Supporting Information

Solvatomorphism and anion effects in predominantly low spin iron(III) Schiff base complexes

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Contents

NMR and IR spectra of HnaphEen and [Fe(naphEen)$_2$]halide

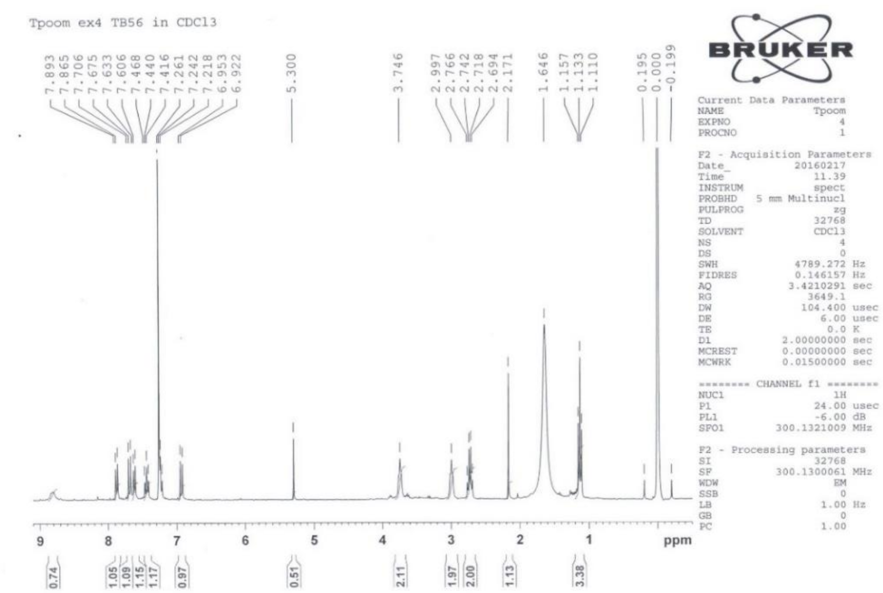


Figure S1 ^{1}H NMR spectrum of HnaphEen. Note that the peak 1.65 ppm is due to water.

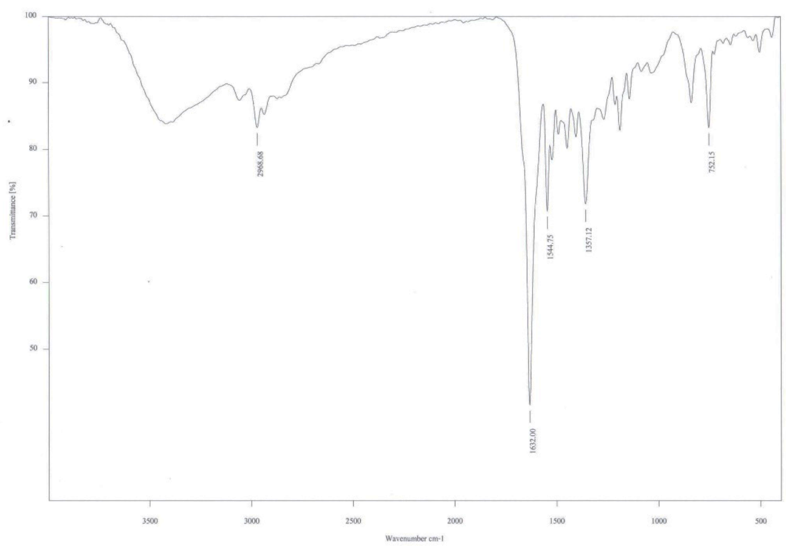
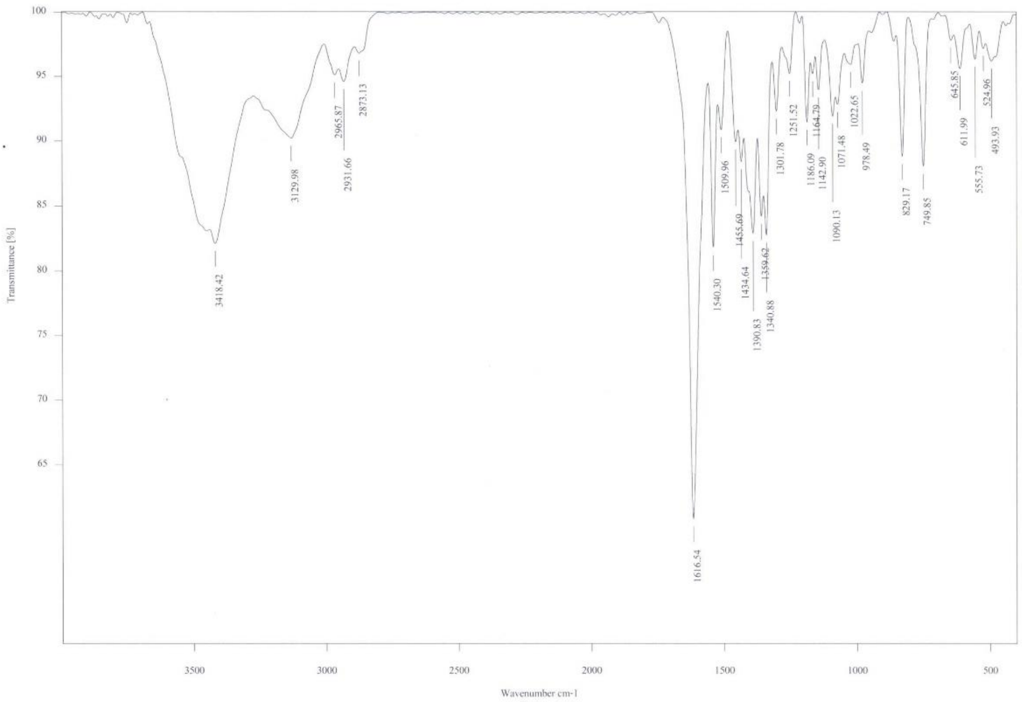


Figure S2 IR spectrum of HnaphEen.

F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Wavenumber cm-1
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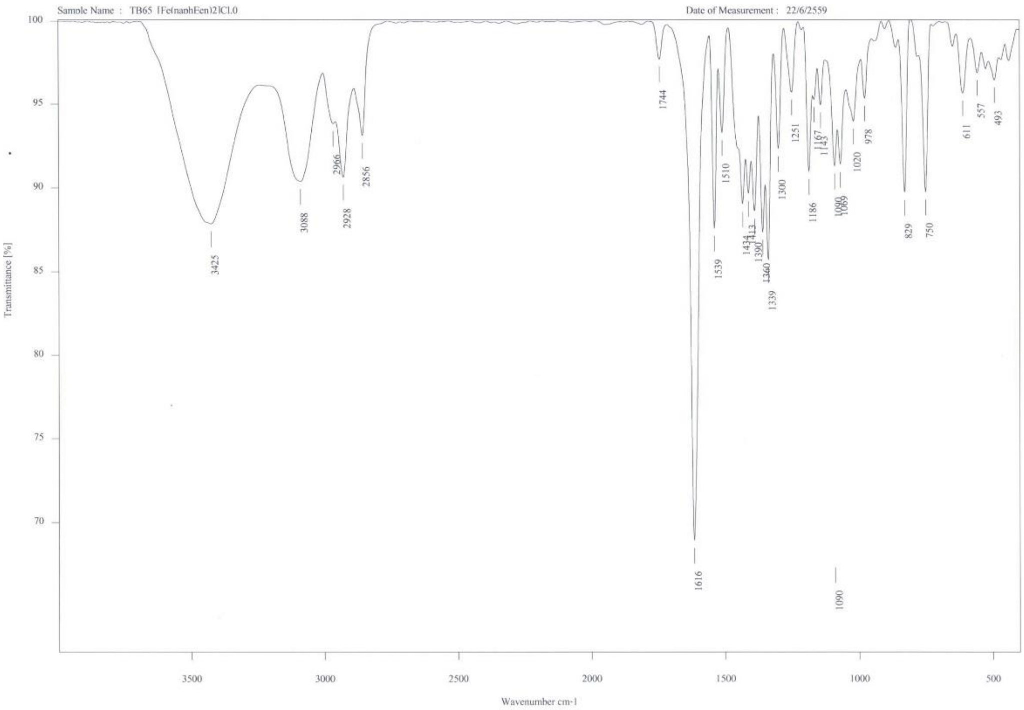
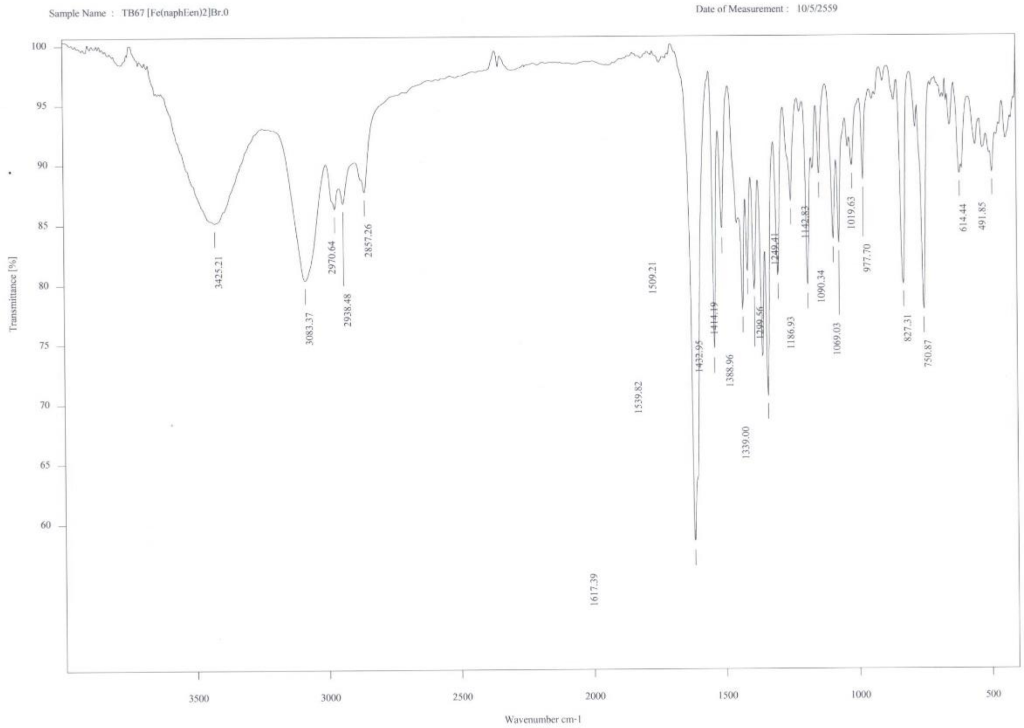
3129.98
2965.87
2931.66
2873.13
1616.54
1540.30
1509.96
1455.69
1434.64
1390.83
1359.62
1340.88
1301.78
1251.52
1186.09
1164.79
1142.90
1090.13
1071.48
1022.65
978.49
829.17
749.85
645.85
611.99
555.73
524.96
493.93

Cl


Sample Name : TB65 [Fe(naphEen)2]Cl.0
Date of Measurement : 22/6/2559
Transmittance [%]
Wavenumber cm-1
3425
3088
2966
2928
2856
1744
1616
1539
1510
1434
1413
1390
1360
1339
1300
1251
1186
1167
1145
1090
1080
1069
1020
978
829
750
611
557
493

Br



I

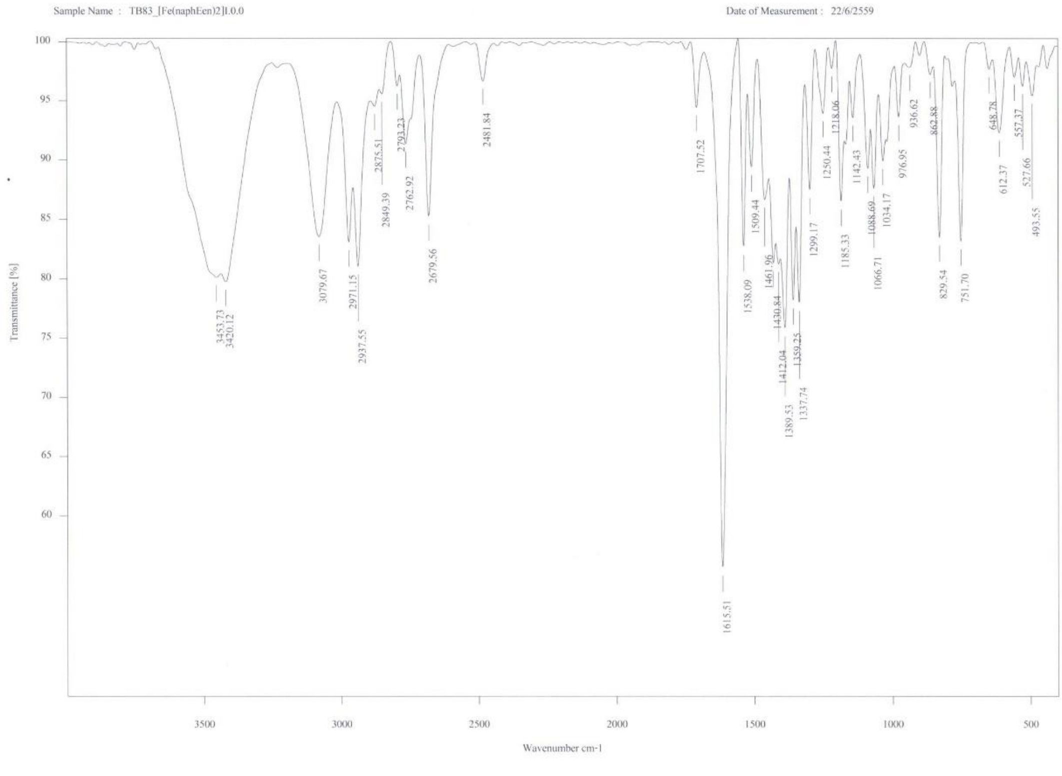


Figure S3 IR spectra of [Fe(naphEen)$_2$]halide.

TGA Studies of [Fe(naphEen)$_2$]F

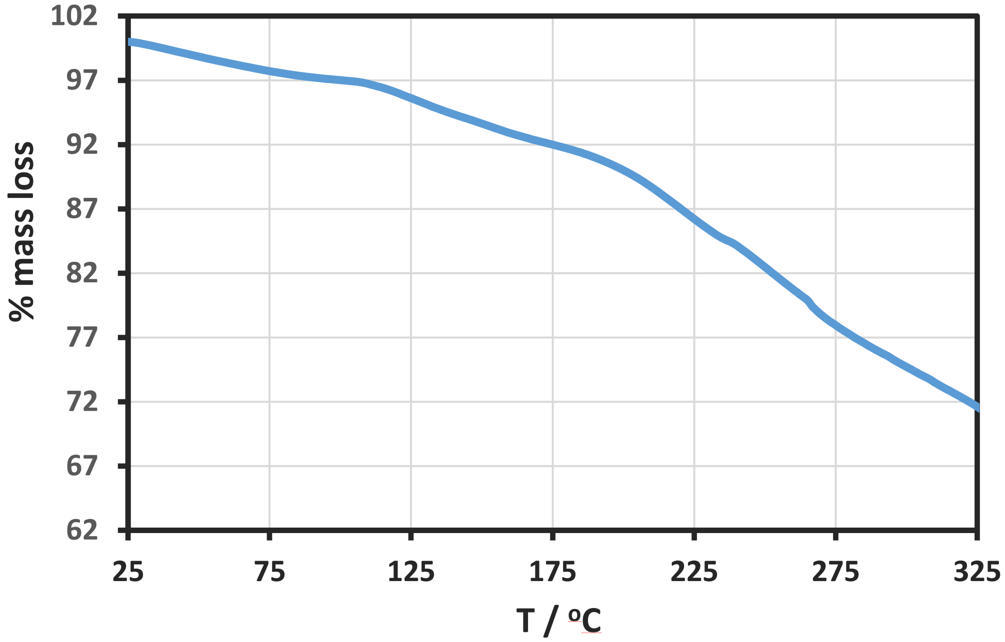
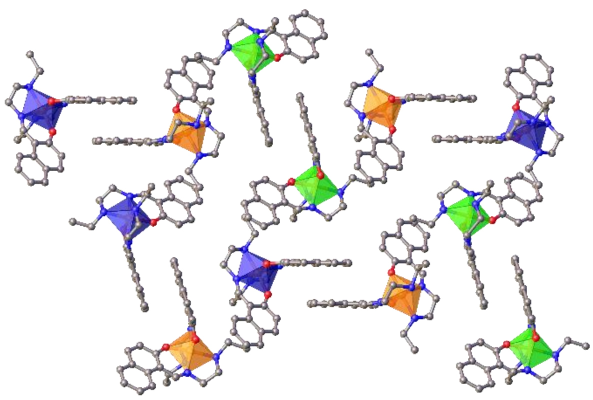
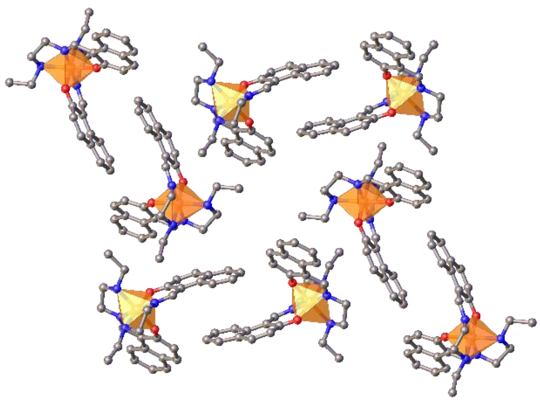


Figure S4 TGA analysis of [Fe(naphEen)$_2$]F.

Crystal Packing



[Fe(naphEen)$_2$]Br·0.5H$_2$O



[Fe(naphEen)$_2$]I

Figure S5 View of the supramolecular squares in **3** and **4** at 293 K. In the case of **3** the Fe1, Fe2 and Fe3 centres are coloured orange, purple and green, respectively.

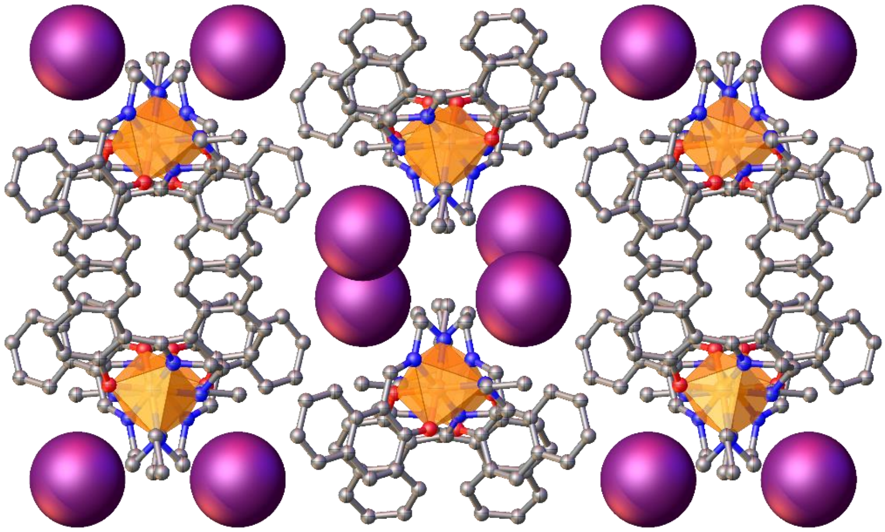


Figure S6 View of the 'Butterfly' motif in [Fe(naphEen)$_2$]I **4** viewed down the *a* axis.

Table S1 Summary of the supramolecular contacts in [Fe(naphEen)$_2$]Cl·H_2O **2** and [Fe(naphEen)$_2$]Br·H_2O **3** that make up the Fe squares.

	2-123 K	**3-123 K**	**3-293 K**
Fe1			**Fe1-Fe2**
C-H···π	2.831(3) {H27B···Cg (C9-C10)}	2.861(4) {H27A···Cg (C9-C10)}	2.86(3) (H52···C18)
π-π	3.253(6) (plane-to-plane) 3.731(4) (Cg ···Cg)	3.283(9) (plane-to-plane) 3.782(6) (Cg···Cg)	3.19(4) (C22···C37)
Fe2			**Fe-3**
C-H···O	2.638(4) (H39···O4)	2.672(5) (H39···O4)	-
C-H···π	2.694(6) (H55···C32)	2.689(8) (H55···C32)	2.781(15) {H90B···Cg (C1-C6)}
C-H···π	2.769(4) {H27B···Cg (C35-C40)}	2.810(5) {H27B···Cg (C35-C40)}	2.79(1) {H87B···Cg (C35-C40)}
C-H···π	-	-	2.82(2) (H82···C33)
π-π	-	-	3.16(6) {C67···C67*)

Table S2 Summary of the supramolecular contacts in [Fe(naphEen)$_2$]I **4** that make up the Fe squares.

	4-293 K
Fe1	
C-H···π	2.84(3) (H23··· C2)
	2.707(9) (H30B···Cg)
π-π	3.30(3) (plane-to-plane)
	4.366(17) (Cg···Cg)
C-H···I	3.089(2) (H18 ··I1)

Mössbauer spectroscopic studies

Table S3 ^{57}Fe Mössbauer spectral properties of **1**.

T (K)	State	δ (mm/s)	ΔE_Q (mm/s)	B (T)	Γ_L (mm/s)	Γ_R (mm/s)	I (%)
291	**HS**	0.39	0.71	-	0.50	0.53	71
	LS	0.16	2.70	-	0.49	0.42	29
5.1	**HS**	0.51	0.69	-	0.56	0.57	36
	HS2	0.50	-	48	0.70	0.70	20
	LS	0.22	2.79		0.61	0.44	44