.246152	-2.111595
H	2.175960	7.269939	-2.563182
H	-0.280745	7.583272	-2.564605
H	0.280541	-7.584099	-2.556247
H	-2.176160	-7.270757	-2.554189
H	7.584263	0.280145	-2.553760
H	-7.271086	2.175736	-2.550277
H	7.270911	-2.176555	-2.550727
H	-7.584445	-0.280965	-2.550375
H	3.176823	4.980297	-2.382407
H	-1.824756	5.618334	-2.384686
H	1.824629	-5.618968	-2.379081
H	-3.176942	-4.980912	-2.375515
H	5.618956	1.824350	-2.378815
H	-4.980990	3.176637	-2.374849
H	4.980889	-3.177261	-2.373221
H	-5.619068	-1.824974	-2.374471
Fe	0.000062	0.000013	-1.768551
C	-4.743180	4.556674	2.470649
C	-5.606070	3.439761	2.470547

C	5.606097	-3.439253	2.471038
C	4.743215	-4.556173	2.470552
C	3.439583	5.606391	2.470934
C	-4.556404	-4.742989	2.468736
C	4.556488	4.743486	2.471016
C	-3.439498	-5.605890	2.468616
C	-3.356768	4.401176	2.376547
C	-5.105723	2.137654	2.376584
C	5.105770	-2.137124	2.377278
C	3.356833	-4.400658	2.376035
C	2.137462	5.106064	2.377015
C	-4.400872	-3.356559	2.374990
C	4.400959	3.357078	2.376928
C	-2.137367	-5.105538	2.374998
C	-2.856718	3.098525	2.279016
C	-3.719105	1.982432	2.279346
C	3.719182	-1.981886	2.279641
C	2.856806	-3.097984	2.278701
C	1.982210	3.719447	2.279787
C	-3.098197	-2.856506	2.277790
C	3.098296	2.857053	2.279423
C	-1.982110	-3.718899	2.278118
C	-1.501307	2.572460	2.182258
C	-2.867904	0.803598	2.182284
C	2.868006	-0.803026	2.182697
C	1.501422	-2.571898	2.181686
C	0.803364	2.868253	2.182772
C	-2.572115	-1.501078	2.181437
C	2.572223	1.501650	2.182655
C	-0.803251	-2.867681	2.181506
N	-1.540915	1.190762	2.121978
N	1.541035	-1.190178	2.121853
N	-0.430317	3.354189	2.199818
N	-3.353837	-0.430086	2.199147
N	3.353938	0.430651	2.200144
N	0.430425	-3.353626	2.198723
N	1.190526	1.541267	2.122414
N	-1.190401	-1.540676	2.121398
H	-5.169254	5.558919	2.545414
H	-6.683383	3.599209	2.544663
H	6.683387	-3.598713	2.545462
H	5.169273	-5.558435	2.545181
H	3.599044	6.683704	2.545040
H	-5.558663	-5.169076	2.543236
H	5.558738	5.169552	2.545758
H	-3.598967	-6.683220	2.542449
H	-2.687086	5.262303	2.376619
H	-5.769870	1.272406	2.375564
H	5.769909	-1.271870	2.376732
H	2.687156	-5.261787	2.375643
H	1.272243	5.770251	2.376049
H	-5.261971	-2.686845	2.375073
H	5.262056	2.687360	2.376986
H	-1.272142	-5.769716	2.373993
O	0.000405	0.001087	0.005023
Fe	0.000102	0.000364	1.780109

116 **Complex 1-O**Coordinates from ORCA-job /home/pavelafanasiev/Desktop/orca28/Fe-CD-O-XAS-
OPT-b

C	1.592378	6.369972	-2.283158
C	0.194148	6.563207	-2.281885
C	-0.193048	-6.563009	-2.280106
C	-1.591280	-6.369775	-2.281573
C	6.563630	-0.193441	-2.280213
C	-6.369262	1.591937	-2.283923
C	6.370378	-1.591669	-2.281767
C	-6.562521	0.193713	-2.282155
C	2.147560	5.091763	-2.176247
C	-0.687082	5.483411	-2.174189
C	0.688165	-5.483182	-2.172641
C	-2.146474	-5.091536	-2.175112
C	5.483811	0.687777	-2.172706
C	-5.091045	2.147132	-2.177189
C	5.092133	-2.146852	-2.175318
C	-5.482743	-0.687500	-2.174138
C	1.265111	4.012448	-2.062817
C	-0.130427	4.205159	-2.061673
C	0.131499	-4.204889	-2.060568
C	-1.264045	-4.012183	-2.061899
C	4.205511	0.131122	-2.060677
C	-4.011747	1.264706	-2.063441
C	4.012798	-1.264411	-2.062052
C	-4.204476	-0.130832	-2.061829
C	1.484712	2.577878	-1.955486
C	-0.730351	2.883617	-1.955109
C	0.731405	-2.883324	-1.954286
C	-1.483675	-2.577577	-1.955096
C	2.883952	0.731032	-1.954342
C	-2.577182	1.484334	-1.956119
C	2.578203	-1.484036	-1.955112
C	-2.882948	-0.730736	-1.954929
N	0.264978	1.919241	-1.898900
N	-0.263932	-1.918929	-1.898568
N	2.693477	2.040240	-1.969533
N	-2.039547	2.693091	-1.970444
N	2.040606	-2.692805	-1.969397
N	-2.692430	-2.039942	-1.969639
N	1.919541	-0.264308	-1.898523
N	-1.918571	0.264600	-1.899083
H	2.249516	7.237194	-2.369030
H	-0.203242	7.576206	-2.367221
H	0.204357	-7.576031	-2.365092
H	-2.248410	-7.237022	-2.367256
H	7.576658	0.203954	-2.365164
H	-7.236468	2.249065	-2.370041
H	7.237620	-2.248801	-2.367488
H	-7.575526	-0.203691	-2.367347
H	3.227282	4.938358	-2.178434
H	-1.767988	5.629134	-2.175228
H	1.769070	-5.628914	-2.173548
H	-3.226195	-4.938135	-2.177453
H	5.629544	1.768680	-2.173541
H	-4.937629	3.226850	-2.179758
H	4.938708	-3.226569	-2.177704
H	-5.628482	-1.768405	-2.174793
Fe	0.000466	0.000176	-1.573642
C	-4.799783	4.524959	2.204428

C	-5.652020	3.400894	2.205825
C	5.650960	-3.401087	2.205531
C	4.798740	-4.525175	2.204306
C	3.400448	5.651386	2.204715
C	-4.525594	-4.799414	2.204221
C	4.524532	4.799173	2.203448
C	-3.401524	-5.651667	2.205345
C	-3.409913	4.380604	2.140365
C	-5.138025	2.101646	2.142743
C	5.136922	-2.101881	2.142254
C	3.408862	-4.380881	2.140221
C	2.101220	5.137336	2.141809
C	-4.381253	-3.409545	2.140303
C	4.380218	3.409281	2.139702
C	-2.102307	-5.137664	2.142086
C	-2.895877	3.081990	2.079339
C	-3.748883	1.956847	2.080684
C	3.747757	-1.957144	2.080196
C	2.894783	-3.082301	2.078974
C	1.956460	3.748172	2.080059
C	-3.082650	-2.895491	2.079101
C	3.081629	2.895185	2.078814
C	-1.957518	-3.748506	2.080148
C	-1.531152	2.568140	2.022517
C	-2.886127	0.781265	2.023102
C	2.885022	-0.781601	2.022509
C	1.530039	-2.568480	2.022231
C	0.780893	2.885424	2.022725
C	-2.568810	-1.530760	2.022527
C	2.567794	1.530431	2.022375
C	-0.781938	-2.885786	2.022607
N	-1.568943	1.189720	1.978954
N	1.567744	-1.190097	1.978445
N	-0.461193	3.353617	2.039894
N	-3.354320	-0.460833	2.040349
N	3.353271	0.460463	2.039815
N	0.460116	-3.354030	2.039881
N	1.189406	1.568187	1.978924
N	-1.190392	-1.568538	1.978727
H	-5.235818	5.524452	2.254124
H	-6.731998	3.551177	2.255961
H	6.730939	-3.551342	2.255703
H	5.234799	-5.524651	2.254147
H	3.550710	6.731377	2.254616
H	-5.525082	-5.235448	2.254019
H	5.524018	5.235241	2.252990
H	-3.551809	-6.731646	2.255416
H	-2.748404	5.247954	2.137969
H	-5.794461	1.230577	2.141819
H	5.793308	-1.230774	2.141213
H	2.747394	-5.248262	2.137962
H	1.230116	5.793723	2.140836
H	-5.248616	-2.748052	2.138114
H	5.247603	2.747818	2.137418
H	-1.231214	-5.794066	2.140958
C	-0.000357	0.000488	0.016220
Fe	-0.000454	-0.000164	2.071173
O	-0.000349	-0.000319	3.752265

116 **Complex 2-O**

Coordinates from ORCA-job /home/pavelafanasiev/Bureau/orca/Fe-ND-O-XAS-OPT-a

H	0.541728	-7.546604	-2.357569
H	-1.923413	-7.317352	-2.359632
C	0.100166	-6.552031	-2.273628
H	4.995918	-5.742863	2.282790
C	-1.306170	-6.421263	-2.274985
H	-3.844847	-6.569324	2.270025
H	2.018782	-5.532550	-2.166782
H	2.524928	-5.364298	2.113192
C	0.932603	-5.435214	-2.167204
H	-1.486632	-5.738949	2.106150
C	4.603275	-4.726607	2.213586
C	-3.647264	-5.497868	2.202140
C	-1.918283	-5.170083	-2.169620
C	3.221739	-4.524952	2.119304
C	-2.326986	-5.043478	2.111250
H	-3.003663	-5.065078	-2.170752
H	6.572639	-3.832904	2.294644
H	-5.748464	-4.984757	2.278911
C	0.318720	-4.182535	-2.057850
C	5.500878	-3.639311	2.220476
C	-4.730981	-4.595818	2.207021
C	-1.083917	-4.052074	-2.059701
H	5.084213	-3.006039	-2.112058
C	2.763110	-3.207673	2.031886
C	-2.120260	-3.663887	2.025170
O	-0.000372	-0.000137	3.565206
N	0.315782	-3.374357	1.959811
H	7.337829	-1.926427	-2.288264
C	0.861200	-2.839354	-1.948037
N	2.160668	-2.597744	-1.939948
C	5.041726	-2.320426	2.133168
C	1.420642	-2.636708	1.941190
C	-0.906389	-2.854279	1.937580
C	5.188940	-1.920595	-2.109225
C	-4.524148	-3.214550	2.120991
C	3.661969	-2.118720	2.039291
C	-1.369873	-2.631923	-1.950060
C	-3.205449	-2.760584	2.030256
C	6.441663	-1.308600	-2.208649
H	5.733768	-1.477240	2.136851
N	-0.177942	-1.915461	-1.902681
H	-5.360584	-2.514247	2.124301
N	-2.602458	-2.155294	-1.941829
C	2.647655	-1.369004	-1.905450
C	4.071290	-1.086584	-2.002669
N	1.520719	-1.264754	1.879310
N	-1.259465	-1.524245	1.876025
H	-5.551251	-2.017342	-2.110188
C	2.848275	-0.907438	1.949942
C	-2.630378	-1.419387	1.944675
C	6.572463	0.096814	-2.208638
H	7.567235	0.538697	-2.288602
N	1.934121	-0.180199	-1.850205
C	-2.854277	-0.857616	-1.905621
C	4.201903	0.315957	-2.001573
C	-5.453660	-0.931143	-2.107677
N	3.366435	0.315457	1.973638
Fe	0.000290	-0.000577	-1.544039

N	0.000303	0.000921	0.063277
Fe	0.000081	0.000928	1.834321
N	-3.366413	-0.313961	1.971514
C	5.454120	0.929491	-2.109394
C	-4.201370	-0.317610	-2.000728
C	2.854799	0.855989	-1.906451
N	-1.933545	0.178500	-1.850183
H	-7.566854	-0.540358	-2.286032
C	-6.572021	-0.098479	-2.206825
C	2.630394	1.420885	1.946899
H	5.551628	2.015701	-2.112653
C	-2.848191	0.908922	1.949127
N	1.259499	1.525811	1.877930
N	-1.520606	1.266357	1.879775
C	-4.070703	1.084937	-2.002630
C	-2.647027	1.367365	-1.905973
N	2.603083	2.153654	-1.943346
N	0.178673	1.913940	-1.904195
H	5.360598	2.515665	2.127029
H	-5.733772	1.478493	2.134142
C	-6.441162	1.306927	-2.207708
C	1.370519	2.630410	-1.951916
C	3.205476	2.762078	2.032548
C	-3.661941	2.120133	2.038948
C	-5.188369	1.918918	-2.109184
C	4.524177	3.215984	2.123509
C	0.906457	2.855857	1.939196
C	-1.420584	2.638251	1.942540
N	-2.159988	2.596038	-1.941519
C	-5.041792	2.321730	2.131506
C	-0.860551	2.837696	-1.950035
H	-7.337347	1.924748	-2.287223
N	-0.315731	3.375914	1.961429
C	2.120317	3.665420	2.027201
C	-2.763118	3.209130	2.032701
H	-5.083615	3.004362	-2.112685
C	1.084531	4.050461	-2.062394
C	4.731075	4.597256	2.209240
C	-0.318122	4.180848	-2.060849
C	-5.501079	3.640553	2.219045
H	5.748575	4.986150	2.281262
H	-6.572923	3.834078	2.292269
H	3.004225	5.063598	-2.173674
C	2.327116	5.045013	2.112972
C	1.918834	5.168478	-2.172687
C	-3.221865	4.526338	2.120452
C	3.647403	5.499361	2.203957
C	-4.603501	4.727876	2.213529
C	-0.932060	5.433425	-2.170867
H	1.486830	5.740575	2.107591
H	-2.525088	5.365721	2.115290
H	-2.018244	5.530689	-2.170649
H	3.845013	6.570835	2.271577
C	1.306660	6.419584	-2.278660
H	-4.996244	5.744090	2.282946
C	-0.099678	6.550271	-2.277574
H	1.923870	7.315684	-2.363513
H	-0.541286	7.544786	-2.362066

116 **Complex 3-O**

Coordinates from ORCA-job /home/pavelafanasiev/Desktop/orca28/Fe-OD-XAS-
OPT-OXO-b

C	1.519227	6.389712	-2.261295
C	0.118390	6.566855	-2.259480
C	-0.118448	-6.567623	-2.255817
C	-1.519287	-6.390485	-2.257800
C	6.567207	-0.118821	-2.257296
C	-6.390168	1.518876	-2.259411
C	6.390068	-1.519660	-2.258724
C	-6.567314	0.118038	-2.257117
C	2.089317	5.117381	-2.169016
C	-0.750612	5.476440	-2.165820
C	0.750544	-5.477162	-2.162671
C	-2.089385	-5.118109	-2.166207
C	5.476758	0.750201	-2.164250
C	-5.117798	2.088986	-2.167812
C	5.117712	-2.089724	-2.166658
C	-5.476864	-0.750936	-2.163651
C	1.219033	4.026373	-2.070844
C	-0.179268	4.203107	-2.068802
C	0.179193	-4.203779	-2.066339
C	-1.219108	-4.027046	-2.068546
C	4.203399	0.178884	-2.067444
C	-4.026752	1.218729	-2.069829
C	4.026670	-1.219416	-2.069097
C	-4.203491	-0.179569	-2.067314
C	1.455620	2.594544	-1.979139
C	-0.764359	2.874937	-1.977452
C	0.764282	-2.875568	-1.975658
C	-1.455706	-2.595174	-1.977587
C	2.875202	0.764003	-1.976702
C	-2.594891	1.455344	-1.978754
C	2.594816	-1.455982	-1.977776
C	-2.875292	-0.764640	-1.976318
N	0.242178	1.919881	-1.934318
N	-0.242259	-1.920478	-1.933048
N	2.670097	2.070959	-1.990750
N	-2.071320	2.669817	-1.990939
N	2.071242	-2.670462	-1.989264
N	-2.670185	-2.071606	-1.989553
N	1.920133	-0.242528	-1.933523
N	-1.920212	0.241905	-1.933825
H	2.166080	7.265609	-2.335928
H	-0.290188	7.576261	-2.333171
H	0.290136	-7.577071	-2.328947
H	-2.166133	-7.266418	-2.332038
H	7.576633	0.289740	-2.330803
H	-7.266093	2.165711	-2.333874
H	7.265990	-2.166535	-2.332881
H	-7.576751	-0.290559	-2.330273
H	3.170714	4.976753	-2.171289
H	-1.833023	5.609939	-2.165814
H	1.832956	-5.610656	-2.162533
H	-3.170781	-4.977484	-2.168614
H	5.610245	1.832614	-2.164545
H	-4.977163	3.170380	-2.170449
H	4.977082	-3.171120	-2.168629
H	-5.610360	-1.833347	-2.163274
Fe	-0.000046	-0.000214	-1.619672
C	-4.754956	4.574569	2.201776

C	-5.618515	3.459464	2.202600
C	5.618596	-3.458752	2.202739
C	4.755042	-4.573859	2.202120
C	3.459073	5.618944	2.201639
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C	4.415071	3.366792	2.139703
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C	1.995238	3.729837	2.082295
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C	-1.995155	-3.729156	2.083193
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