

Supplementary Material

Steric Trapping of the High Spin State in Fe(III)

Quinolyisalicylaldimine Complexes

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Supporting Figures

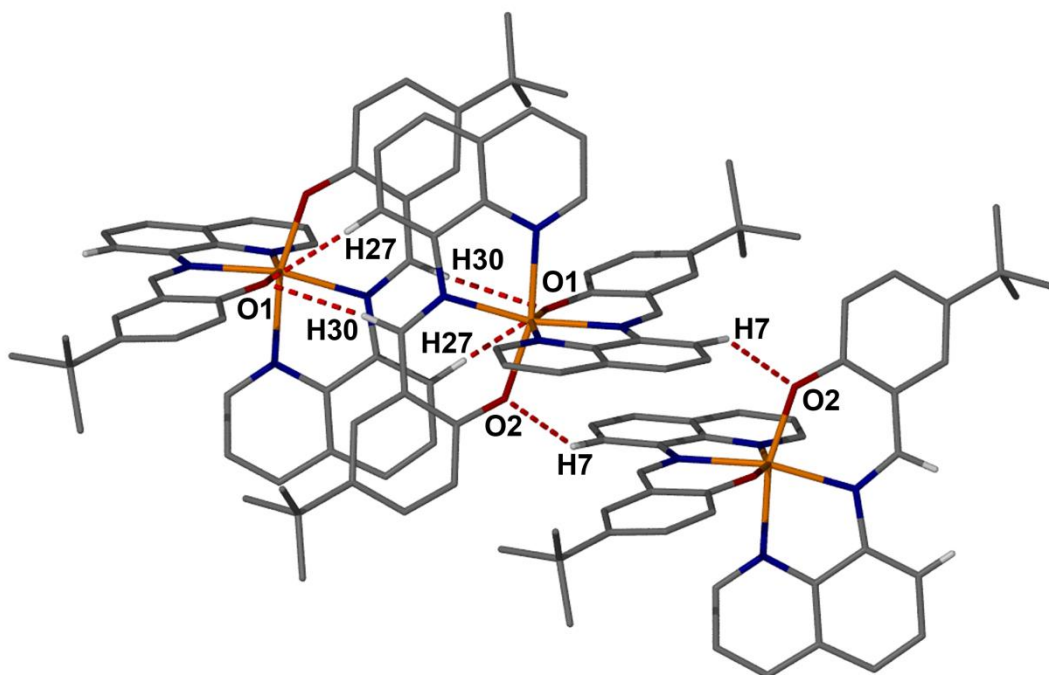


Figure S1 The supplementary C-H...O interactions between the aromatic C-H groups and the phenoxide O atoms in $[\text{Fe}(\text{qsal-5-}t\text{Bu})_2]\text{ClO}_4 \cdot \text{MeOH}$ at 100 K.

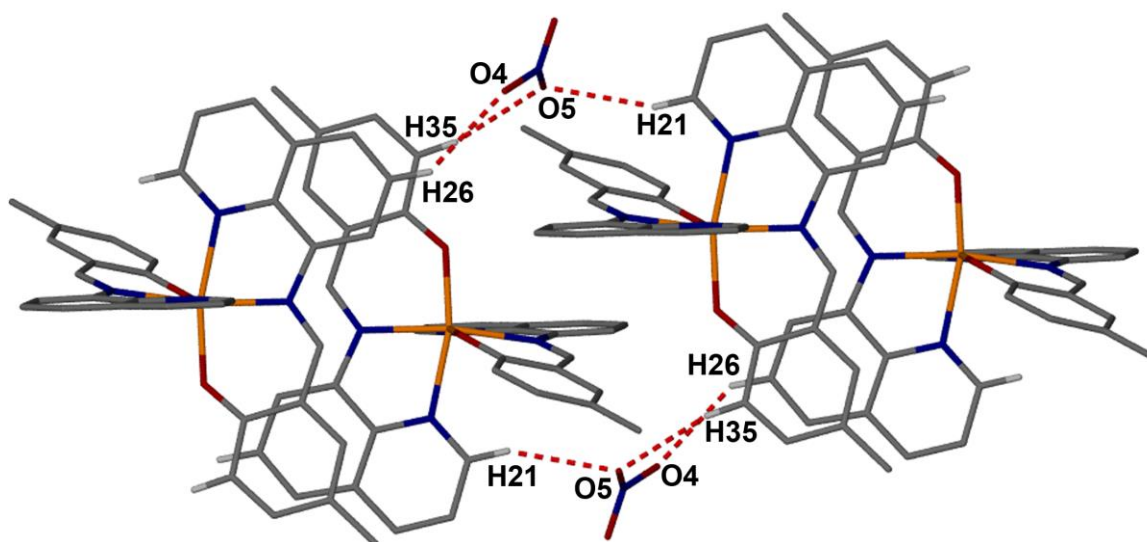


Figure S2 View of the C-H...O interactions which link the nitrate anions to the 1D chains in **3**.

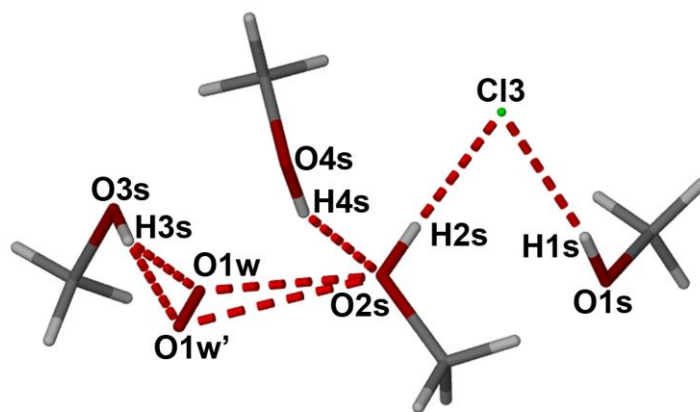


Figure S3 View of the chloride, methanol, water hydrogen bonded chain in **1**.

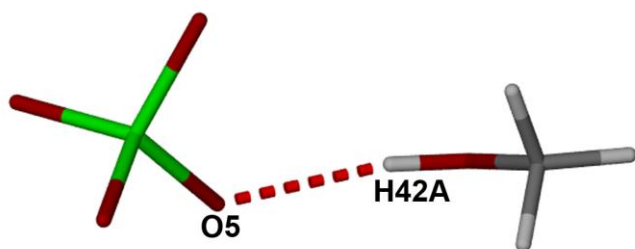


Figure S4 View of the ClO_4^- -MeOH O-H...O hydrogen bond in **2**.

Supporting Table

Table S1 Hydrogen bond geometries for [Fe(qsal-5-*t*Bu)₂]Y **1**, **2** and **3** (Å, °).

	<i>D-H</i> ⋯ <i>A</i>	<i>D-H</i>	<i>H</i> ⋯ <i>A</i>	<i>D</i> ⋯ <i>A</i>	<i>D-H</i> ⋯ <i>A</i>	
1	O1S-H1S⋯Cl3	0.84	2.25	3.089(4)	174	
	O2S-H2S⋯Cl3	0.84	2.21	3.046(4)	173	
	O3S-H3S⋯O1W ⁱ	0.84	1.87	2.876(7)	175	
	O4S-H4S⋯O2S	0.84	1.99	2.770(5)	154	
	C2-H2⋯O1S	0.95	2.45	3.277(6)	145	
	C3-H3⋯O1S	0.95	2.46	3.338(6)	154	
	C7-H7⋯O2 ⁱ	0.95	2.44	3.325(5)	155	
	C10-H10⋯O2 ⁱ	0.95	2.70	2.528(5)	146	
	C21-H21⋯O4S ⁱⁱ	0.95	2.54	3.413(6)	152	
	C27-H27⋯O1 ⁱⁱⁱ	0.95	2.51	3.438(5)	167	
	C34-H34⋯O1W ^{iv}	0.95	2.57	3.419(6)	149	
	2	O7-H42(A)⋯O5	0.82	1.92	2.731(5)	168
		C1-H1⋯O7 ^v	0.93	2.48	3.304(6)	148
		C6-H6⋯O5	0.93	2.47	3.240(5)	140
C7-H7⋯O2 ^{vi}		0.93	2.51	3.310(4)	144	
C21-H21⋯N2		0.93	2.58	3.136(4)	119	
C21-H21⋯O4 ^{vii}		0.93	2.53	3.361(6)	149	
C27-H27⋯O1 ^{viii}		0.93	2.51	3.375(4)	156	
3	C7-H7⋯O2 ^{ix}	0.95	2.54	3.469(5)	16	
	C10-H10⋯O5 ^x	0.95	2.59	2.973(5)	104	
	C27-H27⋯O1 ^{xi}	0.95	2.43	3.327(4)	158	
	C35-H35⋯O5 ^{xi}	0.95	2.56	3.486(6)	165	

Symmetry codes: ⁱ2-x, -y, 1-z; ⁱⁱ2-x, 1-y, 1-z; ⁱⁱⁱ1-x, 1-y, 1-z, ^{iv} 1+x, y, z, ^v 1-x, -y, -z, ^{vi} 2-x, -y, -z, ^{vii} 1+x, y, z, ^{viii} 1-x, -y, 1-z, ^{ix}1-x, 2-y, 1-z; ^x1-x, 1-y, 1-z; ^{xi}x, 1+y, z,
D = Donor, A = Acceptor