Supporting Information

Solvent effects on the spin crossover properties of iron(II) imidazolylimine complexes

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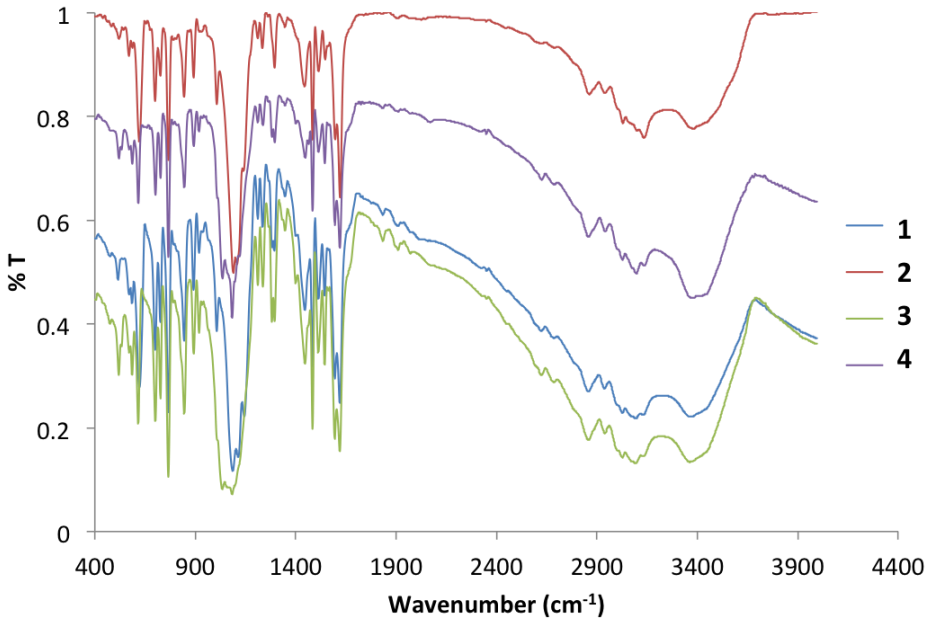


Figure S1 IR spectra of **1**- **4**.

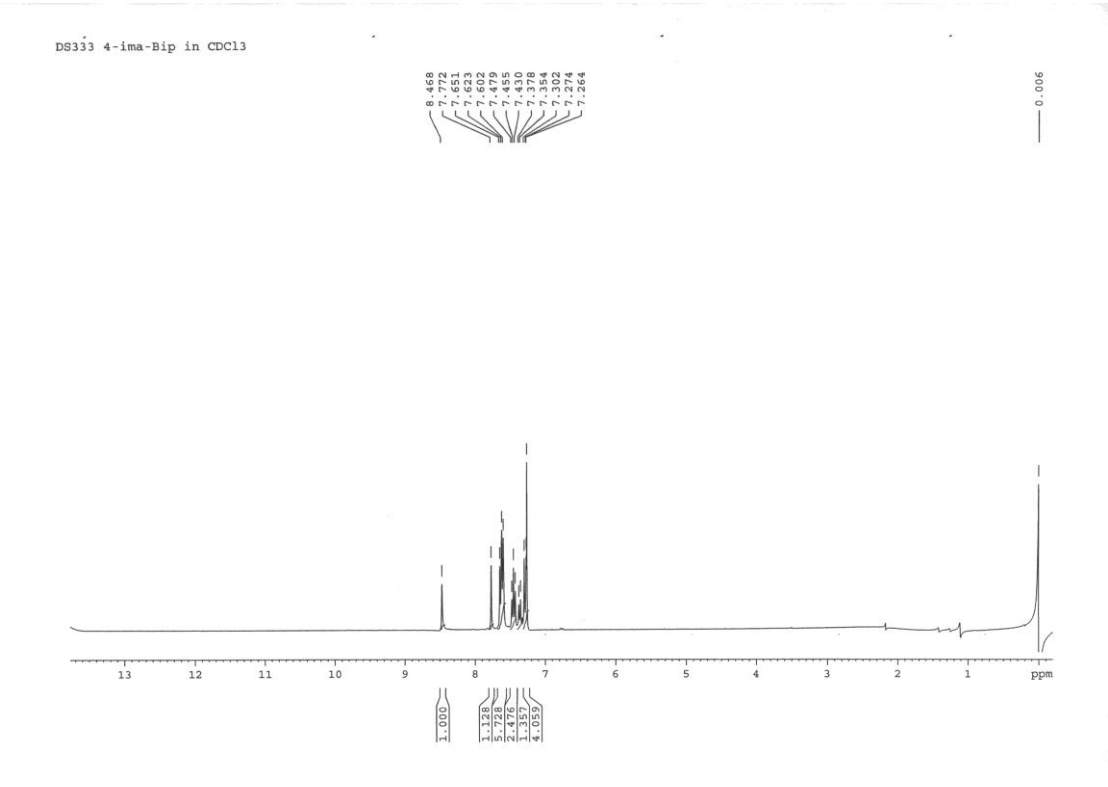


Figure S2 ^{1}H-NMR spectrum of 4-ima-Bp.

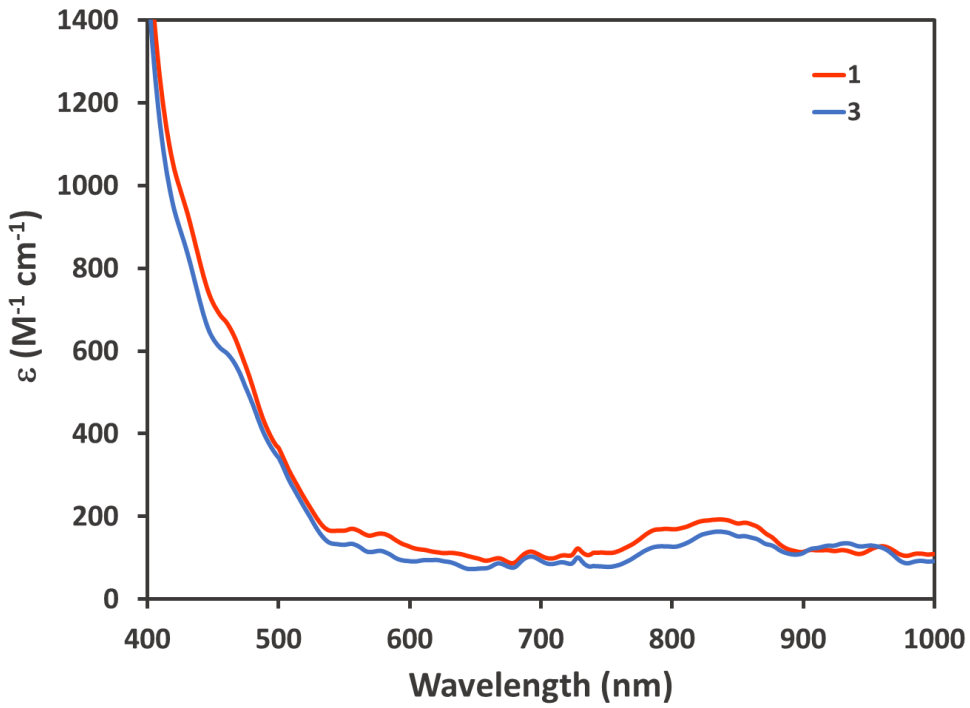


Figure S3 UV-Vis of $[Fe(4\text{-ima-Bp})_3](ClO_4)_2$ **1** and $[Fe(4\text{-ima-Bp})_3](BF_4)_2$ **3** in MeCN in a 0.1 M solution.

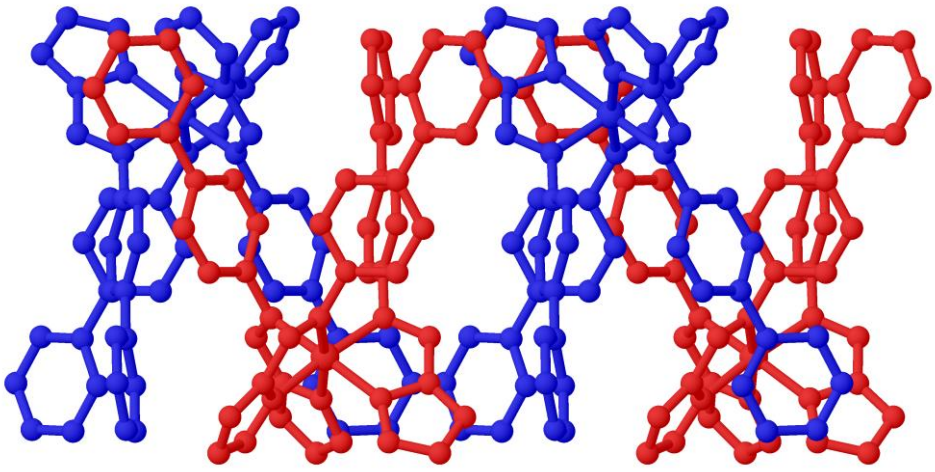


Figure S4 Side-on view of the packing in *fac*-$[Fe(4\text{-ima-Bp})_3](ClO_4)_2 \cdot 3MeOH$ **2**.

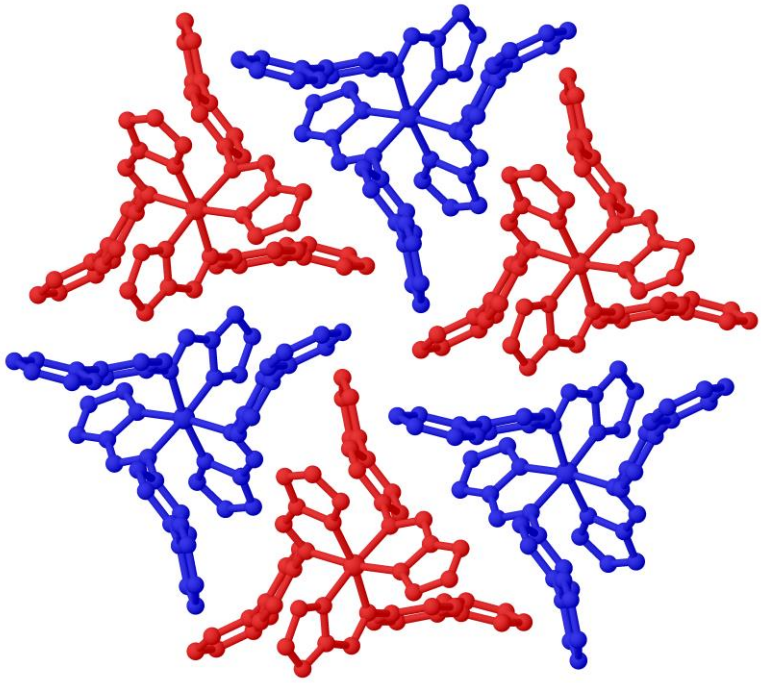
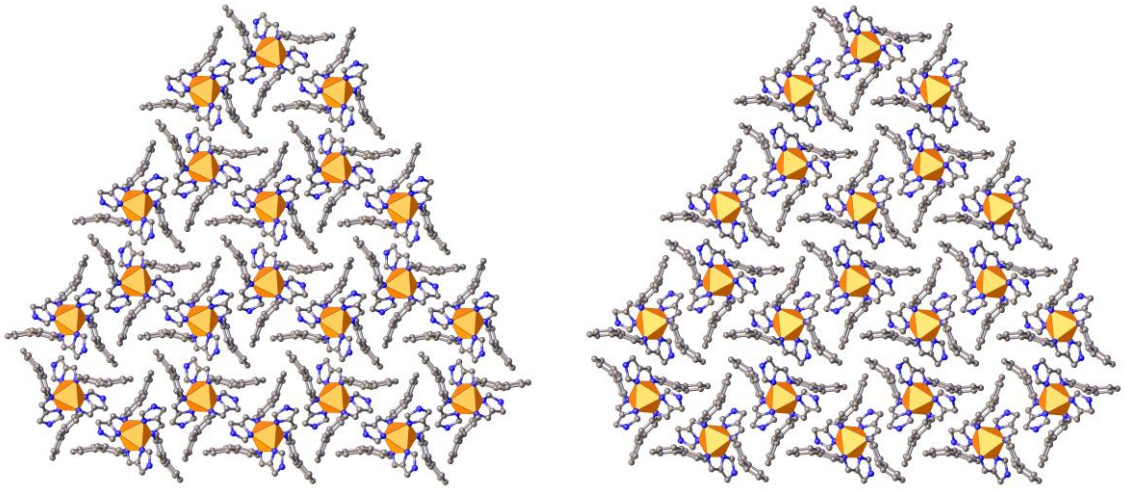


Figure S5 View of the *pseudo*-hexagonal packing motif in *fac*-[Fe(4-ima-Bp)$_3$](BF$_4$)$_2$·3.5MeCN **5**.



MeOH **MeCN**

Figure S6 Comparative view of the hexagonal and *pseudo*-hexagonal packing motifs found in **2** and **5**.

Table S1 Geometric parameters of C-H···π and π–π interactions in **1-2** and **5**.

Complex		Type	Distance
1	C10-H10···π (C5-C10)	*Intramolecular*	2.681 Å
	C7-H7···π (C5-C10)	Intermolecular	2.689 Å
	C13-H13···π (C11-C16)	Intermolecular	2.905 Å
2	C10-H10···π (C5-C10)	*Intramolecular*	2.635 Å
	C7-H7···π (C5-C10)	Intermolecular	2.630 Å
	C13-H13···π (C11-C16)	Intermolecular	2.808 Å
5	C42-H42···π (C5-C10)	*Intramolecular*	2.654 Å
	C10-H10···π (C21-C26)	*Intramolecular*	2.561 Å
	C22-H22···π (C37-C42)	*Intramolecular*	2.657 Å
	C25-H25···π (C5-C10)	Intermolecular	2.716 Å
	C39-H39···π (C21-26)	Intermolecular	2.776 Å
	C45-H45···π (C11-C16)	Intermolecular	3.055 Å
	π-π	-	3.690 Å

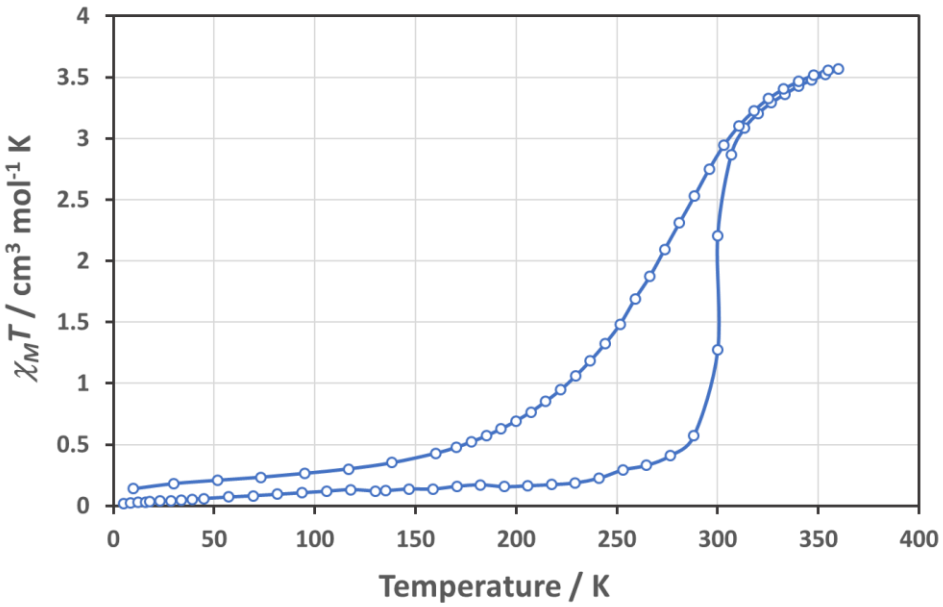


Figure S7 SQUID profile of *fac*-[Fe(4-ima-Bp)$_3$](ClO$_4$)$_2$·3EtOH **1**.

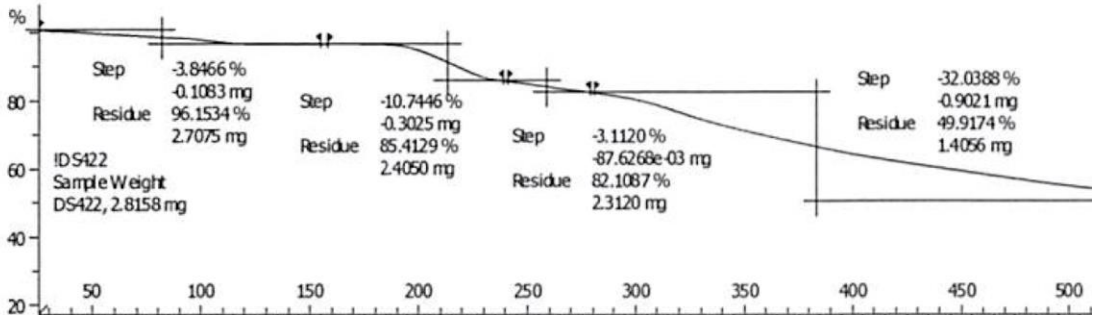


Figure S8 TGA of *fac*-[Fe(4-ima-Bp)$_3$](ClO$_4$)$_2$·3EtOH **1**.

The first mass loss of 3.85% occurs at *ca*. 80 °C and is consistent with one equivalent of EtOH (calculated 4.06%). The second mass loss of 10.74% occurs at ca. 210 °C and is broadly suggestive of loss of the two remaining EtOH molecules (calculated 8.12%).