Supporting Information

Spin Crossover Fe^{III} Complexes with a Substituted Hqnal Ligand: Effects of Anions and Solvents

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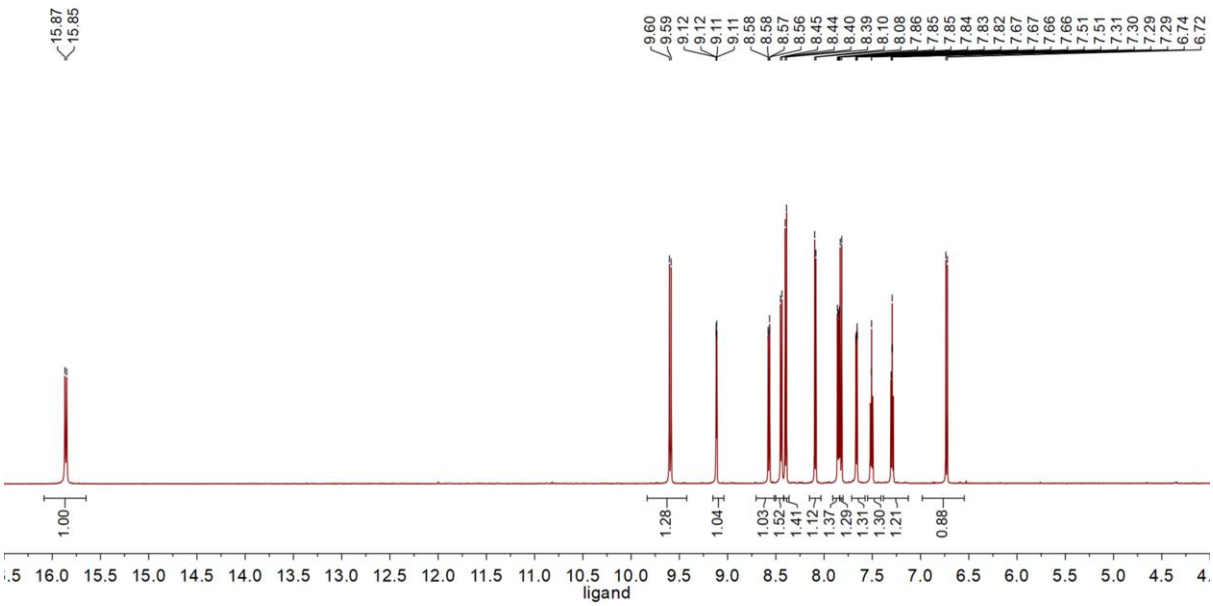

Figure S1. ^{1}H NMR spectrum of ligand Hqnal-5-Br$_q$ in DMSO-d6: δ = 15.86 (d, *J* = 11.0 Hz, 1H), 9.59 (d, *J* = 11.1 Hz, 1H), 9.12 (dd, *J* = 4.1, 1.6 Hz, 1H), 8.57 (dd, *J* = 8.5, 1.6 Hz, 1H), 8.44 (d, *J* = 8.3 Hz, 1H), 8.40 (d, *J* = 8.4 Hz, 1H), 8.09 (d, *J* = 8.3 Hz, 1H), 7.85 (dd, *J* = 8.5, 4.1 Hz, 1H), 7.82 (d, *J* = 9.4 Hz, 1H), 7.66 (dd, *J* = 7.8, 1.4 Hz, 1H), 7.51 (d, *J* = 1.4 Hz, 1H), 7.39–7.13 (m, 1H), 6.73 (d, *J* = 9.4 Hz, 1H).

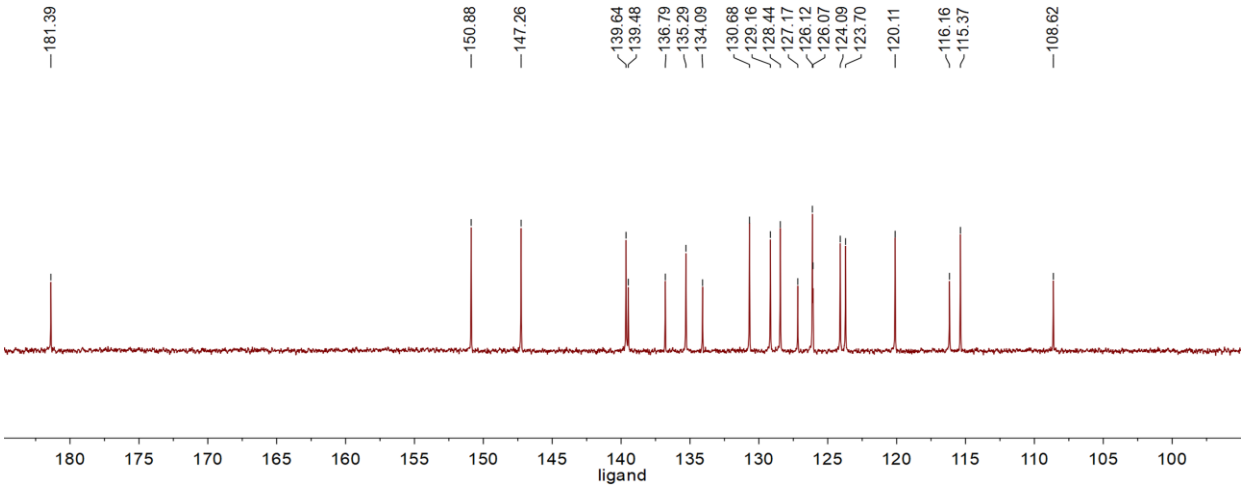

Figure S2. ^{13}C NMR spectrum of ligand Hqnal-5-Br$_q$ in DMSO-d6: δ = 181.39, 150.88, 147.26, 139.64, 139.48, 136.79, 135.29, 134.09, 130.68, 129.16, 128.44, 127.17, 126.12, 126.07, 124.09, 123.70, 120.11, 116.16, 115.37, 108.62.

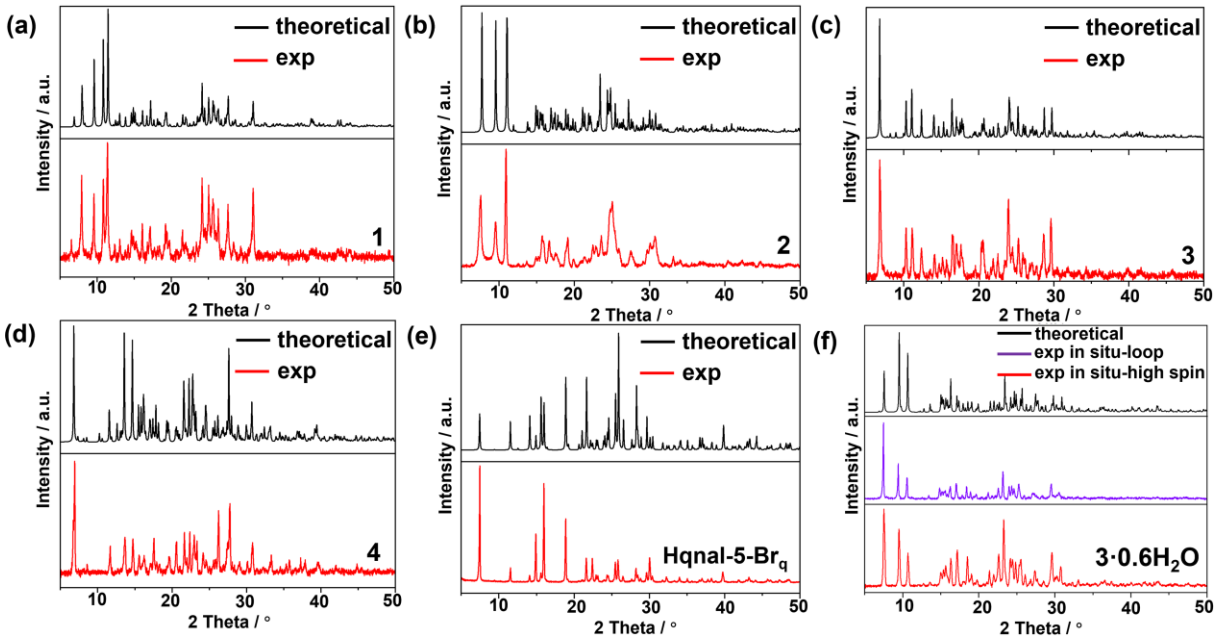

Figure S3. Experimental PXRD patterns (red) measured at 300 K and simulated patterns (black) based on single crystal structures for **1-4** (a-d) and Hqnal-5-Br$_q$ (e); (f) PXRD patterns of the *in-situ* desolvated sample of **3** after the magnetic measurement (purple and red) and the simulated patterns based on the single crystal structure of **3·0.6H$_2$O** (black).

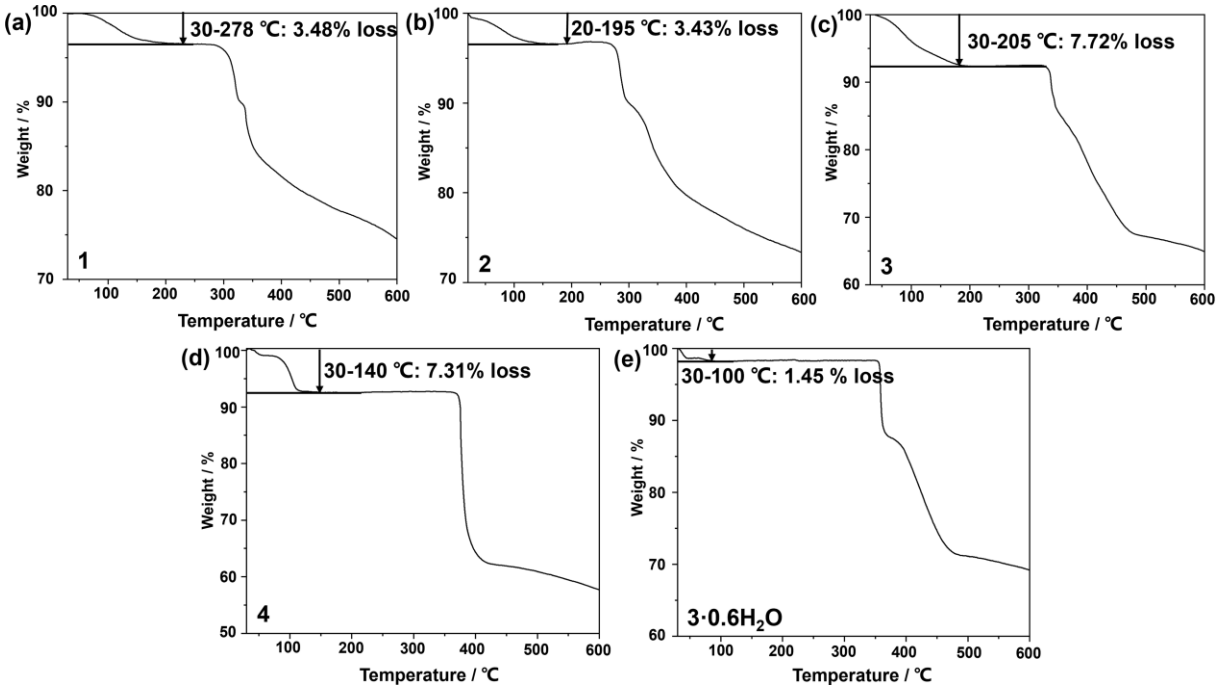

Figure S4. TGA curves of **1-4** (a-d) and **3·0.6H$_2$O** (e)

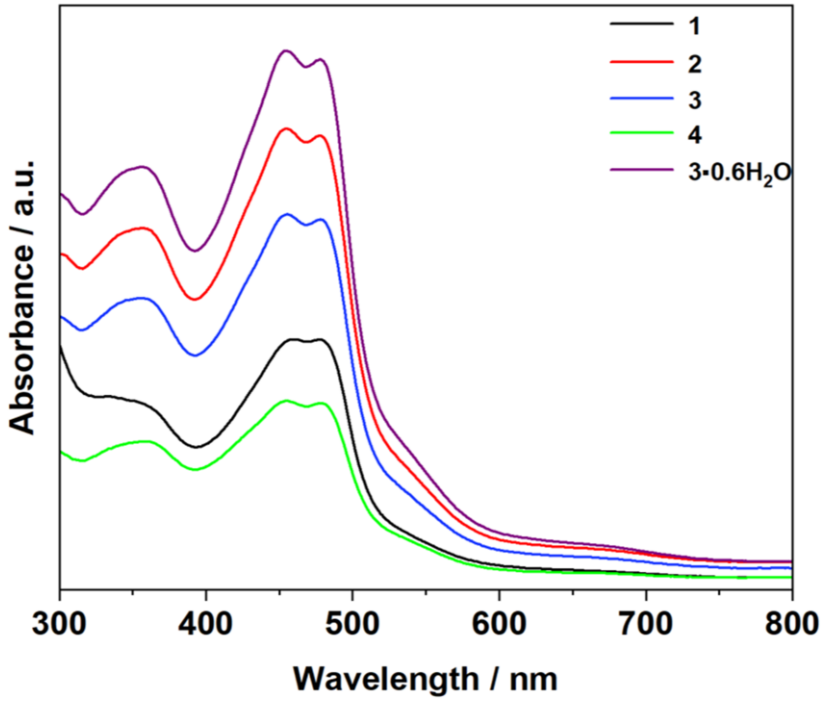

Figure S5. UV-visible spectra of **1**–**4** and **3·0.6H$_2$O** in CH_2Cl_2.

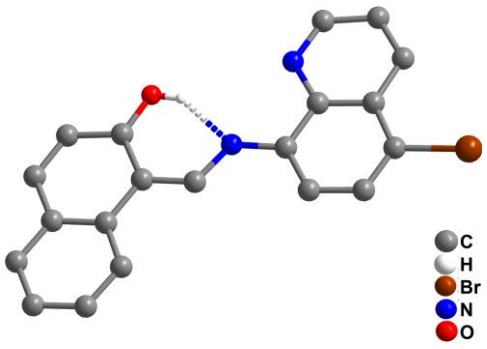

Figure S6. Asymmetric unit of Hqnal-5-Br$_q$ at 193 K.

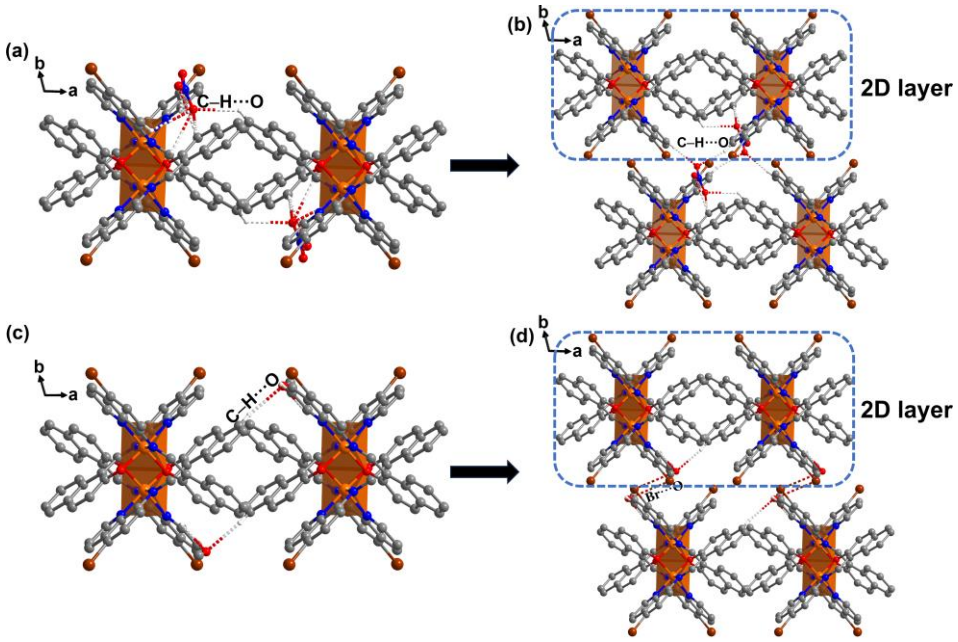

Figure S7. The 2D layers and 3D structure of **1**: the C–H···O interactions between the NO_3^- anions and the cations (a) and (b); the C–H···O and Br···O interactions between the solvents and the cations (c) and (d).

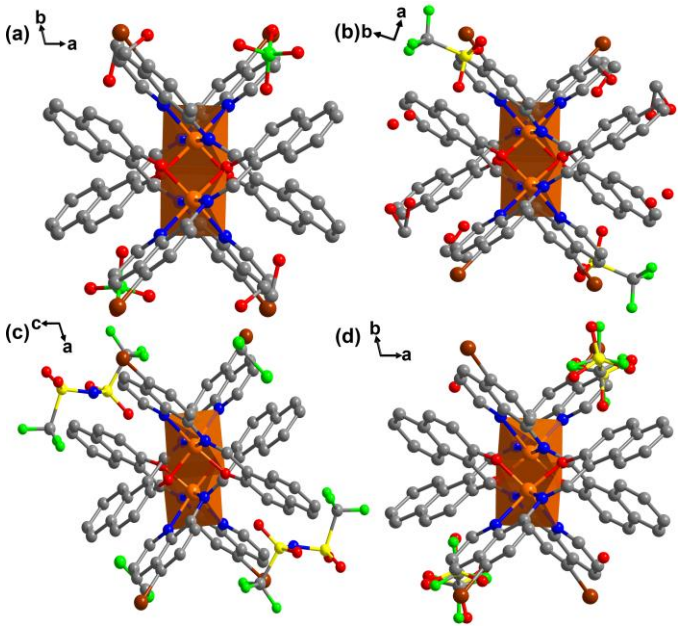

Figure S8. The 1D cross-section of complexes **2-4** (a-c) and **3·0.6H$_2$O** (d).

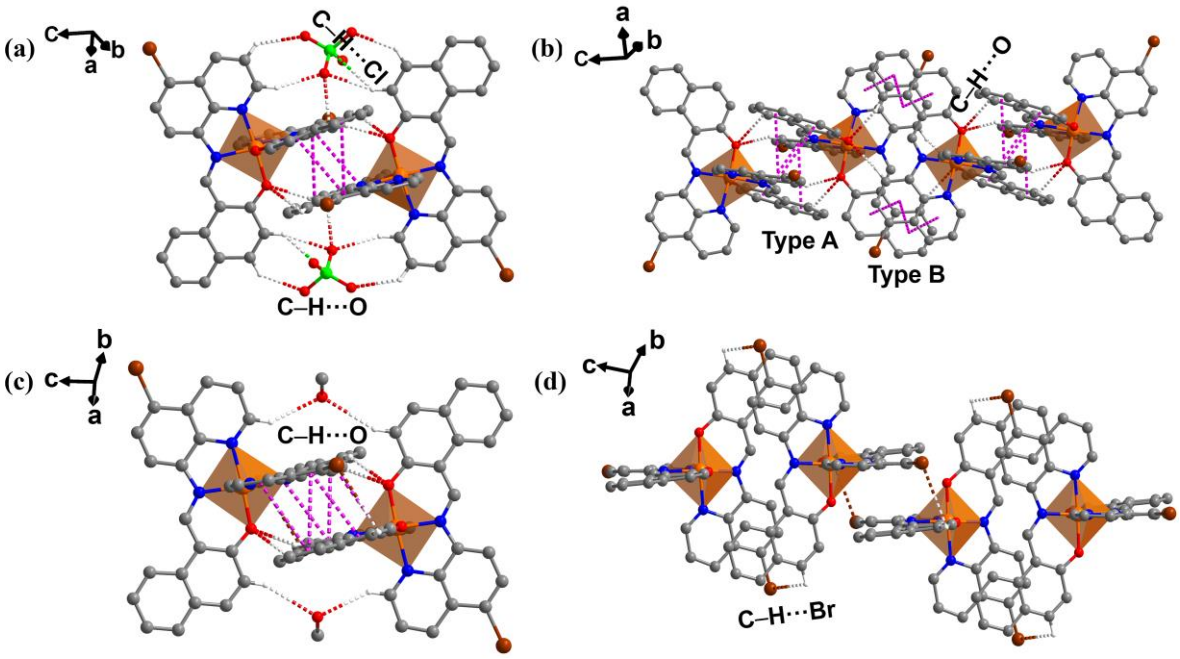

Figure S9. The 1D chain of **2**: (a) the C–H···O/Cl interactions between the ClO_4^- anions and the cations; (b) Type A and Type B π···π interactions and the C–H···O interactions between the cations; (c) the C–H···O interactions between the solvent and the cations; (d) the C–H···Br interactions between the cations.

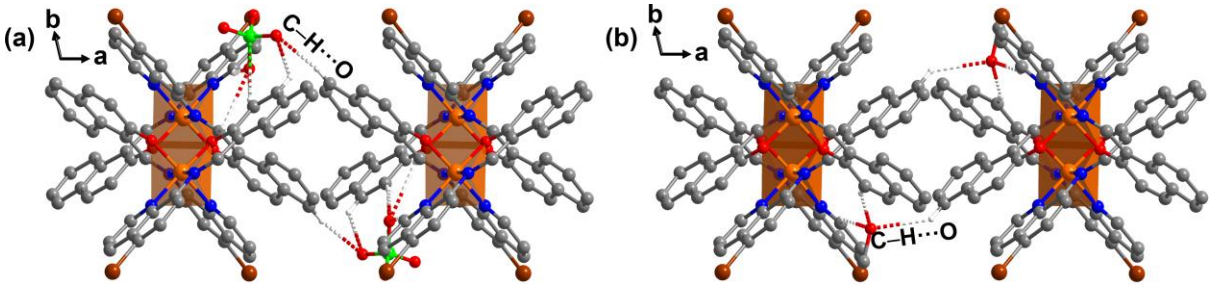

Figure S10. The 2D layer of **2**: (a) the C–H···O interactions between the ClO_4^- anions and the cations; (b) the C–H···O interactions between the solvents and the cations.

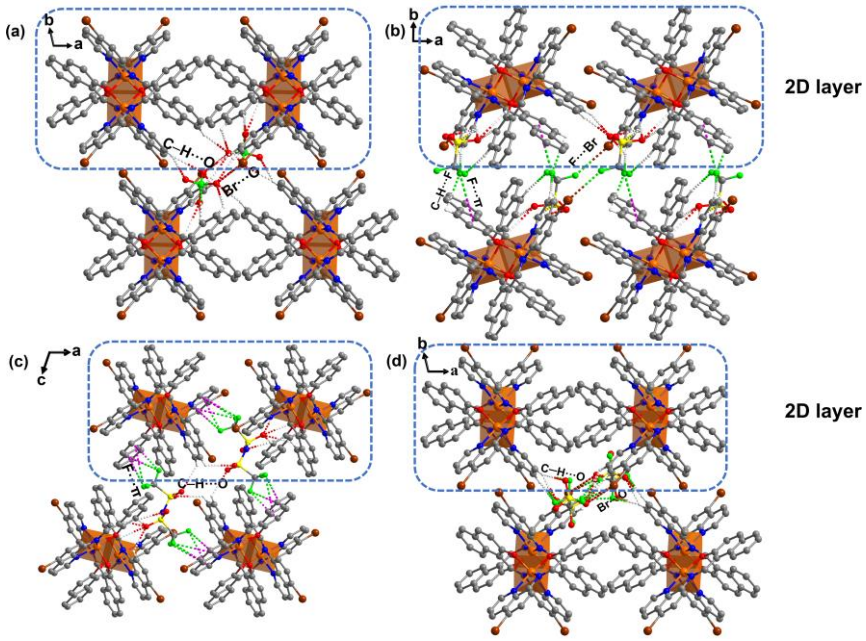

Figure S11. 3D structures of **2-4** and **3·0.6H$_2$O** (a) The C–H···O and Br···O interactions between the 2D layers of **2**; (b) The C–H···O and F···Br/π interactions between the 2D layers of **3**; (c) The C–H···O and F···Br/π interactions between the 2D layers of **4**; (d) The C–H···O and Br···O interactions between the 2D layers of **3·0.6H$_2$O**.

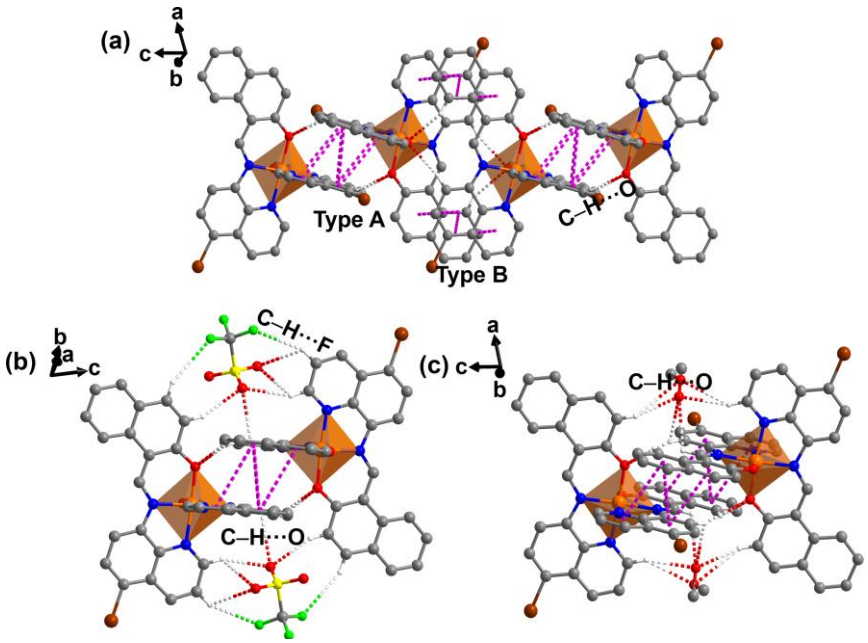

Figure S12. The 1D chain of **3**: (a) Type A and Type B π···π interactions and the C–H···O interactions between the cations; (b) the C–H···O/F interactions between the OTf$^-$ anions and cations; (c) the C–H···O interactions between the solvents and cations.

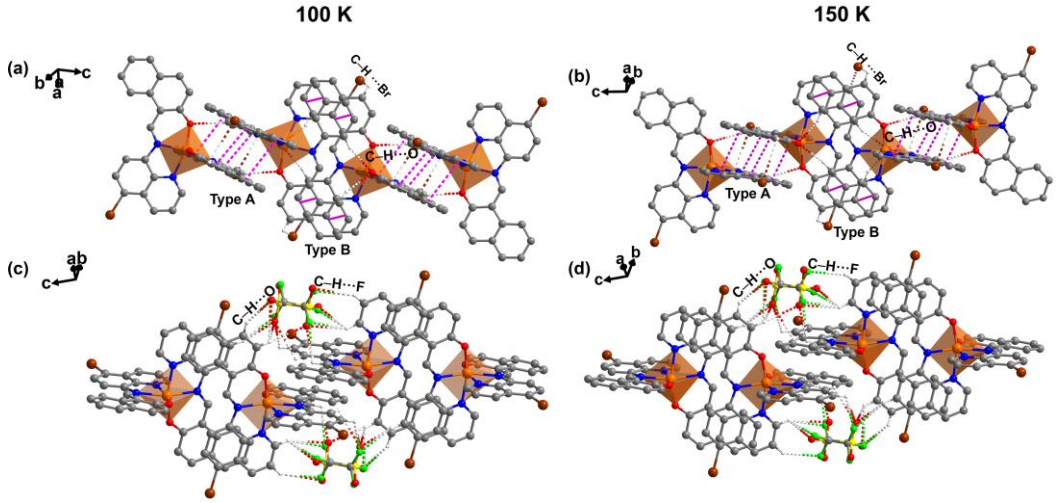

Figure S13. The 1D chain of **3·0.6H$_2$O**: (a-b) Type A and Type B π···π interactions, the C–H···O and the C–H···Br interactions between the cations; (c-d) the C–H···O/F interactions between the OTf^- anions and the cations.

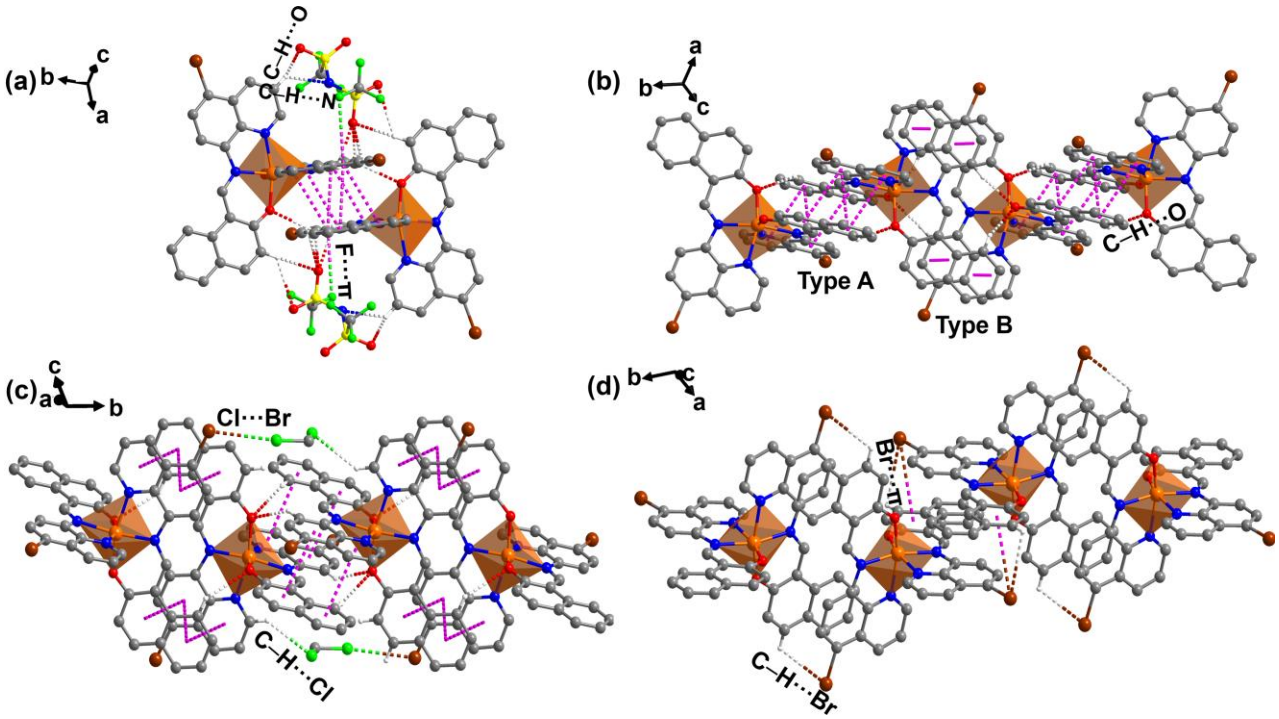

Figure S14. The 1D chain of **4**: (a) the C–H···O/N and F···π interactions between the cations and the NTf_2^- anions; (b) Type A and Type B π···π interactions and the C–H···O interactions between the cations; (c) the C–H···Cl and Cl···Br interactions between the solvents and the cations; (d) the C–H···Br and Br···π interactions between the cations.

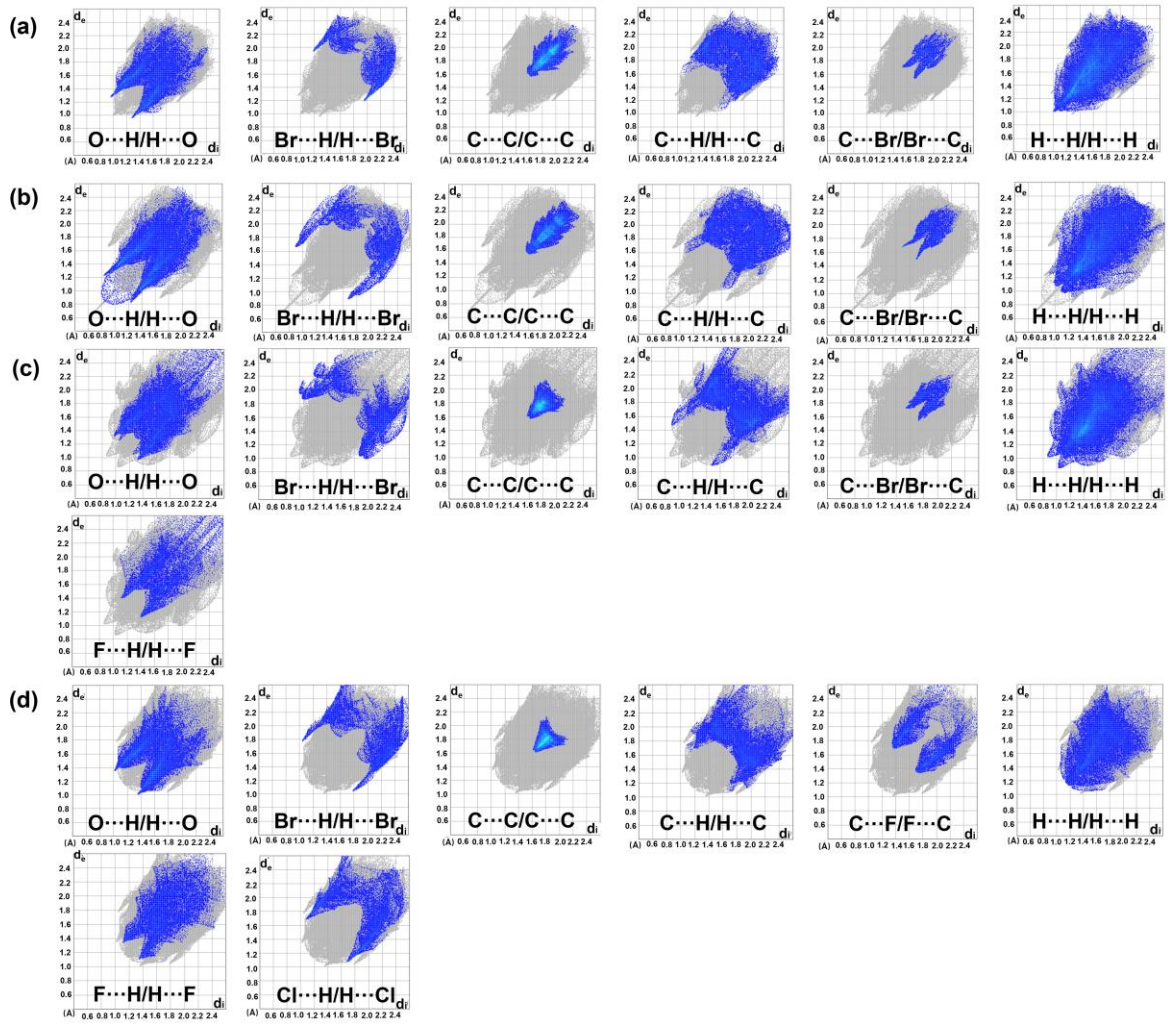

Figure S15. Hirshfeld surface 2D fingerprint plots for **1-4** (a-d) at low temperature.

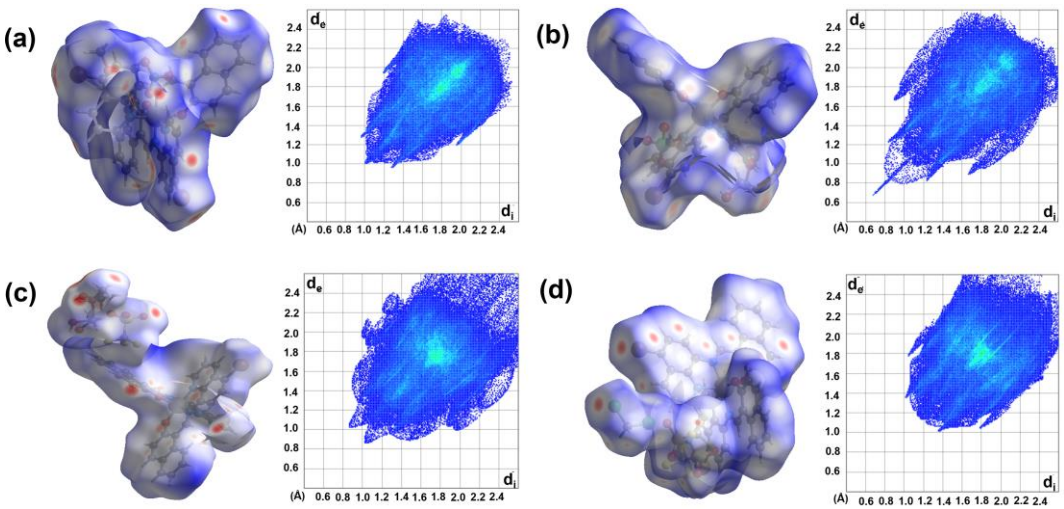

Figure S16. Hirshfeld surface mapped with d_{norm} and Hirshfeld surface 2D fingerprint plots for all contacts for **1-4** (a-d) at low temperature.

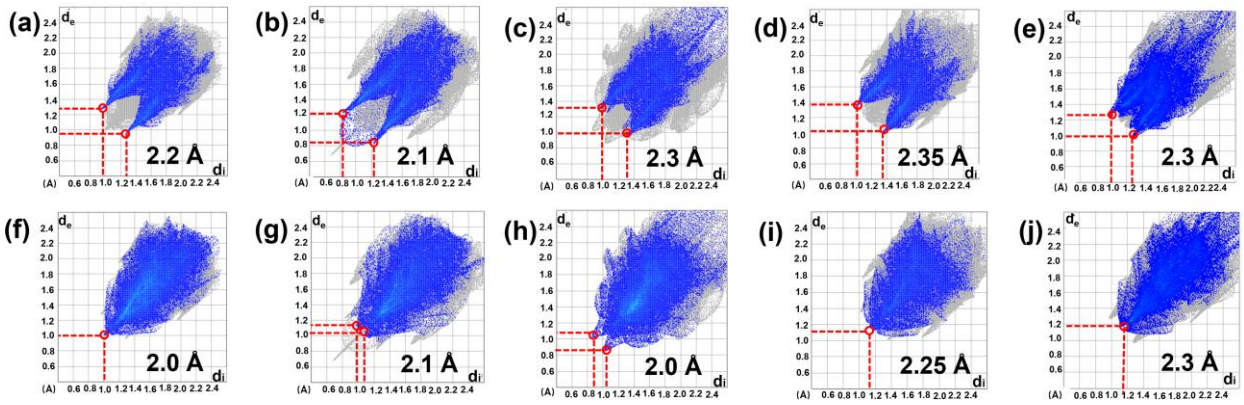

Figure S17. Hirshfeld surface 2D fingerprint plots of H···O/O···H corresponding to (a)-(e) and H···H/H···H corresponding to (f)-(j) for **1-4 and 3·0.6H$_2$O** at low temperature.

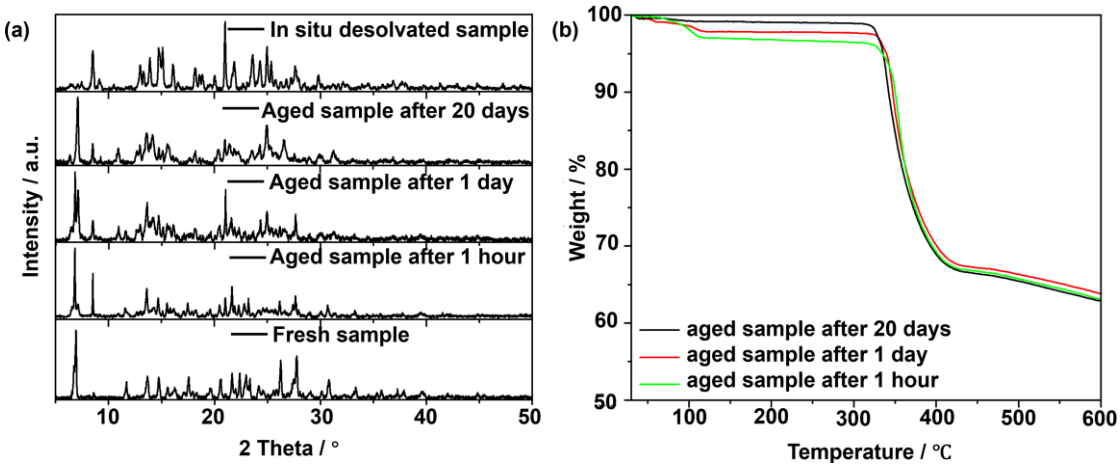

Figure S18. PXRD patterns (a) and TGA curves (b) of complex **4** after different aging times.

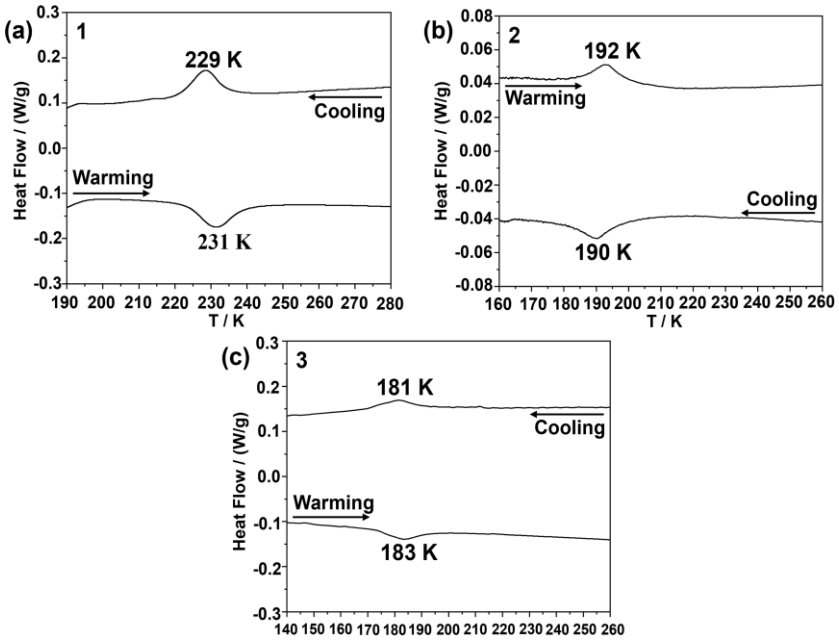

Figure S19. DSC curves at a sweep rate of 5 K·min^{-1} for **1** (a), **2** (b) and **3** (c).

Table S1. Crystallographic data and structure refinement parameters of **1** and **2**.

Complex	**1**		**2**
Formula	$C_{41}H_{28}Br_2FeN_5O_6$		$C_{41}H_{28}Br_2FeN_4O_7$
Formula weight	902.35		939.79
T / K	100	300	90
Crystal system	Triclinic	Triclinic	Triclinic
Space group	$P\bar{1}$	$P\bar{1}$	$P\bar{1}$
a / Å	11.352(3)	11.649(7)	11.811(2)
b / Å	12.600(3)	12.268(8)	12.312(2)
c / Å	13.448(3)	13.964(8)	13.297(2)
α / °	110.230(7)	110.74(3)	106.646(8)
β / °	94.715(8)	95.023(17)	93.560(8)
γ / °	103.082(8)	103.366(19)	101.853(8)
V / Å^3	1730.8(7)	1784.0(18)	1797.9(5)
Z	2	2	2
ρ_{calcd} / g·cm^{-3}	1.731	1.620	1.736
μ / mm^{-1}	4.530	4.366	4.833
F (000)	906.0	870.0	942
R_{int}	-	-	-
GOF on F^2	1.122	1.099	1.006
R_1 / wR_2 ($I \geqslant 2\sigma(I)$)	0.0676 / 0.1924	0.0868 / 0.2052	0.1050 / 0.2356
R_1 / wR_2 (all data)	0.0821/ 0.2265	0.1384 / 0.2316	0.1543 / 0.2632
CCDC	2367591	2367592	2367593
$^aR_1 = \Sigma\|\|F_o\| - \|F_c\|\|/\Sigma\|F_o\|$ $^b wR_2 = \{\Sigma[w(F_o^2 - F_c^2)^2] / \Sigma[w(F_o^2)^2]\}^{1/2}$			

Table S2. Crystallographic data and structure refinement parameters of **3** and **3·0.6H$_2$O**.

Complex	**3**		**3·0.6H$_2$O**	
Formula	$C_{34}H_{34}Br_2F_3FeN_4O_8S$		$C_{41}H_{25.2}Br_2FeN_4O_{5.6}S$	$C_{41}H_{25.2}Br_2FeN_4O_{5.6}S$
Formula weight	1039.47		968.17	968,17
T / K	100	300	150 K	100 K
Crystal system	Triclinic	Triclinic	Triclinic	Triclinic
Space group	$P\bar{1}$	$P\bar{1}$	$P\bar{1}$	$P\bar{1}$
a / Å	12.0896(18)	11.794(8)	12.0862(18)	12.0553(8)
b / Å	13.4142(19)	13.661(8)	12.2200(17)	12.1274(8)
c / Å	13.4157(18)	13.806(7)	13.5092(19)	13.4499(9)
α / º	71.329(5)	72.55(3)	107.475(5)	107.357(2)
β / º	73.875(5)	73.62(3)	90.727(6)	90.604(2)
γ / º	83.853(5)	85.64(3)	102.509(6)	102.644(2)
V / Å^3	1979.7(5)	2036 (2)	1851.5(5)	1825.2(2)
Z	2	2	2	2
ρ_{calcd} / g·cm^{-3}	1.744	1.696	1.737	1.762
μ / mm^{-1}	4.441	4.302	4.673	2.731
F (000)	1046.0	1046.0	966	966
R_{int}	0.0665	0.0376	0.0478	0.0396
GOF on F^2	1.116	1.094	1.085	1.047
R_1 / wR_2 ($I \geqslant 2\sigma(I)$)	0.0630 / 0.1678	0.0531 / 0.1443	0.0430 / 0.1135	0.0375 / 0.0914
R_1 / wR_2 (all data)	0.0919/ 0.1783	0.0768 / 0.1731	0.0522 / 0.1230	0.0435 / 0.0958
CCDC	2367594	2367595	2367596	2384171
$^aR_1 = \Sigma\|\|F_o\| - \|F_c\|\|/\Sigma\|F_o\|$ $^b wR_2 = \{\Sigma[w(F_o^2 - F_c^2)^2] / \Sigma[w(F_o^2)^2]\}^{1/2}$				

Table S3. Crystallographic data and structure refinement parameters of **4** and Hqnal-5-Br_q.

Complex	**4**		Hqnal-5-Br_q
Formula	$C_{43}H_{26}Br_2Cl_2F_6FeN_5O_6S_2$		$C_{32}H_{22}Br_2N_4O_2$
Formula weight	1173.38		377.23
T / K	100	300	193
Crystal system	Triclinic	Triclinic	Orthorhombic
Space group	$P\bar{1}$	$P\bar{1}$	*Pbca*
a / Å	13.346(3)	13.2508(12)	15.340(2)
b / Å	13.720(3)	13.8357(13)	8.4310(13)
c / Å	13.909(3)	14.0684(14)	23.738(4)
α / °	104.951(6)	104.455(3)	90
β / °	101.543(7)	99.916(4)	90
γ / °	112.366(6)	111.885(3)	90
V / Å^3	2145.0(8)	2214.3(4)	3070.2(8)
Z	2	2	8
ρ_{calcd} / g·cm^{-3}	1.817	1.760	1.632
μ / mm^{-1}	5.234	5.070	2.450
F (000)	1166.0	1166.0	1520.0
R_{int}	0.0492	0.0635	0.0700
GOF on F^2	1.101	1.024	1.073
R_1 / wR_2 ($I \geqslant 2\sigma(I)$)	0.0354/ 0.1043	0.0528 / 0.1263	0.0429 / 0.1314
R_1 / wR_2 (all data)	0.0394/ 0.1096	0.0993 / 0.1502	0.0641/ 0.1568
CCDC	2367597	2367598	2367599
$^aR_1 = \Sigma\|\|F_o\| - \|F_c\|\|/\Sigma\|F_o\|$ $^b wR_2 = \{\Sigma[w(F_o^2 - F_c^2)^2] / \Sigma[w(F_o^2)^2]\}^{1/2}$			

Table S4. Selected bond lengths (Å), the averaged Fe−O and Fe−N bonds (Å), and octahedral distortion parameters Θ, Σ, and CShM in **1**, **2**, and **3·0.6H$_2$O**.

Complex	**1**		**2**	**3·0.6H$_2$O**	
T / K	100	300	90	150 K	100 K
Fe1–O1	1.873(3)	1.917(6)	1.893(11)	1.926(2)	1.926(2)
Fe1–O2	1.883(3)	1.923(6)	1.867(11)	1.916(2)	1.917(2)
Fe1–O$_{av}$	1.878(4)	1.920(8)	1.880(16)	1.921(3)	1.922(3)
Fe1–N1	1.936(5)	2.147(7)	1.954(10)	2.139(3)	2.136(3)
Fe1–N2	1.976(7)	2.068(7)	1.936(11)	2.113(3)	2.108(3)
Fe1–N3	1.976(5)	2.145(7)	1.974(14)	2.149(3)	2.148(3)
Fe1–N4	1.929(5)	2.094(7)	1.954(11)	2.104(3)	2.106(2)
Fe1–N$_{av}$	1.954(11)	2.114(14)	1.954(23)	2.126(6)	2.124(5)
V	1730.8(7)	1784.0(18)	2092.4(4)	1851.5(5)	1825.2(2)
Σ	32	69	31	74.5	73.4
Θ	92	249	97	281.6	280.2
CShM	0.180	1.314	0.203	1.626	1.606

Σ is the sum of the deviations of the bite angles from 90˚.
Θ is the sum of the deviation from 60˚ of the 24 trigonal angles of the projection of the octahedron onto its trigonal faces.

Table S5. Selected bond lengths (Å), the averaged Fe−O and Fe−N bonds (Å), and octahedral distortion parameters Θ, Σ, and CShM in **3** and **4**.

Complex	**3**		**4**	
T / K	100	300	100	300
Fe1–O1	1.875(4)	1.900(3)	1.9210(19)	1.915(3)
Fe1–O2	1.876(3)	1.912(3)	1.9248(19)	1.910(3)
Fe1–O$_{av}$	1.876(5)	1.906(4)	1.9229(27)	1.913 (4)
Fe1–N1	1.975(5)	2.136(4)	2.103(2)	2.099(4)
Fe1–N2	1.936(4)	2.090(4)	2.138(2)	2.141(4)
Fe1–N3	1.979(4)	2.132(4)	2.109(2)	2.113(4)
Fe1–N4	1.949(4)	2.105(4)	2.147(2)	2.142(4)
Fe1–N$_{av}$	1.960(9)	2.116(8)	2.124(4)	2.136(8)
V	1979.7(5)	2036.0(2)	2145.0(8)	2214.3(4)
Σ	35.3	69.6	68.1	70.5
Θ	109.3	263.0	265.3	273.4
CShM	0.256	1.472	1.477	1.565

Σ is the sum of the deviations of the bite angles from 90˚.
Θ is the sum of the deviation from 60˚ of the 24 trigonal angles of the projection of the octahedron onto its trigonal faces.

Table S6. Intermolecular interaction distances at different temperatures of **1**

Crystal	**1**	
T / K	100 K	300 K
1D chain		
π···π (Type A1, A2 and A3)	3.691/3.785/-	3.697/3.966/3.913
π···π (Type B1, B2 and B3)	3.876/3.682/3.638	3.817/3.783/3.637
C8–H8/C13–H13···O1	2.786/2.777	2.854/2.879
C27–H27/C33–H33···O2	2.636/2.682	2.764/-
C3–H3···Br2	3.469	3.581
C23–H23···Br1	3.542	3.567
Fe–Fe (Type A and B)	7.182/7.102	7.228/7.283
NO_3 interactions		
C22–H22···O5	2.882	2.813
C40–H40···O3	2.785	-
C40–H40···O4(O5A)	2.455	2.685(2.545)
C22–H22···O4(O3A)	2.505	2.876(2.472)
C7–H7/C13–H13···O4	2.712/2.823	2.452/2.782
2D plane		
π···π (Type C1 and C2)	3.875/3.868	3.783/3.795
NO_3 interactions		
C11–H11···O4(O3A)	2.622	2.630(2.610)
Solvent interactions		
C18–H18/ C19–H19/C30–H30···O6	2.694/2.717/2.561	-/2.716/2.575
3D structure		
Br2···π1/π2	3.697/3.329	3.602/3.294
C3–H3/C23–H23···Br1	3.590/3.330	3.524/3.357
NO_3 interactions		
C18–H18/C38–H38···O3(O5A)	2.372/2.475	2.284(2.524)/2.504(2.706)
Solvent interactions		
Br2···O6	3.565	-

Table S7. Intermolecular interaction distances at 90 K of **2**

Complex	**2**
T / K	90 K
1D chain	
π···π (Type A1 and A2)	3.888/3.677
π···π (Type B1, B2 and B3)	3.848/3.785/3.622
C7–H7/C13–H13···O2	2.564/2.853
C27–H27/C33–H33···O1	2.544/2.697
C18–H18···Br1	3.532
C38–H38···Br2	3.480
Fe–Fe (Type A and B)	7.046/7.022
ClO_4 interactions	
C38–H38···O6	2.575
C39–H39···O3/C11	2.483/3.090
C10–H10/C21–H21···O3	2.668/2.393
C22–H22···O4	2.895
Solvent interactions	
C1–H1/C19–H19···O7	2.526/2.758
2D plane	
ClO_4 interactions	
C16–H16···O6	2.524
Solvent interactions	
C36–H36···O7	2.658
3D structure	
Br1···π1/π2	3.591/3.387
C36–H36···Br2	3.489
ClO_4 interactions	
C16–H16/C23–H23/ C38–H38···O6	2.524/2.309/2.575
C22–H22···O4	2.812
C2–H2···O4/O5	2.673/2.487
Br2···O6	3.408

Table S8. Intermolecular interaction distances at different temperatures of **3**

Crystal	**3**	
T / K	100 K	300 K
1D chain		
π···π (Type A1, A2 and A3)	3.634/3.599/3.748	3.707/-/3.641
π···π (Type B1, B2 and B3)	3.670/3.794/3.805	3.745/3.707/3.605
C27–H27/ C33–H33···O1	2.811/2.641	-/2.786
C7–H7/C13–H13···O2	2.556/2.753	2.564/2.887
C36–H36/C38–H38···Br2	3.542/3.557	3.504/3.581
C18–H18···Br1	3.483	3.504
Fe–Fe (Type A and B)	7.183/7.026	7.370/6.970
OTf interactions		
C22–H22···O4/F1	2.859/2.712	-/2.699
C21–H21···O4/O3	2.697/2.459	2.735/2.733
C10–H10/C39–H39···O3	2.842/2.463	2.681/2.682
C38–H38···F2	2.879	2.749
Solvent interactions		
C1–H1/C19–H19···O8(O8A)	2.557(2.700)/2.396(2.857)	-(2.496)/-(2.578)
C27–H27/C30–H30···O8	2.624/2.626	2.608/-
2D plane		
C18–H18···Br2	3.370	3.481
Br1···π1/π2	3.473/3.479	3.441/3.532
C3–H3···π	3.461	3.444
OTf interactions		
C2–H2/C3–H3···O4	2.509/2.565	2.503/2.811
Solvent interactions		
C42–H42C/H42B/ C42A–H42E···Br2	3.126/3.304/3.479	3.159/-/-
3D structure		
C23–H23···C15	3.142	3.243
C35–H35···C14/C13/π	2.892/3.109/3.519	2.971/3.255/3.540
OTf interactions		
C18–H18···F1(F1A)	2.868	2.821(2.830)
F1···π	3.900	-
Br2···F3(F3A)	3.217	3.207(3.204)

Table S9. Intermolecular interaction distances at 100 K and 150 K of **3·0.6H$_2$O**

Complex	**3·0.6H$_2$O**	
T / K	150 K	100 K
1D chain		
π···π (Type A1 and A2)	3.628/3.884	3.600/3.837
π···π (Type B1 and B2)	3.587/3.656	3.573/3.632
C7–H7···O2	2.694	2.666
C27–H27/C33–H33···O1	2.578/2.711	2.544/2.665
C18–H18···Br2	3.540	3.498
C38-H38···Br1	-	3.703
Fe–Fe (Type A and B)	7.103/6.799	7.069/6.756
OTf interactions		
C22–H22···F1	2.726	2.738
C21–H21···O3A/O5A/F2/F3	2.765/2.767/2.521/2.843	2.699/2.890/2.531/2.775
C26–H26···O5/F3A	2.627/2.858	2.600/2.744
C39–H39···O3A/O4/O5/F1A	2.701/2.821/2.641/2.889	2.713/2.772/2.632/2.816
C38–H38/···O4/F1A	2.704/2.817	2.652/2.824
C6–H6···O5/F3A	2.606/2.698	2.578/2.663
C10–H10···O3A/F2	2.509/2.692	2.471/2.690
C7–H7···O5	2.892	2.871
2D plane		
π···π (Type C)	3.685	3.647
OTf interactions		
C16–H16···O4/O4A/F2	2.635/2.637/2.891	2.601/2.676./2.880
C15–H15···O4A/F2	2.887/2.843	2.853/2.835
Solvent interactions		
C1–H1/C36–H36···O6	2.574/2.865	2.533/2.838
3D structure		
Br2···π	3.525	3.487
Br1···Br1	3.761	3.691
OTf interactions		
Br1···F1A/O4	3.470/3.468	3.513/3.412
C23–H23···F1A/F2A	2.450/2.718	2.440/2.723
C22–H22···O4A/F1	2.534/2.682	2.495/2.685
C2–H2···O3/O5A/F2A/F3	2.502/2.504/2.658/2.500	2.480/2.385/2.623/2.540
C3–H3···O5A/F3	2.426/2.602	2.410/2.564

Table S10. Intermolecular interaction distances at different temperatures of **4**

Crystal	**4**	
T / K	100 K	300 K
1D chain		
π···π (Type A1, A2 and A3)	3.642/3.660/3.670	3.666/3.758/3.748
π···π (Type B1 and B2)	3.600/3.563	3.624/3.719
C10–H10···O1	2.777	2.886
C33–H33/ C28–H28···O2	2.494/2.687	2.596/2.808
C3–H3···Br2	3.516	3.491
C23–H23···Br1	3.406	3.502
Br1···π	3.899	3.981
Fe–Fe (Type A and B)	7.474/6.808	7.448/6.929
NTf_2 interactions		
C22–H22···O4/O3	2.897/2.582	2.889/2.745
C10–H10/C11–H11/ C13–H13···O3	2.682/2.452/2.578	2.771/2.476/2.659
C39–H39···O6/N5	2.611/2.673	2.786/2.722
F2···π	3.700	3.777
Solvent interactions		
C2–H2/C18–H18···Cl1	-/2.886	3.070/2.888
Br2···Cl2	3.602	3.637
2D plane		
C14–H14/ C34–H34/Br1···Br1	3.496/3.506/3.772	3.517/3.522/3.831
C40–H40···Br2	2.968	2.920
NTf_2 interactions		
C19–H19···O5	2.819	-
C20–H20···O6	2.614	2.626
C38–H38···F4	2.887	-
F4/F5/F6···π1	3.656/3.682/3.336	3.592/3.729/3.712
F5/F6···π2	3.630/3.508	3.563/3.689
Solvent interactions		
Br1···Cl2	3.397	3.645
3D structure		
C3–H3···Br2	3.611	-
C31–H31···C7	2.974	-
NTf_2 interactions		
C19–H19···O5	2.757	2.741
Solvent interactions		
C7–H7···Cl2	3.031	3.098

Table S11. Intermolecular interactions contributions for **1-4** calculated by Hirshfeld surface at different temperatures.

Complex	H···H	H···O	H···Br	H···F	H···C	H···N	C···C	C···Br	C···F	O···Br	Other
1(100 K)	35.8	17.7	7.1	-	18.2	2.0	12.9	4.0	-	1.3	1.0
1(300 K)	31.1	23.8	7.2	-	14.5	2.5	12.5	4.2	-	1.7	2.5
2(90 K)	31.2	23.5	8.5	-	16.2	1.3	12.3	4.3	-	1.1	0.2
3(100 K)	32.2	17.3	7.8	8.7	17.1	1.2	7.9	3.5	0.7	0.6	3.0
3(300 K)	28.3	14.5	8.9	13.8	15.8	2.0	9.4	3.8	1.4	0.2	1.9
3·0.6H_2O (150)	25.8	21.0	7.4	8.5	12.5	2.1	13.1	5.8	0.1	0.6	3.1
4(100 K)	18.0	16.2	8.4	11.5	12.1	1.5	8.2	0.9	7.6	0.4	15.2
4(300 K)	19.0	16.3	8.4	11.3	10.8	1.5	8.0	1.0	8.2	0.3	15.2

Table S12 Parameters of **1-3** derived from the domain model

	1	**2**	**3**
n	8.599	10.07	6.122
ΔS ($J \cdot mol^{-1} \cdot K^{-1}$)	28.82	8.964	16.14

Table S13 List of the Fe^{III} SCO complexes with the Hqnal ligand without any substituent groups.

Compound	Type of SCO	$T_{1/2}$	ref
$[Fe(qnal)_2][Pd(dmit)_2]_5$·Acetone	abrupt	$T_{1/2}$ = 220 K	S1
$[Fe(qnal)_2]CF_3SO_3$·MeOH	Abrupt with	$T_{1/2}\uparrow$ = 115 K	S2
	hysteresis loop	$T_{1/2}\downarrow$ = 104 K	
$[Fe(qnal)_2]CF_3SO_3$·acetone	abrupt with	$T_{1/2}\uparrow$ = 133 K	S2
	hysteresis loop	$T_{1/2}\downarrow$ = 130 K	
$[Fe(qnal)_2](NS)$	abrupt with	$T_{1/2}\uparrow$ = 219 K	S3
	hysteresis loop	$T_{1/2}\downarrow$ = 188 K	
$[Fe(qnal)_2]PS \cdot MeOH \cdot CH_2Cl_2$	abrupt	$T_{1/2}$ = 220 K	S3
$[Fe(qnal)_2]NO_3$	low spin	-	S4
$[Fe(qnal)_2]BPh_4$·DCM	gradual	$T_{1/2}$ = 285 K	S4
$[Fe(qnal)_2]NCS$	gradual	$T_{1/2}$ = 340 K	S4

Notes and references

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