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Spin Crossover in Three Schiff-Base Mononuclear Iron (III) Complexes

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Received: 10 July 2019; Accepted: 26 July 2019; Published: date

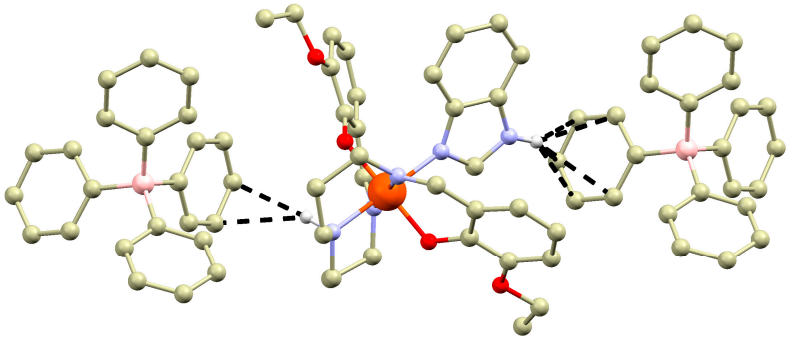

Figure S1. The N-H···p non-covalent interactions (displayed as black dashed lines) in **1a**. Hydrogen atoms (except for those involved in non-covalent interactions) were omitted for clarity.

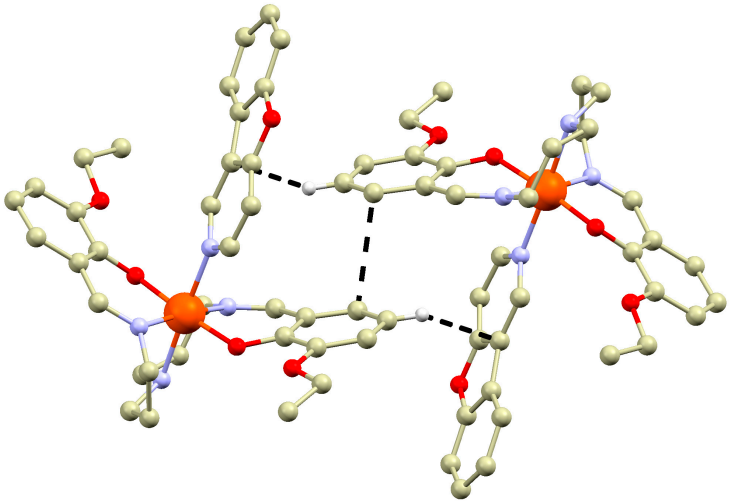

Figure S2. The non-covalent interactions (displayed as black dashed lines) in **2a**. Hydrogen atoms (except for those involved in non-covalent interactionss) were omitted for clarity

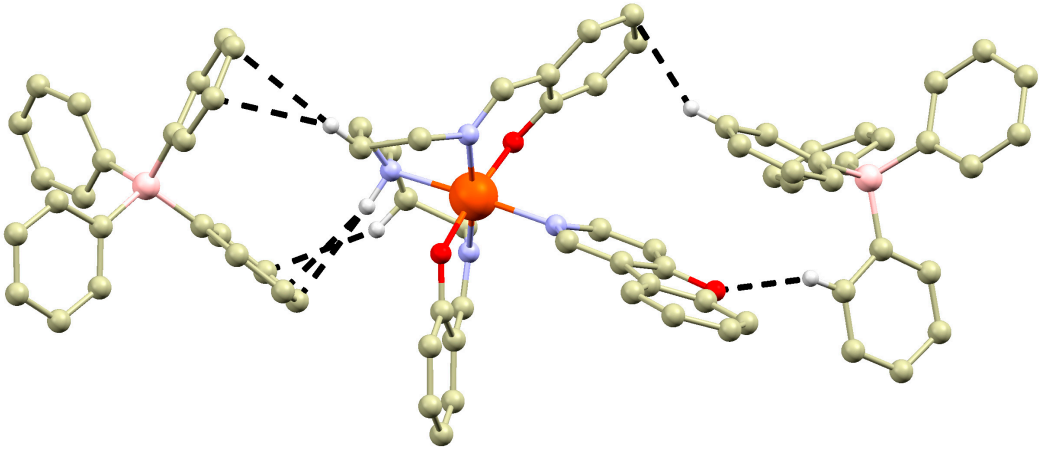

Figure S3. The non-covalent interactions (displayed as black dashed lines) in **2b**. Hydrogen atoms (except for those involved in non-covalent interactions) were omitted for clarity.

Table S1. The interatomic donor-acceptor distances for DFT optimized geometries of $[Fe(R\text{-}LA)(L1)]^+$ of **1a, 2a, 2b** and DAVCEJ, DETBEJ and KISJUS using B3LYP functional.[a]

Compound	Fe-O	Fe-N_{im}	Fe-N_{am}	Fe-N_{hetero}
1a (LS)	1.882/1.904	1.977/1.999	2.070	2.036
2a (LS)	1.881/1.894	1.985/1.992	2.072	2.052
2b (LS)	1.882/1.908	1.984/2.003	2.072	2.049
DAVCEJ (LS)	1.884/1.900	1.983/1.994	2.153	2.033
DETBEJ (LS)	1.881/1.907	1.983/2.006	2.070	2.046
KISJUS (LS)	1.873/1.906	1.978/2.000	2.070	2.014
1a (HS)	1.933/1.950	2.120/2.127	2.312	2.229
2a (HS)	1.935/1.936	2.123/2.127	2.317	2.259
2b (HS)	1.941/1.944	2.122/2.123	2.310	2.255
DAVCEJ (HS)	1.937/1.947	2.111/2.113	2.408	2.226
DETBEJ (HS)	1.940/1.940	2.123/2.126	2.311	2.256
KISJUS (HS)	1.936/1.945	2.124/2.126	2.320	2.198

[a] distances in Å.

Table S2. The interatomic donor-acceptor distances for DFT optimized geometries of $[Fe(R\text{-}LA)(L1)]^+$ of **1a, 2a, 2b** and DAVCEJ, DETBEJ and KISJUS using OPBE functional.[a]

Compound	Fe-O	Fe-N_{im}	Fe-N_{am}	Fe-N_{hetero}
1a (LS)	1.883/1.886	1.936/1.940	2.059	2.041
2a (LS)	1.881/1.884	1.936/1.939	2.056	2.043
2b (LS)	1.880/1.885	1.941/1.946	2.059	2.045
DAVCEJ (LS)	1.883/1.885	1.931/1.939	2.162	2.019
DETBEJ (LS)	1.880/1.884	1.941/1.945	2.060	2.038
KISJUS (LS)	1.878/1.887	1.934/1.941	2.056	2.006
1a (HS)	1.947/1.958	2.113/2.125	2.365	2.311
2a (HS)	1.948/1.950	2.115/2.122	2.360	2.329
2b (HS)	1.946/1.949	2.120/2.125	2.356	2.321
DAVCEJ (HS)	1.949/1.956	2.094/2.096	2.657	2.247
DETBEJ (HS)	1.945/1.947	2.120/2.124	2.357	2.323
KISJUS (HS)	1.950/1.958	2.120/2.121	2.366	2.256

[a] distances in Å.