Electronic Supplementary Material (ESI) for Dalton Transactions.

Supplementary Information for:

Abrupt spin crossover in iron(III) complexes with aromatic anions

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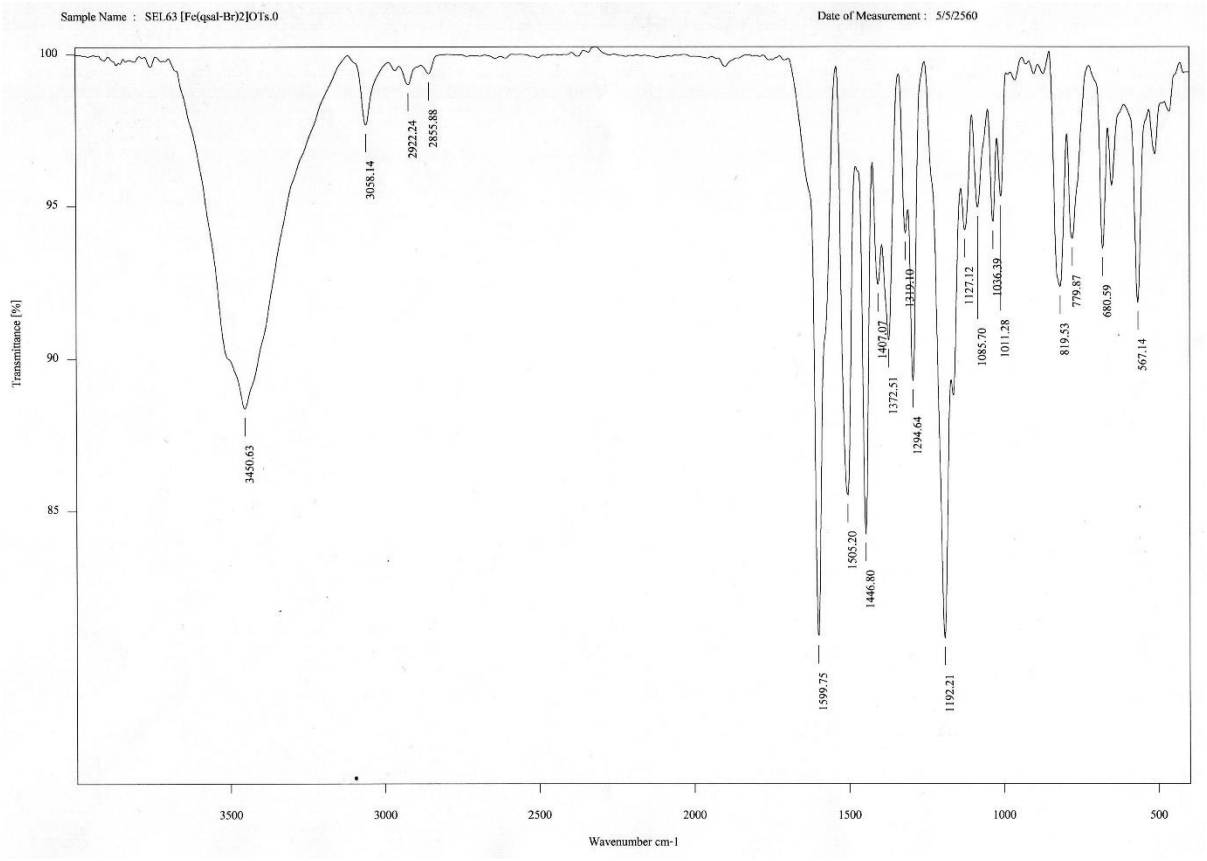
IR spectroscopy



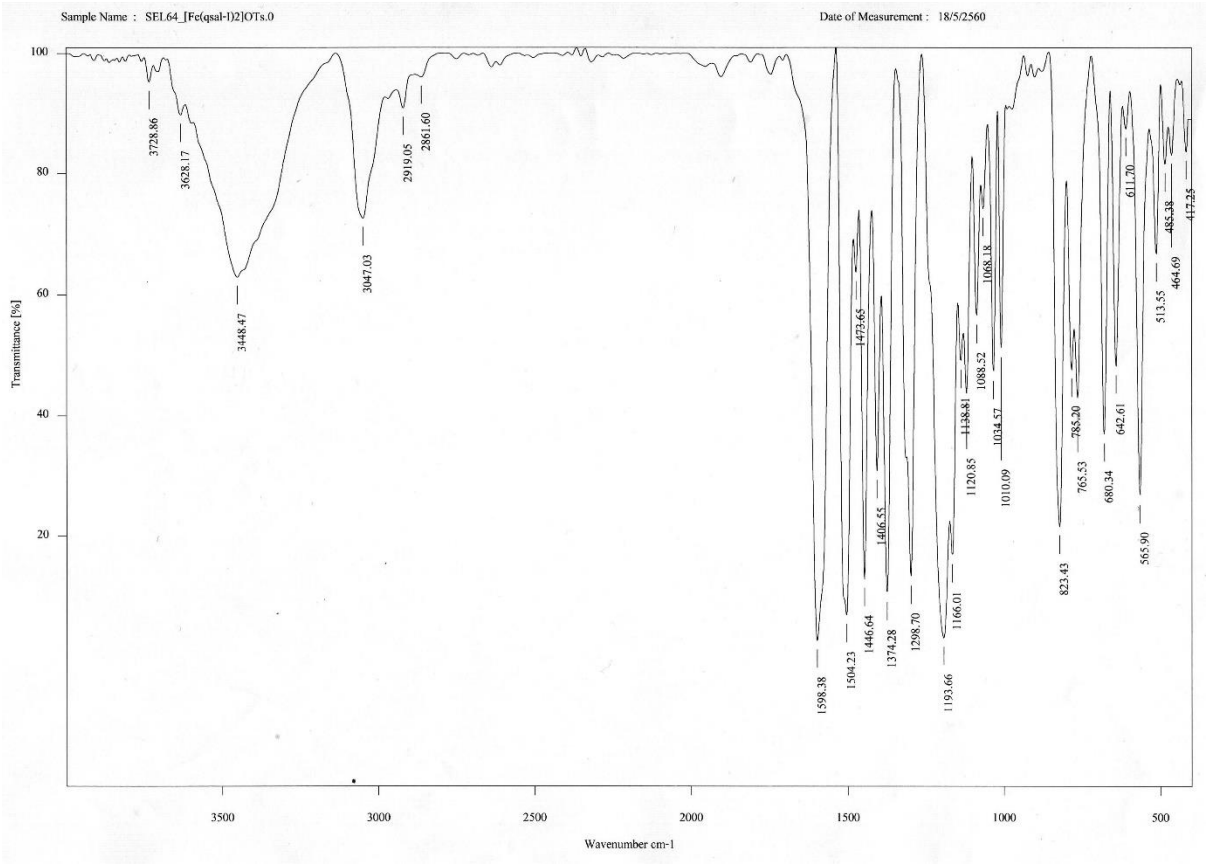


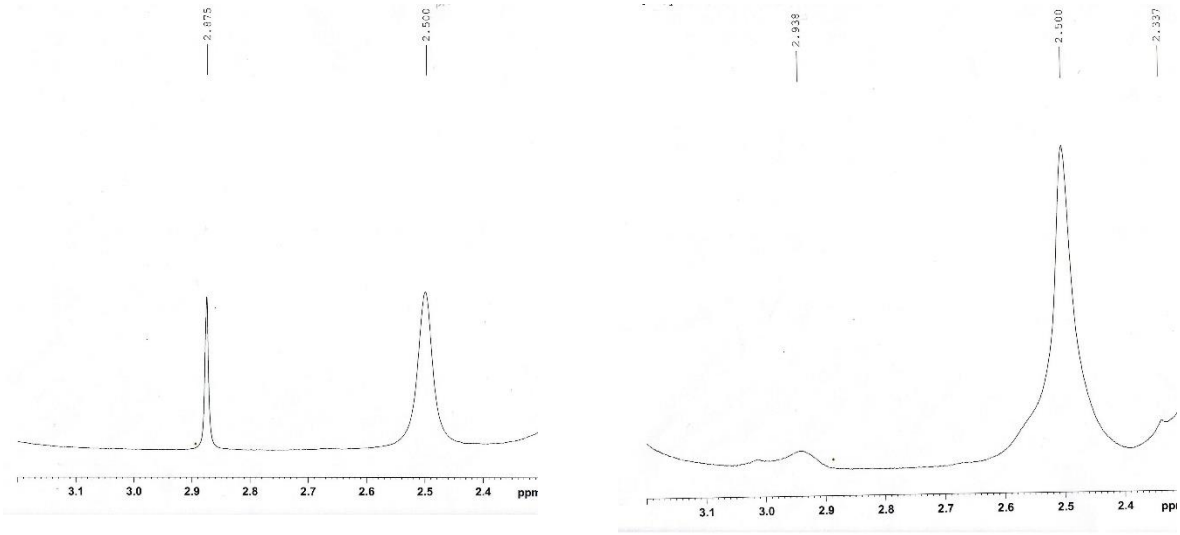
Figure S1 IR spectra of $[Fe(qsal\text{-}X)_2]OTs{\cdot}nH_2O$.

Solution magnetic studies

The ^1H NMR studies to determine the magnetic susceptibility of $[Fe(qsal\text{-}X)_2]OTs$ were recorded at 298 K in d^6-DMSO with TMS added as an internal standard against a reference of DMSO on a 300 MHz Bruker FT-NMR spectrometer following a modified Evan's method. The reference solvent was placed in a co-axial insert with the solution of the complex in a standard NMR tube. The mass susceptibility was calculated using:

$$\chi_g = \chi_o + \frac{3\Delta v}{4\pi v_o c}$$

where χ_o = the mass susceptibility of DMSO (-0.629 x 10^{-6} $cm^3{\cdot}g^{-1}$), $\Delta\upsilon$ (Hz) is the paramagnetic shift of the reference, υ_o is the operating RF frequency of the NMR spectrometer (300.13 x 10^6 Hz) and c is the concentration of the solution in $g{\cdot}cm^{-3}$. The mass susceptibility was then converted to molar susceptibility (χ_M). Diamagnetic corrections were applied and by multiplication with the measurement temperature (298 K) $\chi_M T$ was determined.



X = Br **X = I**

Figure S2 ^{1}H NMR spectrum of [Fe(qsal-X)$_2$]OTs in d^6-DMSO showing the TMS shift.

Table S1 Selected ^{1}H NMR data of **1**-**2** in d^6-DMSO at 298 K.

Compound	**Concentration (g/cm^3)**	**$\Delta\nu$ (Hz)**	**χ_MT (cm^3·mol^{-1}·K)**	**%HS**
[Fe(qsal-Br)$_2$]OTs	0.01	150.05	2.59	55
[Fe(qsal-I)$_2$]OTs	0.01	175.25	3.03	66

X-ray crystallographic studies

Table S2 Crystallographic data and structure refinement parameters for [Fe(qsal-X)$_2$]OTs•nH_2O complexes.

	1·H_2O 103 K	**1**·H_2O 293 K	**2·2**H_2O 103 K
Formula	$C_{39}H_{27}Br_2FeN_4O_5S·H_2O$	$C_{39}H_{27}Br_2FeN_4O_5S·H_2O$	$C_{39}H_{27}I_2FeN_4O_5S·2H_2O$
Formula weight	897.39	897.39	1008.85
Crystal system	Orthorhombic	Orthorhombic	Orthorhombic
Space group	*Pca2$_1$*	*Pca2$_1$*	*Pca2$_1$*
a/Å	12.3433(8)	12.4432(3)	12.7045(3)
b/Å	14.3546(8)	14.6561(4)	14.1173(3)
c/Å	19.2425(14)	19.1005(13)	20.3416(14)
α/°	90	90	90
β/°	90	90	90
γ/°	90	90	90
T/*K*	103	293	103
Cell volume/Å^3	3409.4(4)	3483.3(3)	3648.3(3)
Z	4	4	4
Absorption coefficient (mm^{-1})	7.346	7.190	17.621
Reflections collected	18081	19306	17087
Independent reflections	2928	8805	5211
R_{int}	0.1447	0.1167	0.0791
Max. and min. transition	1.000/0.091	1.000/0.192	1.000/0.350
Restraints/parameters	235/464	21/383	85/486
Final *R* indices [*I*>2σ(*I*)]:	0.0859/0.1901	0.0773/0.2198	0.0622/0.1516
R1,wR2			
CCDC	1920841	1920840	1920842

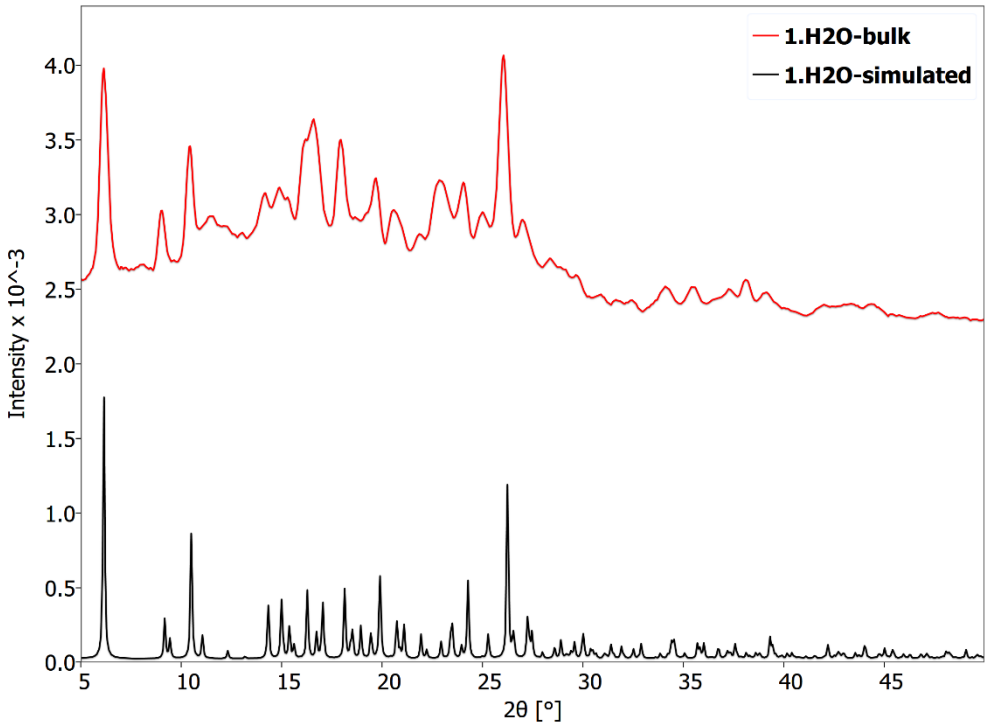


Figure S3 PXRD of $[Fe(qsal\text{-}Br)_2]OTs{\cdot}H_2O$.

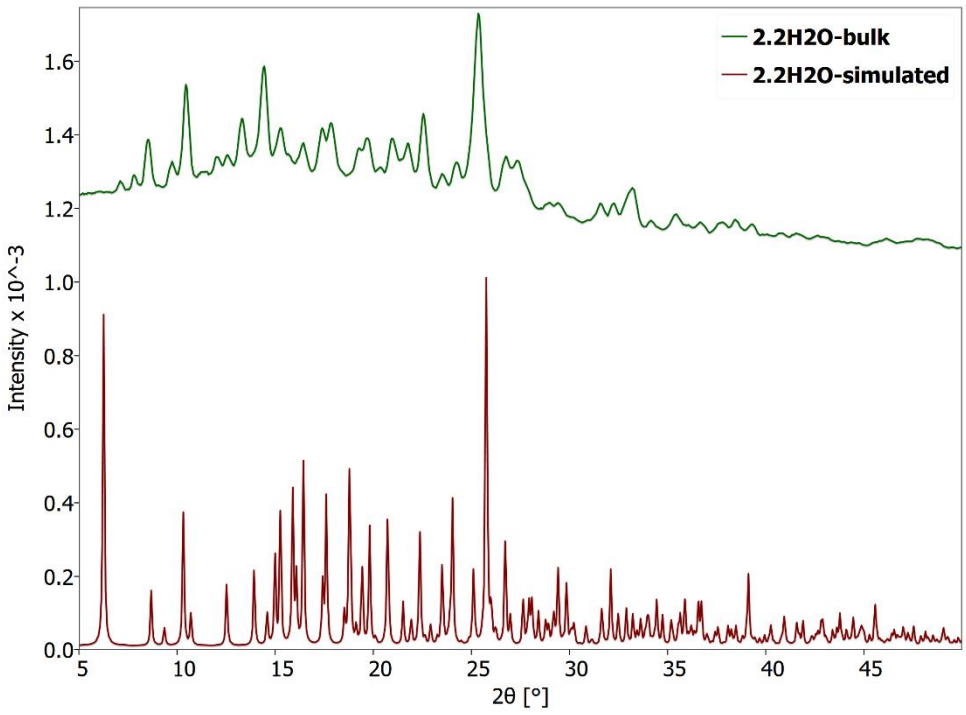


Figure S4 PXRD of $[Fe(qsal\text{-}I)_2]OTs{\cdot}2H_2O$.

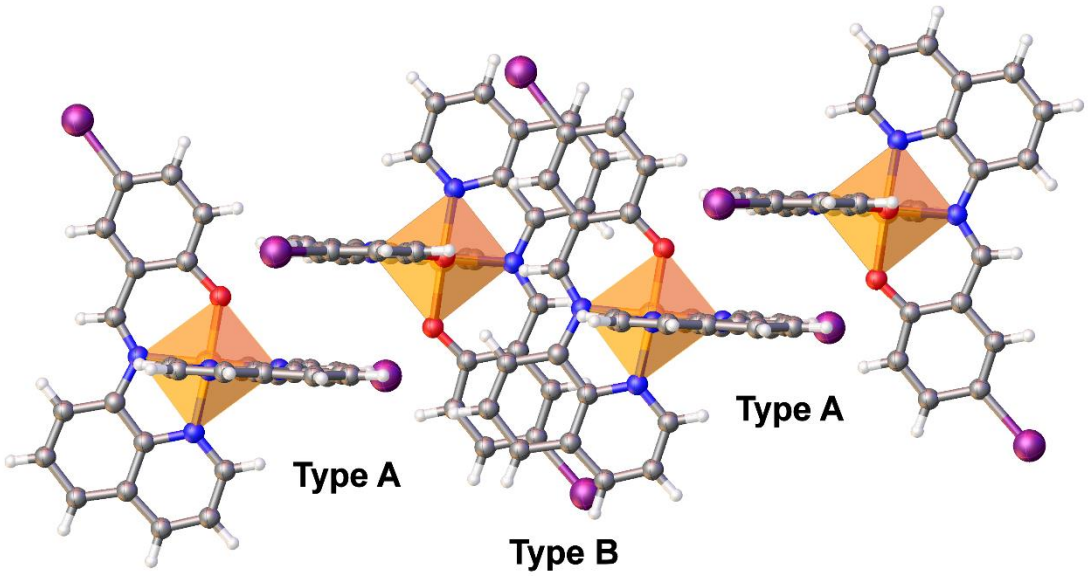


Figure S5 View of the Type A and Type B π-π interactions in [Fe(qsal-I)$_2$]OTs·2H$_2$O **2**·2H$_2$O.

DSC and TGA studies

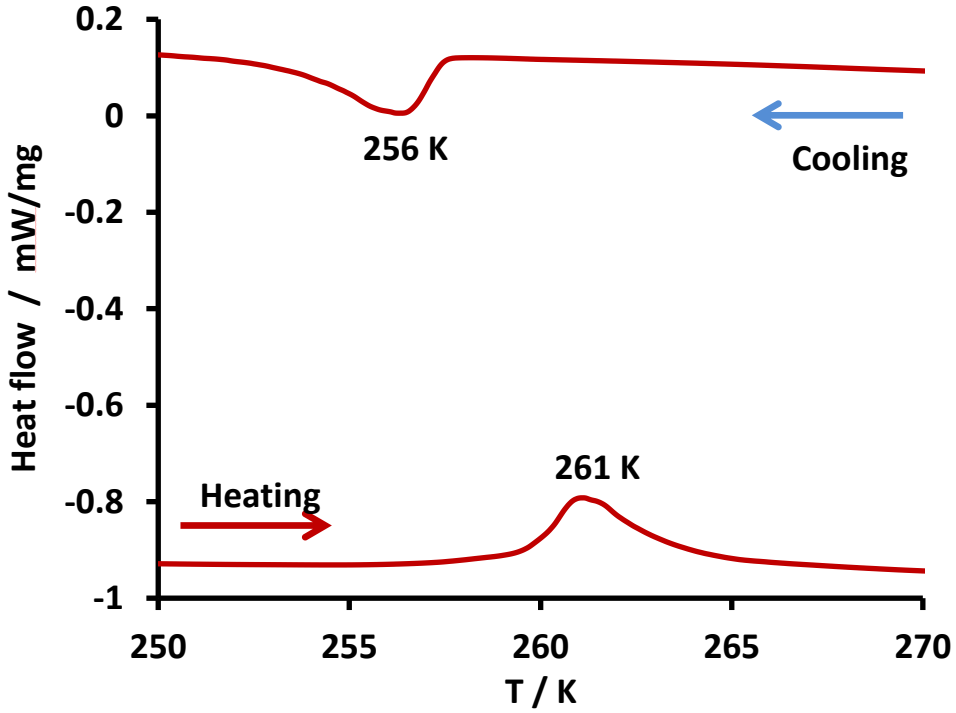


Figure S6 DSC plot for [Fe(qsal-Br)$_2$]OTs.

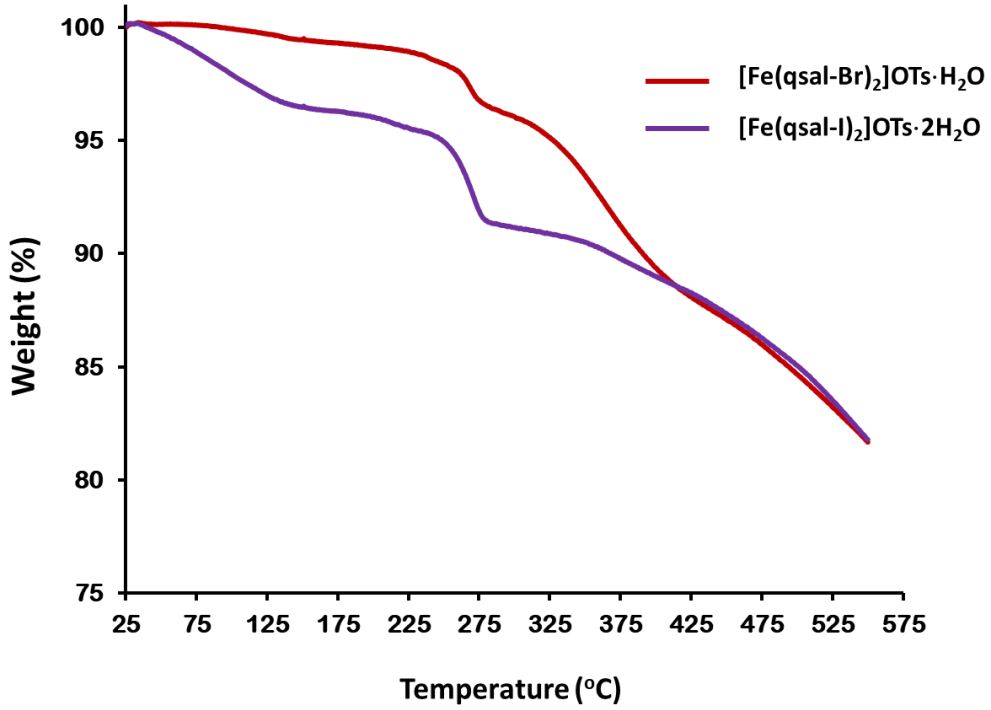


Figure S7 TGA studies of [Fe(qsal-X)$_2$]OTs.