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Table S1. Triple Zeta Basis Sets and the Expansion Coefficients Used in DFT Calculations with a Frozen Core Approximation and with Core Orbitals Unfrozen

Iron		Carbon		Nitrogen		Oxygen		Hydrogen	
2p frozen		1s frozen		1s frozen		1s frozen			
1S	19.55	1S	5.40	1S	6.38	1S	7.36	1S	0.69
2S	9.45	2S	1.28	2S	1.50	2S	1.72	1S	0.92
2P	10.90	2S	2.10	2S	2.50	2S	2.88	1S	1.58
3S	3.50	2S	4.60	2S	5.15	2S	7.58	2P	1.25
3S	5.45	2P	0.82	2P	1.00	2P	1.12		
3P	3.15	2P	1.48	2P	1.88	2P	2.08		
3P	5.15	2P	2.94	2P	3.68	2P	4.08		
3D	1.40	3D	2.00	3D	2.00	3D	2.00		
3D	3.05								
3D	6.40								
4S	0.90								
4S	1.40								
4S	2.30								
4P	1.39								
unfrozen		unfrozen		unfrozen		unfrozen			
1S	23.90	1S	5.00	1S	5.90	1S	6.80	1S	0.69
1S	30.45	1S	7.68	1S	8.74	1S	9.80	1S	0.92
2S	6.35	2S	1.28	2S	1.50	2S	1.72	1S	1.58
2S	10.05	2S	2.10	2S	2.50	2S	2.88	2S	1.25
2P	9.20	2S	4.60	2S	5.15	2S	7.58		
2P	14.60	2P	0.82	2P	1.00	2P	1.12		
3S	3.50	2P	1.48	2P	1.88	2P	2.08		
3S	5.45	2P	2.94	2P	3.68	2P	4.08		
3P	3.15	3D	2.00	3D	2.00	3D	2.00		
3P	5.15								
3D	1.40								
3D	3.05								
3D	6.40								
4S	0.90								
4S	1.40								
4S	2.30								
4P	1.39								

Table S2-a. Composition of The Molecular Orbitals for Model Compound I ($^4A_{2u}$ state, α -spin)

MO (α)	energy (EV)	occu.	primary contributors(%)	group population(%)				overlap population(%)		
				Fe	O	Por	Im	Fe-O	Fe-Por	Fe-Im
21a''	-13.172	1.0	Fe dxy(17.7), N(Por) 2px(12.4), N(Por) 2py(12.4), C β 2px(15.0), C β 2py(14.8), H β 1s (18.8),	17.7	0.0	82.3	0.0	0.0	7.7	0.0
36a'	-13.097	1.0	Fe dz ² (29.3), O 2pz(6.5), N(Por) 2px(5.3), N(Por) 2py(9.0), C β 2px(5.5), Im 2pz(19.9),	30.7	7.3	36.0	25.5	1.1	5.4	3.9
37a'	-13.031	1.0	N(Por) 2px(8.9), N(Por) 2py(6.7), C α 2px(8.0), C α 2py(7.0), C β 2px(6.1), C β 2py(6.8), Cm 2px(5.1), Cm 2py(5.5), H β 1s (15.6), Hm 1s (17.9),	3.6	0.2	95.3	0.9	0.0	1.9	0.0
22a''	-12.606	1.0	N(Por) 2py(9.7), C α 2py(19.4), C β 2py(30.6), H β 1s (23.8),	1.2	1.1	97.0	0.7	0.3	0.8	0.1
38a'	-12.596	1.0	N(Por) 2px(9.5), C α 2px(19.7), C β 2px(30.6), H β 1s (23.5),	1.4	1.5	97.0	0.0	0.4	0.8	0.0
23a''	-12.363	1.0	C α 2px(16.4), C α 2py(18.4), C β 2px(13.2), C β 2py(16.0), H β 1s (23.4),	0.0	0.0	99.9	0.0	0.0	0.0	0.0
24a''	-12.235	1.0	Fe dxy(15.0), C α 2px(11.3), C α 2py(9.1), C β 2px(21.2), C β 2py(18.5),	15.1	0.0	84.9	0.0	0.0	4.6	0.0
39a'	-12.003	1.0	Fe dxz(14.6), O 2px(26.0), N(Por) 2px(9.3), C α 2px(10.6), C β 2px(8.5),	19.3	26.2	54.4	0.2	7.3	1.5	-0.1
25a''	-12.003	1.0	Fe dyz(20.9), O 2py(28.2), N(Por) 2py(6.7), C α 2py(7.2), C β 2pz(5.1), C β 2py(5.7),	24.0	28.5	44.5	3.1	7.9	1.1	0.4
40a'	-11.923	1.0	C α 2pz(45.7), Cm 2pz(44.6),	0.2	0.6	98.3	0.8	0.0	0.0	0.0

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26a''	-11.914	1.0	Fe dyz(8.0), N(Por) 2py(8.4), C α 2py(7.8), C β 2py(5.6), Im 2py(43.6),	11.9	0.2	43.3	45.6	0.0	1.6	4.6
41a'	-11.381	1.0	Fe dxz(23.1), O 2px(10.3), N(Por) 2px(13.5), N(Por) 2py(9.3), C α 2px(6.4),	25.7	12.2	60.3	1.4	2.3	5.1	-1.2
42a'	-11.224	1.0	Fe dz2(5.2), O 2pz(55.5), Im 2pz(15.6),	9.2	57.7	12.6	21.0	-1.6	-3.2	2.5
27a''	-10.895	1.0	Fe dyz(7.9), O 2py(8.9), N(Por) 2px(6.0), N(Por) 2py(7.3), C α 2pz(5.5), Cm 2pz(5.7), Im 2py(41.6),	8.2	9.0	38.2	43.8	1.8	1.8	-3.1
43a'	-10.801	1.0	C α 2pz(36.9), C β 2pz(20.2), Cm 2pz(30.7),	1.2	1.6	96.7	0.5	0.2	0.0	0.0
28a''	-10.779	1.0	C α 2pz(34.4), C β 2pz(19.1), Cm 2pz(27.0),	2.3	3.5	90.5	3.9	0.5	0.2	-0.4
29a''	-9.901	1.0	N(Por) 2pz(11.1), C β 2pz(23.7), Im 2py(57.8),	0.1	1.1	37.4	61.6	0.1	-0.1	0.0
44a'	-9.836	1.0	N(Por) 2pz(21.6), C β 2pz(65.6),	0.6	2.7	93.3	3.3	0.1	1.8	-2.2
30a''	-9.653	1.0	N(Por) 2pz(22.9), C β 2pz(37.5), Im 2py(33.4),	0.0	0.5	64.1	35.4	0.0	-0.1	0.0
45a'	-9.556	1.0	O 2px(15.2), N(Por) 2pz(29.7), C β 2pz(46.3),	1.0	15.1	83.7	0.2	1.2	-1.5	0.0
31a''	-9.537	1.0	O 2py(11.8), N(Por) 2pz(30.3), C β 2pz(47.3),	1.3	11.8	84.9	2.0	1.1	-1.6	0.1
46a'	-9.387	1.0	Fe dx2-y2(93.4),	93.4	0.0	6.5	0.0	0.1	-2.8	0.0
47a'	-8.985	1.0	N(Por) 2pz(26.2), C β 2pz(5.6), Cm 2pz(56.5),	0.4	0.9	96.5	1.5	0.0	1.5	-1.8
32a''	-8.709	1.0	C α 2pz(72.8), C β 2pz(21.4),	0.0	0.0	99.8	0.1	0.0	0.0	0.0
48a'	-8.606	1.0	Fe dxz(52.3), O 2px(38.7),	52.8	38.7	7.9	0.6	-9.2	-5.3	0.0
33a''	-8.562	1.0	Fe dyz(51.9), O 2py(38.4),	52.4	38.4	6.2	3.0	-9.2	-4.6	-1.5
49a'	-6.671	0.0	N(Por) 2pz(9.3), C α 2pz(31.3), C β 2pz(25.6), Cm 2pz(25.8),	1.3	0.0	98.6	0.1	0.1	-0.9	0.0
34a''	-6.659	0.0	N(Por) 2pz(9.9), C α 2pz(30.5), C β 2pz(25.1), Cm 2pz(26.4),	1.4	0.0	98.5	0.1	0.1	-1.0	0.0
35a''	-6.412	0.0	Fe dxy(62.5), N(Por) 2s(8.3), N(Por) 2px(9.6), N(Por) 2py(9.6),	62.5	0.0	37.4	0.1	0.0	-26.6	0.0
50a'	-5.664	0.0	Fe dz2(55.0), O 2pz(21.2),	56.3	21.4	13.2	8.2	-7.7	-7.2	-13.2
51a'	-5.187	0.0	C α 2pz(11.6), C β 2pz(51.6), Cm 2pz(29.8),	0.0	0.0	100.0	0.0	0.0	0.0	0.0

Table S2-b. Composition of the molecular orbitals for model compound I ($^4A_{2u}$ state, β -spin)

MO (β)	energy (eV)	occu.	primary contributors(%)	group population(%)				overlap population(%)			
				Fe	O	Por	Im	Fe-O	Fe-Por	Fe-Im	
21a''	-13.066	1.0	Fe dxy(12.4), N(Por) 2px(11.6), N(Por) 2py(11.8), Cβ 2px(17.0), 12.4 Cβ 2py(17.1), Hβ 1s(19.4),								
36a'	-13.002	1.0	N(Por) 2px(6.7), N(Por) 2py(10.3), Cα 2px(6.7), Cα 2py(8.9), Cβ 2px(6.2), Cβ 2py(5.2), Cm 2px(5.7), Cm 2py(6.1), Hβ 1s(13.5), Hm 1s(21.0),	2.5	0.0	97.4	0.0	0.0	1.8	-0.1	
37a'	-12.881	1.0	Fe dz2(24.5), N(Por) 2px(7.2), N(Por) 2py(5.3), Im 2pz(31.8),	26.1	4.8	27.9	40.6	0.7	5.0	5.0	
22a''	-12.595	1.0	N(Por) 2py(8.8), Cα 2py(20.1), Cβ 2py(32.1), Hβ 1s (23.6),	0.8	0.2	98.2	0.8	0.1	0.7	0.1	
38a'	-12.583	1.0	N(Por) 2px(8.5), Cα 2px(20.7), Cβ 2px(32.5), Cm 2px(5.4), Hβ 1s(23.4),	0.7	0.2	98.9	0.1	0.1	0.7	0.0	
23a''	-12.362	1.0	Cα 2px(17.1), Cα 2py(18.1), Cβ 2px(13.9), Cβ 2py(15.2), Hβ 1s(23.1),	0.0	0.0	100.0	0.0	0.0	0.0	0.0	
24a''	-12.116	1.0	Fe dxy(15.8), N(Por) 2px(7.1), N(Por) 2py(7.3), Cα 2px(10.5), Cα 2py(9.3), Cβ 2px(18.2), Cβ 2py(17.0),	15.8	0.0	84.1	0.0	0.0	6.3	0.0	
25a''	-11.873	1.0	Fe 4py(5.2), N(Por) 2px(6.7), N(Por) 2py(14.6), Cα 2py(12.6), Cβ 2px(6.2), Cβ 2py(8.9), Im 2py(30.7),	6.0	0.8	61.8	32.2	0.3	3.0	2.7	
39a'	-11.712	1.0	Fe 4px(6.1), N(Por) 2px(22.1), N(Por) 2py(12.4), Cα 2px(15.1), Cβ 2px(10.2), Cβ 2py(8.0),	7.3	3.7	88.8	0.0	1.4	5.7	-0.4	
40a'	-11.701	1.0	Cα 2pz(47.2), Cm 2pz(38.0),	0.6	0.5	98.1	0.8	0.1	0.3	0.0	

...Cont.

26a''	-11.469	1.0	Fe dyz(8.5), O 2py(5.9), N(Por) 2px(5.2), N(Por) 2py(7.9), C β 2pz(5.0), Im 2py(45.1),	9.9	6.0	37.2	47.2	2.2	2.4	1.0
41a'	-10.763	1.0	Fe dz ² (8.5), O 2pz(61.4), C β 2pz(5.3), Im 2pz(9.2),	10.9	64.3	12.6	12.8	-1.9	-4.3	1.5
42a'	-10.685	1.0	N(Por) 2pz(8.3), C α 2pz(39.7), C β 2pz(7.6), Cm 2pz(31.5),	4.5	2.6	92.1	0.7	0.9	0.6	-0.1
27a''	-10.634	1.0	C α 2pz(44.3), C β 2pz(15.1), Cm 2pz(30.5),	0.3	0.1	98.5	0.8	0.1	0.0	-0.1
43a'	-10.467	1.0	Fe dxz(23.8), O 2px(15.7), N(Por) 2pz(9.3), C β 2pz(38.0),	23.8	16.1	59.0	1.0	4.9	3.7	-0.5
28a''	-10.299	1.0	Fe dyz(18.6), O 2py(14.8), N(Por) 2pz(11.8), C β 2pz(24.8), Im 2py(20.2),	18.6	15.0	44.7	21.6	4.5	3.0	-2.0
29a''	-9.844	1.0	N(Por) 2pz(8.7), C β 2pz(18.0), Im 2py(65.1),	0.7	1.1	28.9	69.3	0.3	0.0	-0.2
44a'	-9.752	1.0	N(Por) 2pz(20.0), C β 2pz(64.0),	0.9	4.6	90.9	3.5	0.1	1.7	-2.4
30a''	-9.577	1.0	N(Por) 2pz(26.9), C β 2pz(43.6), Im 2py(23.7),	0.0	0.0	74.8	25.1	0.0	0.0	0.0
31a''	-9.010	1.0	Fe dyz(18.0), O 2py(24.5), N(Por) 2pz(17.3), C β 2pz(29.8),	18.2	24.6	56.7	0.5	6.7	-6.0	-0.1
45a'	-9.002	1.0	Fe dxz(18.2), O 2px(24.0), N(Por) 2pz(18.0), C α 2pz(5.1), C β 2pz(29.8),	18.3	24.0	57.5	0.2	6.6	-6.0	0.0
32a''	-8.752	1.0	C α 2pz(73.2), C β 2pz(21.2),	0.0	0.0	99.8	0.2	0.0	0.0	0.0
46a'	-8.598	1.0	Fe dx ² -y ² (88.2),	88.3	0.1	11.5	0.1	0.1	-1.8	-0.2
47a'	-8.574	0.0	Fe dx ² -y ² (5.4), N(Por) 2pz(26.1), Cm 2pz(51.9),	5.9	0.9	91.4	1.1	0.0	1.3	-1.7
48a'	-6.883	0.0	Fe dxz(38.1), O 2px(47.0),	39.2	47.0	13.2	0.9	-8.4	-2.7	0.2
33a''	-6.878	0.0	Fe dyz(37.1), O 2py(45.6),	38.3	45.5	12.6	3.8	-8.1	-2.3	-0.5
49a'	-6.428	0.0	Fe dxz(10.5), N(Por) 2pz(10.9), C α 2pz(22.7), C β 2pz(21.5), Cm 2pz(25.9),	10.6	2.0	87.2	0.0	-1.0	-3.4	0.0
34a''	-6.405	0.0	Fe dyz(10.4), N(Por) 2pz(11.5), C α 2pz(22.2), C β 2pz(21.2), Cm 2pz(26.4),	10.5	1.8	87.5	0.1	-1.0	-3.4	0.1

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35a''	-5.706	0.0	Fe dxy(67.6), N(Por) 2s(7.5), N(Por) 2px(7.8), N(Por) 2py(7.8), 67.6	0.0	32.2	0.2	0.0	-27.9	-0.1
50a'	-5.009	0.0	C α 2pz(8.2), C β 2pz(53.9), Cm 2pz(30.3),	0.1	0.1	99.7	0.1	0.0	-0.1
51a'	-4.888	0.0	Fe dz2(57.3), O 2pz(20.1),	59.1	20.4	12.0	7.4	-7.8	-8.4 -13.9

Table S2-c. Composition of The Molecular Orbitals for Model Compound I ($^4A_{1u}$ cation, α spin)

MO (α)	energy (EV)	occu.	primary contributors(%)	group population(%) overlap population(%)						
				Fe	O	Por	Im	Fe-O	Fe-Por	Fe-Im
21a''	-13.135	1.0	Fe dxy(14.2), N(Por) 2px(11.1), N(Por) 2py(11.2), C β 2px(16.7), 14.2, C β 2py(16.9), H β 1s(18.6), Hm 1s(15.9),							
36a'	-12.952	1.0	Fe dz2(7.0), N(Por) 2py(14.4), C α 2py(10.1), Cm 2px(7.3), Cm 2py(7.6), Hm 1s (21.4), Im 2pz(6.2),	9.5	2.0	80.5	7.8	0.3	2.4	1.2
37a'	-12.935	1.0	Fe dz2(23.7), O 2pz(6.6), N(Por) 2px(10.7), C α 2px(5.8), Hm 1s(6.2), Im 2pz(23.7),	25.3	7.4	36.6	30.5	1.1	3.4	4.3
22a''	-12.693	1.0	N(Por) 2py(7.4), C α 2py(21.2), C β 2py(33.7), Cm 2py(6.1), H β 1s(22.6),	0.8	0.6	98.1	0.5	0.2	0.6	0.0
38a'	-12.681	1.0	N(Por) 2px(7.2), C α 2px(21.5), C β 2px(33.6), Cm 2px(6.3), H β 1s(22.3),	0.9	0.8	98.1	0.1	0.2	0.6	0.0
23a''	-12.489	1.0	C α 2px(17.5), C α 2py(18.4), C β 2px(13.8), C β 2py(15.0), H β 1s(22.5),	0.0	0.0	100.0	0.0	0.0	0.0	0.0
24a''	-12.227	1.0	Fe dxy(18.6), N(Por) 2px(6.7), N(Por) 2py(6.9), C α 2px(10.3), C α 2py(9.0), C β 2px(17.6), C β 2py(16.3),	18.6	0.0	81.3	0.0	0.0	6.4	0.0
39a'	-11.904	1.0	Fe dxz(12.2), Fe 4px(5.5), O 2px(24.6), N(Por) 2px(13.2), N(Por) 2py(5.5), C α 2px(10.4), C β 2px(6.7), C β 2py(5.3),	17.9	24.8	57.2	0.0	6.9	2.8	-0.1
25a''	-11.903	1.0	Fe dyz(10.5), Fe 4py(5.9), O 2py(23.2), N(Por) 2px(5.9), N(Por) 2py(14.6), C α 2py(11.1), C β 2px(5.7), C β 2py(7.0),	16.6	23.4	59.7	0.3	6.5	3.0	0.0

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40a'	-11.842	1.0	C α 2pz(51.0), C μ 2pz(38.6),	0.2	0.5	98.4	0.8	0.0	0.0	0.0
26a''	-11.810	1.0	Fe dyz(17.9), O 2py(5.5), C β 2pz(6.4), Im 2py(47.4),	19.5	5.5	26.4	49.6	1.5	1.2	5.0
41a'	-11.240	1.0	Fe dxz(26.0), O 2px(13.7), N(Por) 2px(12.3), N(Por) 2py(8.8), C α 2px(5.0), C β 2pz(6.1),	28.1	15.1	55.1	1.3	3.1	5.2	-1.3
42a'	-11.038	1.0	Fe dz2(5.4), O 2pz(55.7), Im 2pz(14.9),	9.3	57.9	13.3	20.0	-1.7	-3.2	2.5
43a'	-10.804	1.0	C α 2pz(43.1), C β 2pz(21.3), C μ 2pz(27.1),	0.4	0.6	98.4	0.6	0.0	0.1	0.0
27a''	-10.794	1.0	C α 2pz(43.1), C β 2pz(15.2), C μ 2pz(26.8),	0.6	0.5	94.0	4.4	0.1	0.1	-0.3
28a''	-10.739	1.0	Fe dyz(9.7), O 2py(12.4), N(Por) 2px(6.0), N(Por) 2py(7.4), C β 2pz(6.2), Im 2py(40.8),	10.0	12.4	34.5	43.1	2.3	2.0	-3.3
44a'	-9.871	1.0	N(Por) 2pz(19.1), C β 2pz(64.7),	0.5	3.7	91.8	4.0	0.1	1.5	-2.0
29a''	-9.859	1.0	N(Por) 2pz(18.7), C β 2pz(34.5), Im 2py(39.8),	0.1	0.8	56.7	42.5	0.1	-0.1	0.0
30a''	-9.604	1.0	N(Por) 2pz(16.7), C β 2pz(25.1), Im 2py(50.7),	0.0	1.0	45.3	53.7	0.1	-0.1	0.0
45a'	-9.517	1.0	O 2px(15.0), N(Por) 2pz(29.0), C β 2pz(43.9),	1.9	15.0	83.0	0.2	1.6	-2.0	0.0
31a''	-9.505	1.0	O 2py(11.6), N(Por) 2pz(29.3), C β 2pz(45.1),	2.1	11.6	83.9	2.5	1.4	-2.0	0.2
46a'	-9.067	1.0	Fe dx2-y2(93.7),	93.7	0.0	6.2	0.1	0.1	-2.4	0.0
32a''	-9.013	1.0	C α 2pz(73.6), C β 2pz(20.8),	0.0	0.0	99.7	0.3	0.0	0.0	0.0
47a'	-8.586	1.0	N(Por) 2pz(29.7), C μ 2pz(54.1),	0.5	0.8	96.3	1.5	0.0	1.8	-2.0
48a'	-8.392	1.0	Fe dxz(52.4), O 2px(39.5),	52.9	39.5	7.0	0.6	-9.4	-4.7	0.0
33a''	-8.357	1.0	Fe dyz(52.0), O 2py(39.0),	52.5	39.0	5.5	3.1	-9.3	-4.0	-1.5
49a'	-6.625	0.0	N(Por) 2pz(12.6), C α 2pz(25.4), C β 2pz(23.5), C μ 2pz(29.8),	1.9	0.0	98.0	0.1	0.1	-1.3	0.0
34a''	-6.602	0.0	N(Por) 2pz(13.3), C α 2pz(24.6), C β 2pz(23.0), C μ 2pz(30.4),	1.9	0.0	98.0	0.1	0.1	-1.3	0.0
35a''	-6.157	0.0	Fe dxy(63.4), N(Por) 2s(8.5), N(Por) 2px(9.1), N(Por) 2py(9.1),	63.4	0.0	36.5	0.1	0.0	-26.8	0.0
50a'	-5.444	0.0	Fe dz2(55.1), O 2pz(20.9),	56.6	21.2	13.1	8.2	-7.8	-7.0	-13.5
51a'	-5.158	0.0	C α 2pz(7.4), C β 2pz(53.8), C μ 2pz(31.3),	0.0	0.0	99.9	0.1	0.0	0.0	0.0

Table S2-d. Composition of the molecular orbitals for model compound I ($^4A_{1u}$, β -spin)

MO (β)	energy (eV)	occu.	primary contributors(%)	group population(%)				overlap population(%)		
				Fe	O	Por	Im	Fe-O	Fe-Por	Fe-Im
21a''	-13.067	1.0	Fe dxy(10.0), N(Por) 2px(10.4), N(Por) 2py(10.6), C β 2px(18.2), 10.0 C β 2py(18.5), H β 1s(19.0),	10.0	0.0	90.0	0.0	0.0	5.6	0.0
36a'	-12.933	1.0	N(Por) 2px(8.0), N(Por) 2py(10.7), C α 2px(7.2), C α 2py(8.9), Cm 2px(8.7), Cm 2py(9.4), H β 1s(7.0), Hm 1s(26.6),	2.3	0.0	97.6	0.0	0.0	1.6	-0.1
37a'	-12.754	1.0	Fe dz2(24.2), N(Por) 2px(5.6), Im 2pz(37.0),	25.8	5.2	21.1	47.3	0.7	4.2	5.6
22a''	-12.662	1.0	N(Por) 2py(7.4), C α 2py(21.3), C β 2py(33.5), Cm 2py(6.1), H β 1s(22.9),	0.6	0.2	98.7	0.5	0.0	0.6	0.0
38a'	-12.648	1.0	N(Por) 2px(7.2), C α 2px(21.6), C β 2px(33.5), Cm 2px(6.4), H β 1s(22.4),	0.7	0.2	98.6	0.4	0.1	0.6	0.0
23a''	-12.447	1.0	C α 2px(17.6), C α 2py(18.2), C β 2px(14.0), C β 2py(14.8), H β 1s(22.5),	0.0	0.0	100.0	0.0	0.0	0.0	0.0
24a''	-12.088	1.0	Fe dxy(18.0), N(Por) 2px(9.1), N(Por) 2py(9.3), C α 2px(9.7), C α 2py(8.8), C β 2px(15.8), C β 2py(15.0),	18.0	0.0	81.9	0.0	0.0	7.7	0.0
25a''	-11.809	1.0	Fe 4py(5.7), N(Por) 2px(8.2), N(Por) 2py(17.4), C α 2py(12.4), C β 2px(6.3), C β 2py(7.8), Im 2py(26.7),	6.3	1.0	65.3	28.0	0.3	3.8	2.4
39a'	-11.668	1.0	C α 2pz(45.9), Cm 2pz(40.0),	0.5	0.4	98.2	0.8	0.1	0.3	0.0
40a'	-11.656	1.0	Fe 4px(6.3), N(Por) 2px(23.9), N(Por) 2py(13.6), C α 2px(14.2), C β 2px(8.9), C β 2py(7.7),	7.4	3.6	88.7	0.1	1.3	6.1	-0.5

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26a''	-11.371	1.0	Fe dyz(8.5), O 2py(5.4), N(Por) 2py(7.0), C β 2pz(6.0), Im 2py(48.7),	9.6	5.5	34.3	51.0	2.0	2.3	1.3
41a'	-10.654	1.0	N(Por) 2pz(6.1), C α 2pz(40.2), C β 2pz(11.2), Cm 2pz(34.0),	1.9	1.0	96.4	0.6	0.4	0.3	0.0
42a'	-10.617	1.0	Fe dz ² (8.4), O 2pz(58.3), N(Por) 2pz(5.1), C β 2pz(8.6), Im 2pz(8.0),	10.9	61.2	17.3	11.2	-1.8	-4.2	1.3
27a''	-10.617	1.0	C α 2pz(42.0), C β 2pz(17.9), Cm 2pz(31.9),	0.1	0.0	99.3	0.4	0.0	0.0	0.0
43a'	-10.422	1.0	Fe dxz(22.4), O 2px(14.3), N(Por) 2pz(14.6), C β 2pz(38.9),	22.5	15.1	61.2	1.1	4.5	4.2	-0.5
28a''	-10.239	1.0	Fe dyz(15.5), O 2py(12.1), N(Por) 2pz(15.4), C β 2pz(26.3), Im 2py(20.9),	15.6	12.3	49.7	22.2	3.7	3.1	-1.9
29a''	-9.814	1.0	N(Por) 2pz(19.2), C β 2pz(35.4), Im 2py(38.4),	0.4	0.6	58.0	41.0	0.2	0.1	-0.1
44a'	-9.799	1.0	O 2pz(7.5), N(Por) 2pz(17.8), C β 2pz(61.3),	1.1	7.4	86.8	4.7	0.1	1.3	-2.1
30a''	-9.577	1.0	N(Por) 2pz(17.4), C β 2pz(25.5), Im 2py(50.9),	0.0	0.1	45.9	53.9	0.0	-0.1	0.0
31a''	-8.946	1.0	Fe dyz(21.8), O 2py(27.9), N(Por) 2pz(14.6), C α 2pz(5.5), C β 2pz(24.4),	22.0	28.1	49.1	0.9	7.7	-6.2	-0.2
45a'	-8.937	1.0	Fe dxz(21.9), O 2px(27.3), N(Por) 2pz(15.5), C α 2pz(5.6), C β 2pz(24.7),	22.0	27.4	50.4	0.2	7.6	-6.2	-0.1
32a''	-8.669	0.0	C α 2pz(71.7), C β 2pz(22.5),	0.0	0.0	99.8	0.2	0.0	0.0	0.0
46a'	-8.623	1.0	N(Por) 2pz(28.3), Cm 2pz(55.3),	0.5	1.2	96.0	1.4	0.1	1.5	-1.8
47a'	-8.425	1.0	Fe dx ² -y ² (93.7),	93.7	0.0	6.2	0.1	0.1	-1.8	0.0
33a''	-6.731	0.0	Fe dyz(29.9), O 2py(41.7), C α 2pz(8.0), C β 2pz(6.1), Cm 2pz(5.6),	30.9	41.7	24.2	3.5	-6.8	-1.2	-0.5
48a'	-6.729	0.0	Fe dxz(29.9), O 2px(42.0), C α 2pz(9.0), C β 2pz(7.0), Cm 2pz(6.0),	30.9	41.9	26.7	0.9	-6.9	-1.2	0.2

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49a'	-6.407	0.0	Fe dxz(19.0), O 2px(6.8), N(Por) 2pz(9.1), C α 2pz(18.4), C β 2pz(19.1), Cm 2pz(21.7),	19.3	6.8	73.6	0.1	-2.5	-4.7	0.1
34a''	-6.390	0.0	Fe dyz(17.5), O 2py(5.8), N(Por) 2pz(9.7), C α 2pz(18.6), C β 2pz(19.4), Cm 2pz(22.7),	17.7	5.8	75.8	0.5	-2.3	-4.3	0.0
35a''	-5.525	0.0	Fe dxy(68.3), N(Por) 2s(7.5), N(Por) 2px(7.5), N(Por) 2py(7.5),	68.3	0.0	31.5	0.2	0.0	-27.8	-0.1
50a'	-5.077	0.0	C α 2pz(8.2), C β 2pz(55.1), Cm 2pz(29.4),	0.0	0.0	99.9	0.1	0.0	0.0	0.0
51a'	-4.732	0.0	Fe dz ² (57.4), O 2pz(20.1),	59.3	20.5	11.7	7.4	-7.7	-8.3	-13.9

Table S-2e. Composition of The Molecular Orbitals for Model Compound II (α spin)

MO (α)	energy (EV)	occu.	primary contributors(%)	group population(%)				overlap population(%)		
				Fe	O	Por	Im	Fe-O	Fe-Por	Fe-Im
21a''	-9.710	1.0	Fe dxy(14.5), N(Por) 2px(11.2), N(Por) 2py(11.4), C β 2px(15.2), 14.5 C β 2py(15.4), H β 1s(17.4),	0.0	85.5	0.0	0.0	6.8	0.0	
36a'	-9.581	1.0	Fe dz ² (24.5), N(Por) 2px(13.8), N(Por) 2py(14.1), C α 2px(5.3), 27.1 C α 2py(5.6), C β 2px(8.1), C β 2py(7.9), Im 2pz(6.2),	2.7	62.0	7.9	0.7	8.5	1.9	
37a'	-9.488	1.0	N(Por) 2px(9.8), N(Por) 2py(10.0), C α 2px(8.3), C α 2py(8.5), Cm 2px(9.2), Cm 2py(10.0), Hm 1s(28.1),	3.0	0.0	96.9	0.0	1.8	-0.1	
22a''	-9.221	1.0	N(Por) 2py(8.6), C α 2py(21.6), C β 2py(30.6), Cm 2py(6.3), H β 1s(21.1),	1.1	0.8	96.5	1.6	0.8	0.2	
38a'	-9.202	1.0	N(Por) 2px(8.2), C α 2px(22.2), C β 2px(31.1), Cm 2px(6.9), H β 1s(20.8),	1.2	1.1	97.7	0.0	0.8	0.0	
23a''	-8.958	1.0	C α 2px(18.1), C α 2py(19.3), C β 2px(13.1), C β 2py(14.5), Cm 2py(5.3), H β 1s(20.0),	0.0	0.0	100.0	0.0	0.0	0.0	
24a''	-8.694	1.0	Fe dxy(18.9), N(Por) 2px(6.4), N(Por) 2py(6.6), C α 2px(10.4), C α 2py(8.9), C β 2px(17.7), C β 2py(16.2),	18.9	0.0	81.1	0.1	6.2	0.0	
25a''	-8.660	1.0	Fe dyz(10.9), C β 2pz(6.0), Im 2py(63.6),	11.9	2.7	20.2	66.5	-0.6	5.1	
39a'	-8.415	1.0	Fe dxz(15.4), O 2px(28.1), N(Por) 2px(10.3), C α 2px(9.5), C β 2px(6.5),	20.2	28.3	51.4	0.1	1.7	0.0	
26a''	-8.412	1.0	Fe dyz(12.2), Fe 4py(5.3), O 2py(25.9), N(Por) 2py(12.2), C α 2py(10.7), C β 2px(5.2), C β 2py(7.2),	17.7	26.1	55.3	0.9	2.0	0.0	

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40a'	-8.182	1.0	C α 2pz(47.8), C β 2pz(5.1), Cm 2pz(41.4),	0.2	0.9	98.2	0.6	0.0	0.0	0.0
41a'	-7.783	1.0	Fe dxz(18.3), O 2px(7.8), O 2pz(14.1), N(Por) 2px(11.8), N(Por) 2py(8.0), C α 2px(5.2), C β 2pz(6.0),	22.7	22.4	50.8	4.1	1.3	3.6	-0.4
42a'	-7.731	1.0	Fe dxz(5.4), O 2pz(46.0), Im 2pz(10.7),	13.2	50.0	22.4	14.7	-0.7	-1.7	1.3
27a''	-7.489	1.0	Fe dyz(15.0), O 2py(11.2), N(Por) 2px(8.6), N(Por) 2py(11.5), Im 2py(27.9),	16.0	11.2	42.5	29.7	2.3	4.1	-3.8
43a'	-7.170	1.0	C α 2pz(39.1), C β 2pz(23.2), Cm 2pz(30.5),	0.0	0.1	99.3	0.5	0.0	0.0	0.0
28a''	-7.145	1.0	C α 2pz(41.0), C β 2pz(22.1), Cm 2pz(30.6),	0.0	0.0	99.9	0.0	0.0	0.0	0.0
29a''	-6.854	1.0	Im 2py(86.0),	0.4	1.4	6.9	91.3	0.2	0.0	-0.2
44a'	-6.439	1.0	N(Por) 2pz(20.1), C β 2pz(65.6),	0.7	2.7	93.7	3.1	0.1	1.9	-2.5
30a''	-6.258	1.0	N(Por) 2pz(35.0), C β 2pz(54.8),	0.0	0.0	95.3	4.6	0.0	0.0	0.0
45a'	-6.047	1.0	O 2px(15.4), N(Por) 2pz(30.8), C β 2pz(40.8),	1.5	15.3	83.0	0.2	1.3	-1.7	0.0
31a''	-6.038	1.0	O 2py(13.1), N(Por) 2pz(31.3), C β 2pz(42.2),	1.6	13.0	84.7	0.6	1.2	-1.7	0.1
46a'	-5.636	1.0	Fe dx ² -y ² (93.6),	93.6	0.0	6.3	0.1	0.1	-2.6	0.0
32a''	-5.233	1.0	C α 2pz(70.6), C β 2pz(23.8),	0.0	0.0	99.9	0.1	0.0	0.0	0.0
47a'	-5.110	1.0	N(Por) 2pz(29.1), Cm 2pz(55.5),	0.6	0.6	96.7	1.2	0.0	2.0	-2.2
48a'	-5.010	1.0	Fe dxz(52.3), O 2px(39.0),	52.8	39.0	7.6	0.6	-9.4	-4.9	0.1
33a''	-4.991	1.0	Fe dyz(51.8), O 2py(38.8),	52.3	38.8	6.3	2.6	-9.4	-4.3	-1.0
49a'	-3.051	0.0	N(Por) 2pz(11.1), C α 2pz(25.8), C β 2pz(26.7), Cm 2pz(28.0),	1.5	0.0	98.4	0.1	0.1	-1.0	0.0
34a''	-3.030	0.0	N(Por) 2pz(11.8), C α 2pz(25.1), C β 2pz(26.0), Cm 2pz(28.7),	1.6	0.0	98.3	0.2	0.1	-1.1	0.0
35a''	-2.709	0.0	Fe dxy(62.4), N(Por) 2s(8.4), N(Por) 2px(9.4), N(Por) 2py(9.4),	62.4	0.0	37.3	0.3	0.0	-26.8	-0.1
50a'	-2.106	0.0	Fe dz ² (54.4), O 2pz(20.8),	56.1	21.1	12.8	8.5	-8.8	-5.3	-15.1
51a'	-1.676	0.0	C α 2pz(6.8), C β 2pz(57.3), Cm 2pz(28.4),	0.0	0.0	99.9	0.1	0.0	0.0	0.0
36a''	-1.615	0.0	Im 2py(88.8),	1.2	0.1	2.1	96.9	-0.2	-0.7	-0.1

Table S2-f. Composition of the molecular orbitals for model compound II (β spin)

MO (β)	energy (EV)	occu.	primary contributors(%)	group population(%)				overlap population(%)		
				Fe	O	Por	Im	Fe-O	Fe-Por	Fe-Im
21a''	-9.641	1.0	Fe dxy(10.3), N(Por) 2px(10.6), N(Por) 2py(10.8), C β 2px(17.2), 10.3 C β 2py(17.6), H β 1s(18.1),		0.0	89.7	0.0	0.0	5.7	0.0
36a'	-9.485	1.0	N(Por) 2px(8.1), N(Por) 2py(12.0), C α 2px(7.3), C α 2py(9.7), Cm 2px(9.2), Cm 2py(9.9), Hm 1s(28.2),	2.5	0.0	97.5	0.0	0.0	1.7	-0.1
37a'	-9.445	1.0	Fe dz2(22.0), N(Por) 2px(14.8), N(Por) 2py(11.6), C α 2px(5.4), 24.3 C β 2px(6.2), C β 2py(6.8), Im 2pz(14.0),		1.8	55.5	17.9	0.5	8.0	3.1
22a''	-9.219	1.0	N(Por) 2py(8.3), C α 2py(21.8), C β 2py(31.2), Cm 2py(6.6), H β 1s(21.1),	0.9	0.2	97.3	1.7	0.1	0.8	0.1
38a'	-9.198	1.0	N(Por) 2px(7.7), C α 2px(22.7), C β 2px(32.0), Cm 2px(7.4), H β 1s(20.8),	0.8	0.2	98.9	0.0	0.1	0.7	0.0
23a''	-8.961	1.0	C α 2px(18.4), C α 2py(19.0), C β 2px(13.4), C β 2py(14.2), Cm 2py(5.2), H β 1s(20.0),	0.0	0.0	100.0	0.0	0.0	0.0	0.0
24a''	-8.600	1.0	C α 2py(5.3), Im 2py(67.8),	4.3	0.0	25.9	70.9	0.0	0.0	3.9
25a''	-8.571	1.0	Fe dxy(18.4), N(Por) 2px(9.0), N(Por) 2py(9.2), C α 2px(9.6), C α 2py(8.7), C β 2px(15.5), C β 2py(14.7),	18.4	0.0	81.2	0.4	0.0	7.6	0.0
39a'	-8.183	1.0	C α 2pz(48.1), C β 2pz(5.1), Cm 2pz(41.7),	0.1	0.2	98.9	0.7	0.0	0.0	0.0
40a'	-8.132	1.0	Fe 4px(6.6), N(Por) 2s(5.0), N(Por) 2px(24.7), N(Por) 2py(13.6), 7.9 C α 2px(15.0), C β 2px(9.5), C β 2py(7.9),	4.3	87.6	-0.1	1.5	6.2	-0.4	

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26a''	-8.050	1.0	O 2py(6.0), N(Por) 2px(11.7), N(Por) 2py(20.1), C α 2py(10.6), C β 2px(5.9), C β 2py(6.7), Im 2py(12.3),	8.7	6.1	72.1	12.9	2.2	5.2	-0.7
41a'	-7.311	1.0	Fe dz ₂ (9.3), O 2pz(62.6), C β 2pz(6.3), Im 2pz(7.4),	11.3	65.5	13.4	10.5	-1.9	-5.0	1.2
42a'	-7.181	1.0	C α 2pz(40.5), C β 2pz(15.6), Cm 2pz(33.2),	0.9	0.5	97.9	0.6	0.2	0.1	0.0
27a''	-7.150	1.0	C α 2pz(41.5), C β 2pz(20.8), Cm 2pz(31.1),	0.0	0.0	99.8	0.0	0.0	0.0	0.0
43a'	-7.024	1.0	Fe dxz(24.0), O 2px(15.6), N(Por) 2pz(16.1), C β 2pz(35.0),	24.0	16.1	58.9	1.0	4.8	4.6	-0.5
28a''	-6.986	1.0	Fe dyz(11.3), O 2py(7.6), N(Por) 2pz(8.8), C β 2pz(14.9), Im 2py(49.1),	11.3	7.7	28.6	52.4	2.3	2.2	-0.6
29a''	-6.742	1.0	Fe dyz(8.1), O 2py(7.2), N(Por) 2pz(9.9), C β 2pz(14.9), Im 2py(50.0),	8.2	7.3	31.1	53.2	2.1	1.7	-1.3
44a'	-6.419	1.0	O 2pz(5.5), N(Por) 2pz(18.5), C β 2pz(63.3),	1.1	5.4	90.2	3.4	0.1	1.7	-2.4
30a''	-6.255	1.0	N(Por) 2pz(35.0), C β 2pz(54.8),	0.0	0.0	95.3	4.7	0.0	0.0	0.0
31a''	-5.542	1.0	Fe dyz(20.1), O 2py(27.2), N(Por) 2pz(15.6), C α 2pz(6.4), C β 2pz(24.9),	20.2	27.3	51.9	0.6	7.2	-5.9	-0.1
45a'	-5.528	1.0	Fe dxz(20.2), O 2px(27.2), N(Por) 2pz(16.2), C α 2pz(6.4), C β 2pz(24.7),	20.3	27.3	52.3	0.2	7.1	-5.9	0.0
32a''	-5.239	1.0	C α 2pz(70.6), C β 2pz(23.7),	0.0	0.0	99.9	0.1	0.0	0.0	0.0
46a'	-5.105	1.0	N(Por) 2pz(29.4), Cm 2pz(55.2),	0.7	0.9	96.4	1.1	0.0	1.8	-2.0
47a'	-4.978	1.0	Fe dx ² -y ² (93.6),	93.6	0.0	6.4	0.1	0.1	-2.0	0.0
33a''	-3.369	0.0	Fe dyz(33.8), O 2py(43.3), C α 2pz(5.9),	34.8	43.3	17.5	4.8	-7.7	-1.6	-0.1
48a'	-3.350	0.0	Fe dxz(34.6), O 2px(43.4), C α 2pz(7.0), C β 2pz(5.4),	35.6	43.4	20.4	0.9	-8.0	-1.5	0.3
49a'	-2.966	0.0	Fe dxz(15.3), N(Por) 2pz(10.1), C α 2pz(18.8), C β 2pz(21.6), Cm 2pz(23.8),	15.4	4.1	80.1	0.1	-1.8	-4.2	0.1

...Cont.

34a"	-2.948	0.0	Fe dyz(13.3), N(Por) 2pz(10.8), C α 2pz(19.1), C β 2pz(22.0), Cm 2pz(25.0),	13.4	3.1	82.8	0.3	-1.5	-3.8	0.1
35a"	-2.065	0.0	Fe dxy(67.2), N(Por) 2s(7.4), N(Por) 2px(7.5), N(Por) 2py(7.5),	67.2	0.0	32.0	0.9	0.0	-27.6	-0.2
50a'	-1.679	0.0	C α 2pz(6.8), C β 2pz(57.3), Cm 2pz(28.4),	0.0	0.0	99.9	0.1	0.0	0.0	0.0
36a"	-1.563	0.0	Im 2py(86.3),	3.3	0.6	2.1	94.3	-0.5	-0.6	-0.7
51a'	-1.403	0.0	Fe dz2(53.4), O 2pz(18.7), H(Im) 1s(8.0),	55.7	19.0	10.6	12.9	-8.5	-6.0	-13.9

Table S3-a. Mulliken Charges, Spin Populations and ESP Charges in $^4A_{2u}$ State of Compound I

Atom types	Indices	Mulliken charge	α -spin	β -spin	Net spin	ESP charge
Fe	1	0.655	8.292	7.053	1.239	0.781
O	2	-0.428	3.707	2.721	0.986	-0.477
N1.Po	3 4	-0.389	2.728	2.660	0.068	-0.174
N2.Po	5 6	-0.393	2.729	2.663	0.066	-0.197
N1.Im	7	-0.301	2.637	2.664	-0.027	-0.436
N2.Im	8	0.028	2.488	2.484	0.004	-0.316
C α 1	9 11	0.266	1.849	1.885	-0.036	0.305
C α 2	10 12	0.254	1.855	1.891	-0.036	0.296
C α 3	13 15	0.264	1.851	1.885	-0.034	0.307
C α 4	14 16	0.245	1.859	1.895	-0.036	0.319
C β 1	17 19	0.197	1.901	1.902	-0.001	-0.262
C β 2	18 20	0.201	1.899	1.900	-0.001	-0.260
C β 3	21 23	0.196	1.901	1.903	-0.002	-0.254
C β 4	22 24	0.200	1.900	1.900	0.000	-0.276
Cm1	25 27	0.165	2.024	1.811	0.213	-0.349
Cm2	26	0.122	2.044	1.834	0.210	-0.293
Cm3	28	0.128	2.043	1.829	0.214	-0.278
C1.Im	29	0.467	1.773	1.759	0.014	0.272
C2.Im	30	0.350	1.827	1.823	0.004	-0.003
C3.Im	31	0.239	1.880	1.881	-0.001	-0.063
H β 1	32 34	-0.194	0.597	0.596	0.001	0.187
H β 2	33 35	-0.194	0.597	0.596	0.001	0.183
H β 3	36 38	-0.193	0.597	0.596	0.001	0.186
H β 4	37 39	-0.194	0.597	0.596	0.001	0.187
Hm1	40 42	-0.168	0.577	0.592	-0.015	0.211
Hm2	41	-0.164	0.574	0.590	-0.016	0.184
Hm3	43	-0.165	0.574	0.590	-0.016	0.186
Hn.Im	44	-0.005	0.502	0.503	-0.001	0.348
H1.Im	45	-0.125	0.562	0.563	-0.001	0.020
H2.Im	46	-0.177	0.588	0.589	-0.001	0.091
H3.Im	47	-0.151	0.575	0.575	0.000	0.162

Table S3-b. Mulliken Charges, Spin Populations and ESP Charges in $^4A_{1u}$ State of Compound I

Atom types	Indices	Mulliken charge	α -spin	β -spin	Net spin	ESP charge
Fe	1	0.656	8.248	7.095	1.153	1.016
O	2	-0.438	3.709	2.729	0.980	-0.506
N1.Po	3 4	-0.403	2.673	2.730	-0.057	-0.337
N2.Po	5 6	-0.406	2.675	2.731	-0.056	-0.359
N1.Im	7	-0.302	2.631	2.671	-0.040	-0.467
N2.Im	8	0.027	2.489	2.485	0.004	-0.321
C α 1	9 11	0.288	1.928	1.784	0.144	0.447
C α 2	10 12	0.276	1.935	1.789	0.146	0.437
C α 3	13 15	0.285	1.928	1.786	0.142	0.447
C α 4	14 16	0.267	1.937	1.796	0.141	0.458
C β 1	17 19	0.204	1.912	1.884	0.028	-0.272
C β 2	18 20	0.207	1.907	1.886	0.021	-0.273
C β 3	21 23	0.203	1.910	1.887	0.023	-0.266
C β 4	22 24	0.206	1.909	1.885	0.024	-0.286
Cm1	25 27	0.128	1.910	1.961	-0.051	-0.507
Cm2	26	0.085	1.933	1.982	-0.049	-0.448
Cm3	28	0.091	1.928	1.981	-0.053	-0.434
C1.Im	29	0.463	1.776	1.760	0.016	0.279
C2.Im	30	0.347	1.829	1.824	0.005	0.006
C3.Im	31	0.237	1.881	1.882	-0.001	-0.067
H β 1	32 34	-0.191	0.594	0.597	-0.003	0.193
H β 2	33 35	-0.192	0.595	0.597	-0.002	0.189
H β 3	36 38	-0.192	0.594	0.597	-0.003	0.191
H β 4	37 39	-0.192	0.594	0.597	-0.003	0.192
Hm1	40 42	-0.172	0.586	0.585	0.001	0.220
Hm2	41	-0.167	0.584	0.583	0.001	0.192
Hm3	43	-0.168	0.585	0.583	0.002	0.194
Hn.Im	44	-0.007	0.503	0.503	0.000	0.347
H1.Im	45	-0.127	0.563	0.564	-0.001	0.016
H2.Im	46	-0.179	0.589	0.590	-0.001	0.086
H3.Im	47	-0.152	0.576	0.576	0.000	0.161

Table S3-c. Mulliken Charges, Spin Populations and ESP Charges in Compound II

Atom types	Indices	Mulliken charge	α -spin	β -spin	Net spin	ESP charge
Fe	1	0.658	8.264	7.079	1.185	1.113
O	2	-0.463	3.709	2.754	0.955	-0.568
N1.Po	3 4	-0.405	2.690	2.715	-0.025	-0.296
N2.Po	5 6	-0.408	2.692	2.716	-0.024	-0.319
N1.Im	7	-0.293	2.627	2.666	-0.039	-0.475
N2.Im	8	0.018	2.493	2.489	0.004	-0.338
Ca1	9 11	0.261	1.869	1.871	-0.002	0.370
Ca2	10 12	0.249	1.875	1.876	-0.001	0.362
Ca3	13 15	0.258	1.870	1.872	-0.002	0.371
Ca4	14 16	0.241	1.879	1.881	-0.002	0.386
C β 1	17 19	0.169	1.915	1.916	-0.001	-0.303
C β 2	18 20	0.173	1.913	1.914	-0.001	-0.303
C β 3	21 23	0.169	1.915	1.916	-0.001	-0.296
C β 4	22 24	0.172	1.914	1.914	0.000	-0.318
Cm1	25 27	0.102	1.948	1.949	-0.001	-0.522
Cm2	26	0.060	1.969	1.970	-0.001	-0.464
Cm3	28	0.066	1.966	1.967	-0.001	-0.449
C1.Im	29	0.465	1.776	1.759	0.017	0.287
C2.Im	30	0.360	1.823	1.817	0.006	0.020
C3.Im	31	0.213	1.893	1.895	-0.002	-0.094
H β 1	32 34	-0.219	0.610	0.610	0.000	0.170
H β 2	33 35	-0.220	0.610	0.610	0.000	0.166
H β 3	36 38	-0.220	0.610	0.610	0.000	0.168
H β 4	37 39	-0.220	0.610	0.610	0.000	0.169
Hm1	40 42	-0.199	0.599	0.599	0.000	0.211
Hm2	41	-0.196	0.598	0.598	0.000	0.183
Hm3	43	-0.196	0.598	0.598	0.0000	0.185
Hn.Im	44	-0.022	0.511	0.511	0.000	0.333
H1.Im	45	-0.126	0.562	0.564	-0.002	0.011
H2.Im	46	-0.180	0.589	0.591	-0.002	0.082
H3.Im	47	-0.168	0.584	0.584	0.000	0.145