Supporting Information

Trigonal prismatic anionic iron (III) complex of a radical *o*-imino-benzo-semiquinonate derivative: Structural and spectral analysis

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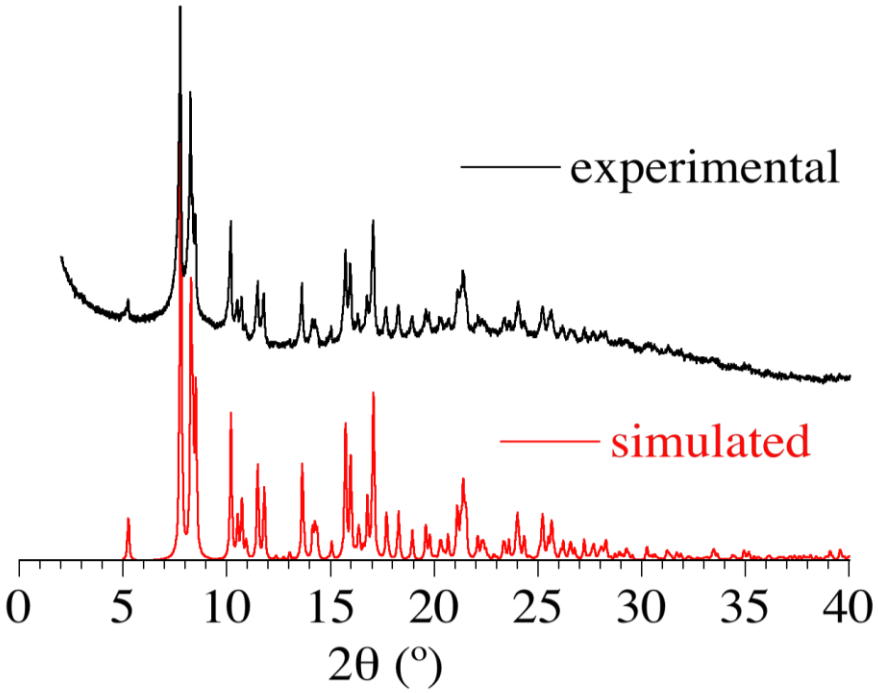

Fig. S1: (a) Simulated and (b) powder X-ray diffraction pattern of complex **1**.

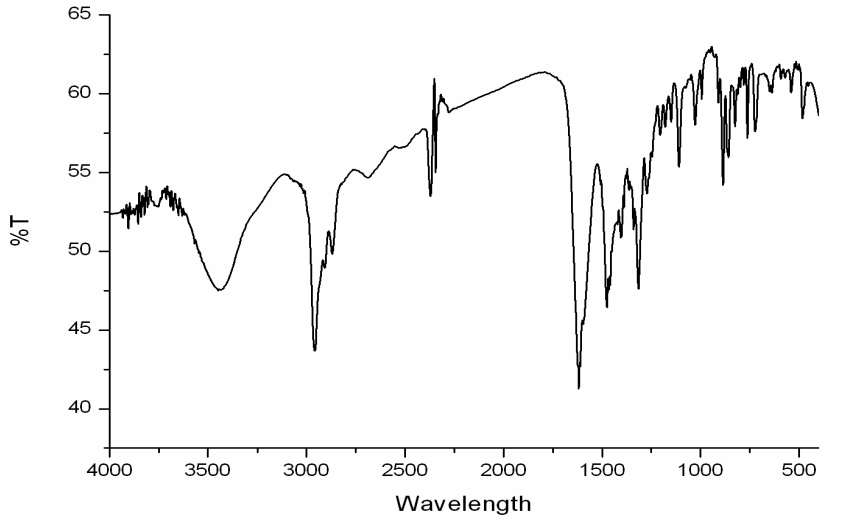

Fig. S2: IR spectrum of complex **1**.

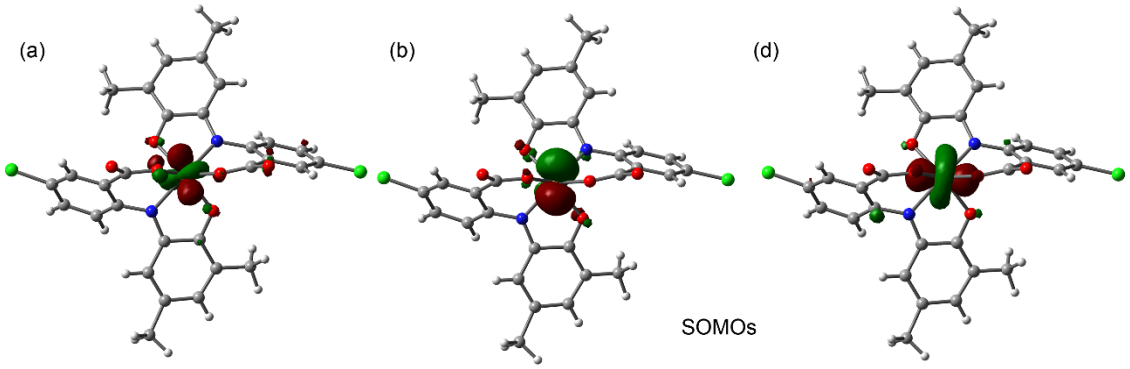

Fig. S3: Plot of the three highest *alpha* SOMOs of complex **1**.

Table **S1.** Selected bond lengths (Å) for **1**.

atoms	**distance**	**atoms**	**distance**	**atoms**	**distance**	**atoms**	**distance**
Fe1-O6	2.006(2)	O2-C7	1.223(5)	C5-C6	1.360(6)	C23-C24	1.388(6)
Fe1-O3	2.008(3)	O3-C9	1.290(4)	C8-C13	1.419(5)	C24-C25	1.377(6)
Fe1-O1	2.018(3)	O4-C28	1.280(5)	C8-C9	1.443(5)	C25-C26	1.363(7)
Fe1-N1	2.045(3)	O5-C28	1.235(5)	C9-C10	1.417(5)	C26-C27	1.383(7)
Fe1-O4	2.053(3)	O6-C30	1.281(4)	C10-C11	1.375(5)	C29-C34	1.413(5)
Fe1-N2	2.055(3)	C1-C2	1.393(5)	C11-C12	1.427(5)	C29-C30	1.449(5)
N1-C8	1.339(4)	C1-C6	1.399(5)	C12-C13	1.354(5)	C30-C31	1.432(5)
N1-C2	1.409(5)	C1-C7	1.498(6)	C22-C23	1.387(5)	C31-C32	1.368(5)
N2-C29	1.338(4)	C2-C3	1.385(5)	C22-C27	1.389(6)	C32-C33	1.428(5)
N2-C23	1.417(5)	C3-C4	1.384(5)	C22-C28	1.505(6)	C33-C34	1.348(5)
O1-C7	1.290(5)	C4-C5	1.380(6)				

Table **S2.** Selected bond angles (º) for **1**.

Atoms	**angle**	**Atoms**	**angle**	**Atoms**	**angle**
O1-Fe1-O3	135.17(11)	O3-Fe1-O4	85.62(11)	O4-Fe1-N1	128.13(12)
O1-Fe1-O4	77.98(12)	O3-Fe1-O6	129.83(12)	O4-Fe1-N2	82.70(13)
O1-Fe1-O6	87.54(12)	O3-Fe1-N1	76.27(12)	O6-Fe1-N1	88.72(12)
O1-Fe1-N1	81.75(12)	O3-Fe1-N2	87.39(12)	O6-Fe1-N2	76.25(13)
O1-Fe1-N2	130.40(12)	O4-Fe1-O6	136.74(11)	N1-Fe1-N2	142.64(13)