Electronic Supplementary Material (ESI) for Dalton Transactions.

Supporting Information for

Spin Crossover in Hydrogen-Bonded Frameworks of Fe^{II} Complexes with Organodisulfonate Anions

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General Procedures

Elemental analyses for C, H and N were performed on a Perkin-Elmer 240C analyzer. IR spectra were obtained for KBr pellets on a Nicolet 170SX FT-IR spectrophotometer in the 4000–400 cm^{-1} region. DSC measurement was performed on a TA DSC Q2000 instrument under nitrogen atmosphere at a scan rate of 5 $K \cdot min^{-1}$ in both heating and cooling modes. TG analyses were recorded on a NETZSCH TG209F3 thermo analyzer by being filled into alumina crucibles under N_2 atmosphere within the temperature range of 300−1000 K at a heating rate of 10 $K \cdot min^{-1}$. Variable-temperature magnetic susceptibilities were measured with Quantum Design SQUID VSM system. Samples were prepared rapidly to avoid any loss of solvent for magnetic measurements. The experimental susceptibilities were corrected for the sample holder and that of the compounds according to Pascal's constants.[S1]

X-ray Crystallography

Suitable single crystals of complexes $\mathbf{1_{NDS}}$–$\mathbf{4_{NDS}}$ were carefully selected under an optical microscope. The diffraction data were collected on an APEX DUO diffractometer with a CCD area detector (graphite monochromated Mo Kα radiation, λ = 0.71070 Å) under a nitrogen flow. The intensity data of $\mathbf{1_{NDS}}$–$\mathbf{4_{NDS}}$ (123(2), 298(2) K) were collected by the ω scan technique. The structures were solved by direct methods and refined with full-matrix least-squares technique (*SHELXTL*-2014). Absorption corrections were applied upon using multiscan program SADABS.[S2] Hydrogen atoms of organic ligands were generated geometrically by the riding mode and all the non-hydrogen atoms were refined anisotropically through full-matrix least-squares technique on F^2 with the *SHELXTL* program package.[S3] Selected bond lengths and bond angles are listed in Table S2–S5.

Syntheses of $[Fe(H_2O)_6]$·NDS and $[Fe(H_2O)_6]$·BPDS

$[Fe(H_2O)_6]$·NDS. This starting material was A 10 mL aqueous solution of $FeSO_4 \cdot 7H_2O$ (10 mmol, 2.78 g) was added to 10 mL of aqueous solution of NaOH (20 mmol, 0.80 g). The resulting mixture was stirred at room temperature for 20 min and then filtrated. The residue was added to 20 mL of H_2O containing 2.88 g (10 mmol) of H_2NDS, and the resulting mixture was stirred for 10 min and then filtrated to remove the remaining insoluble material. The pale yellow filtrate was concentrated under vacuum at 80 ℃ to 5 mL and then cooled to room temperature. The white powder products were obtained by filtration and washed with cold water. Yield: 3.96 g (88%). Elemental analysis (%) calc. for $C_{12}H_{20}S_2FeO_{12}$: C, 30.85; H, 3.77; Found: C, 30.62; H, 3.66. IR (KBr, cm^{-1}): 3386(b, s), 1639 (m), 1502(s), 1221(m), 1203(m), 1176(s), 1157(s), 1045(s), 1124(s), 795(m), 771(m), 607(m), 525(m).

$[Fe(H_2O)_6]$·BPDS. This compound was synthesized by a similar method as that for $[Fe(H_2O)_6]$·NDS by using H_2BPDS (0.63 g, 10 mmol). Yield: 1.63 g (~34%, based on Fe). Elemental analysis (%) calc. for $C_{11}H_{16}S_2FeO_{10}$: C, 30.26; H, 4.23; Found: C, 30.28; H, 4.27. IR (KBr, cm^{-1}): 3497(b, s), 1631(m), 1625(s), 1226(s), 1195(s), 1173(s), 1135(s), 1047(s), 999(m), 813(m), 731(m), 617(m), 556(m).

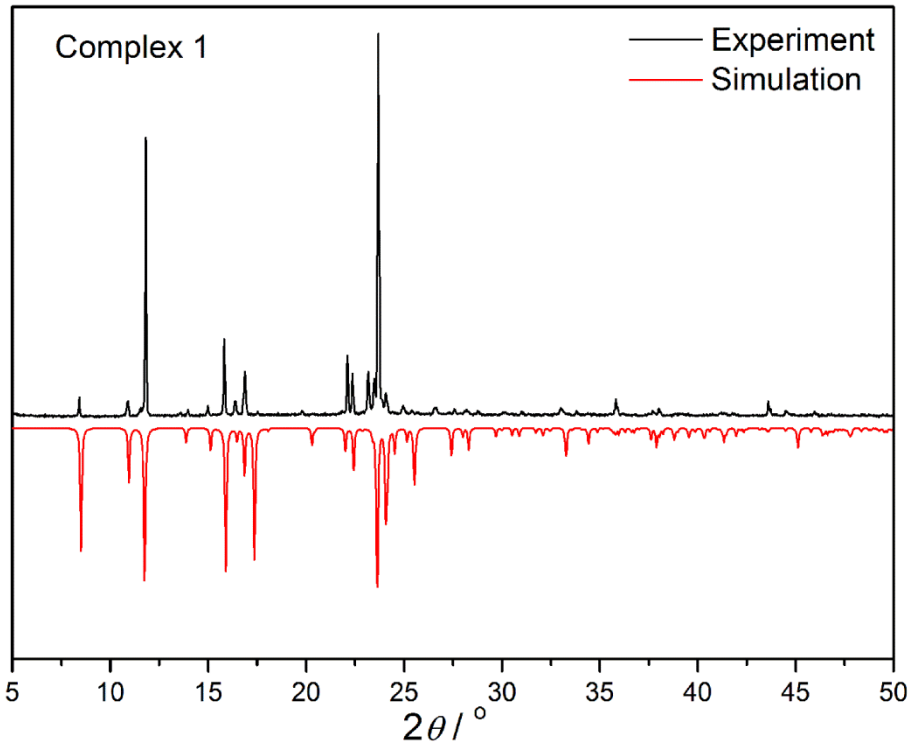

Figure S1. Experimental and simulated powder X-ray diffraction patterns for $\mathbf{1}_{\mathbf{NDS}}$.

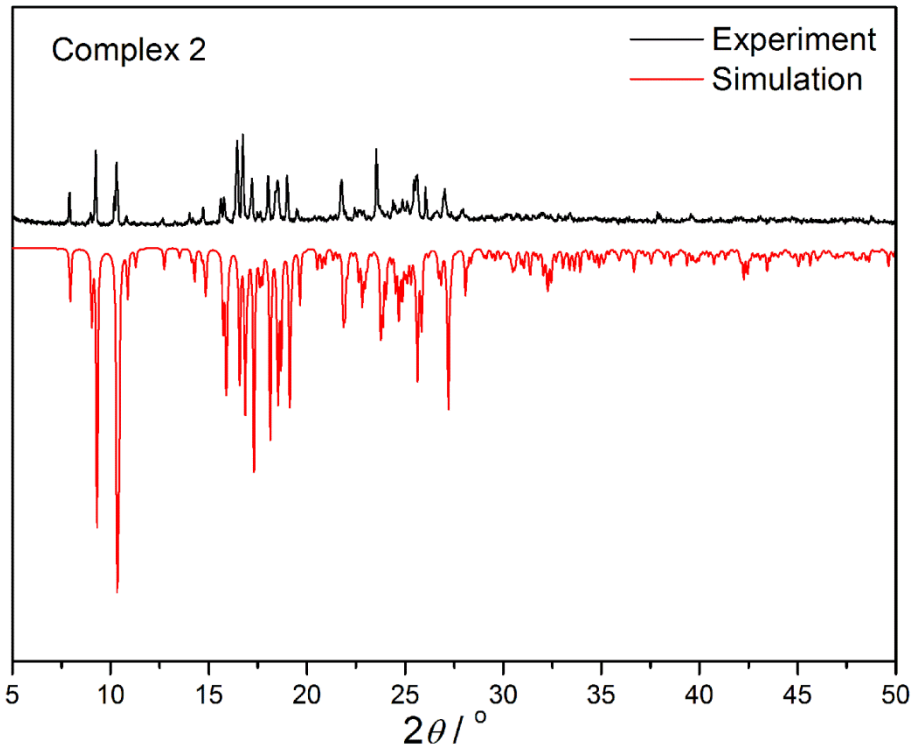

Figure S2. Experimental and simulated powder X-ray diffraction patterns for $\mathbf{2}_{\mathbf{BPDS}}$.

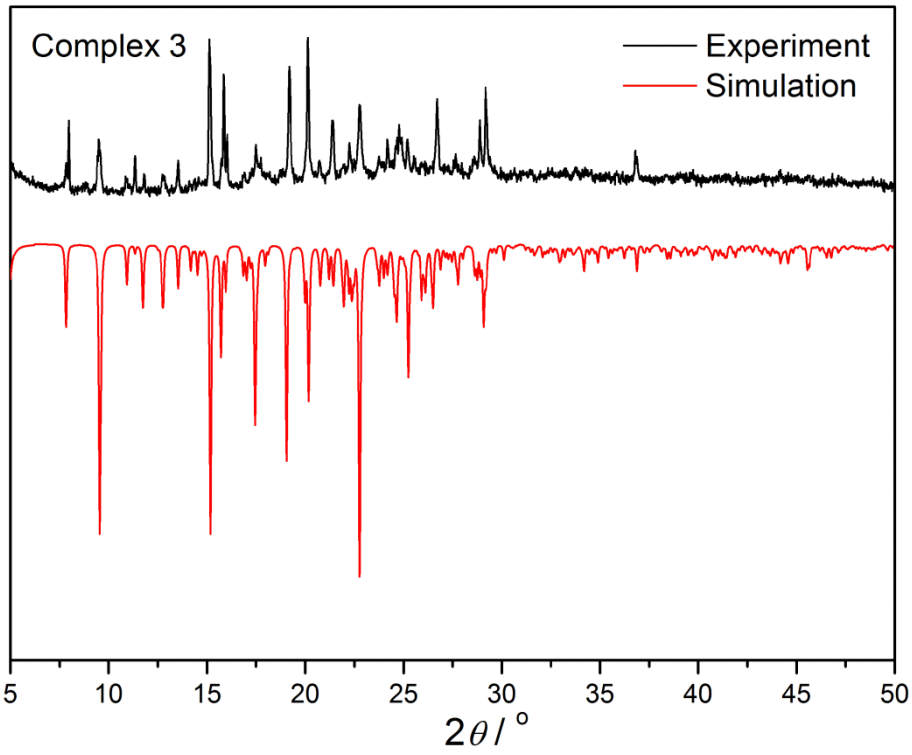

Figure S3. Experimental and simulated powder X-ray diffraction patterns for $\mathbf{3}_{\mathbf{ABDS}}$.

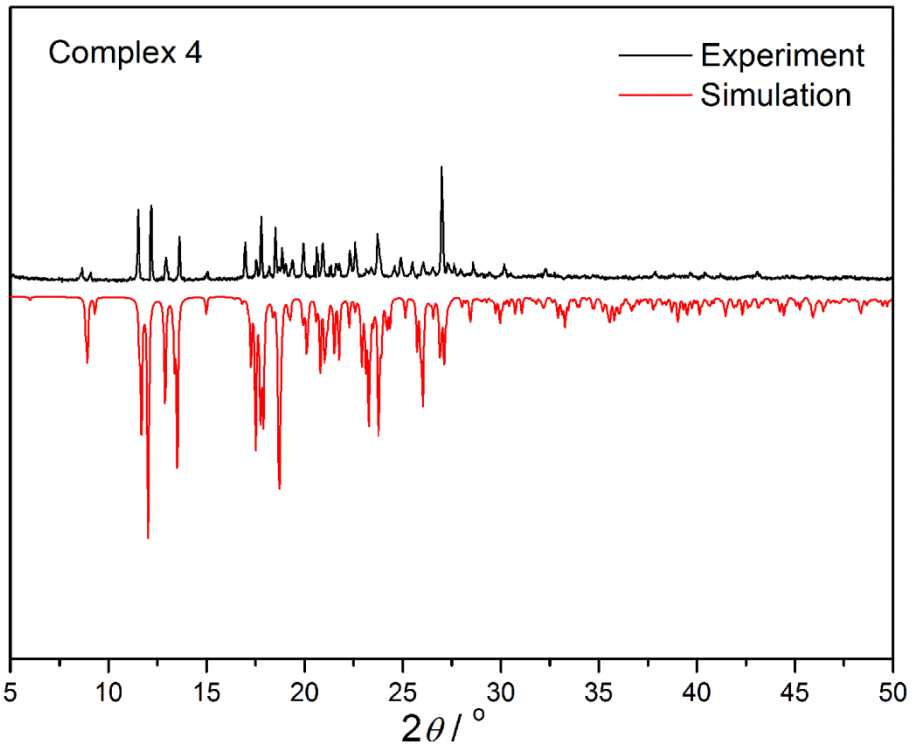

Figure S4. Experimental and simulated powder X-ray diffraction patterns for $\mathbf{4}_{\mathbf{DNDS}}$.

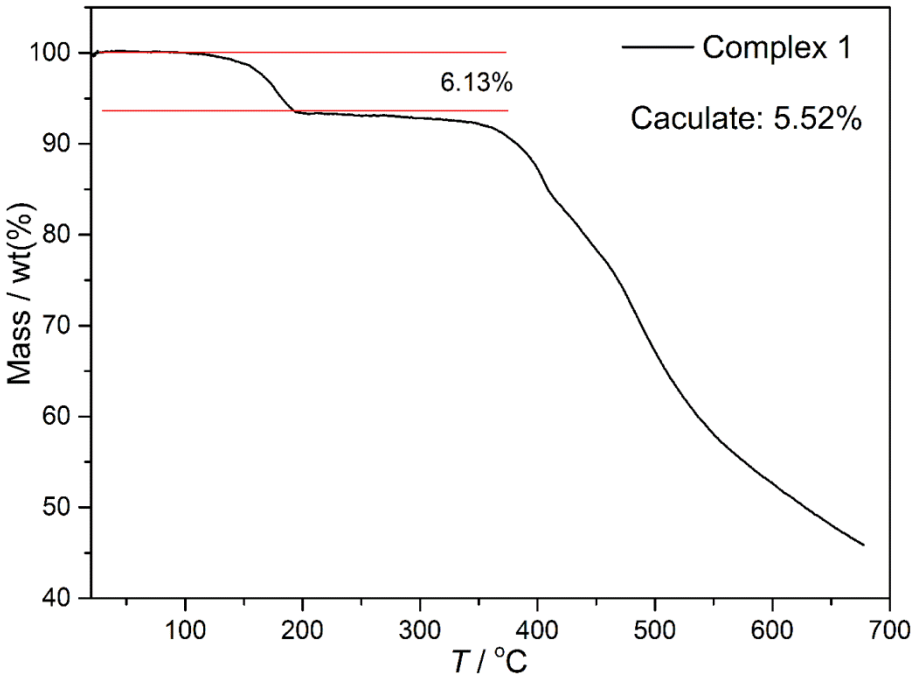

Figure S5. TG curve of compound $\mathbf{1}_{\mathbf{NDS}}$ at a rate of 10 K·min^{-1} under at N_2 atmosphere.

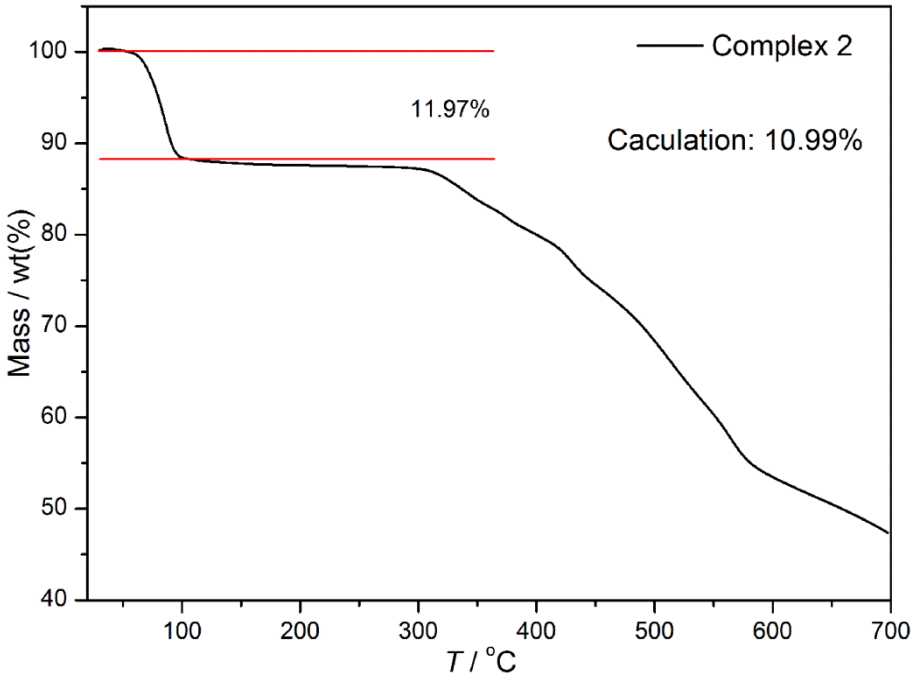

Figure S6. TG curve of compound $\mathbf{2}_{\mathbf{BPDS}}$ at a rate of 10 K·min^{-1} under at N_2 atmosphere.

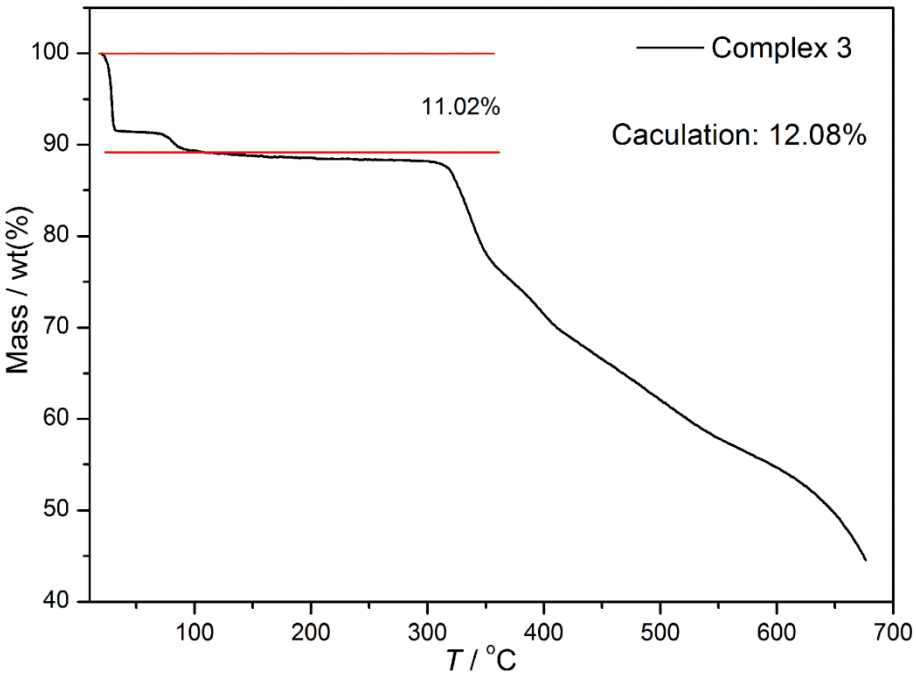

Figure S7. TG curve of compound $\mathbf{3}_{\mathbf{ABDS}}$ at a rate of 10 K·min^{-1} under at N_2 atmosphere.

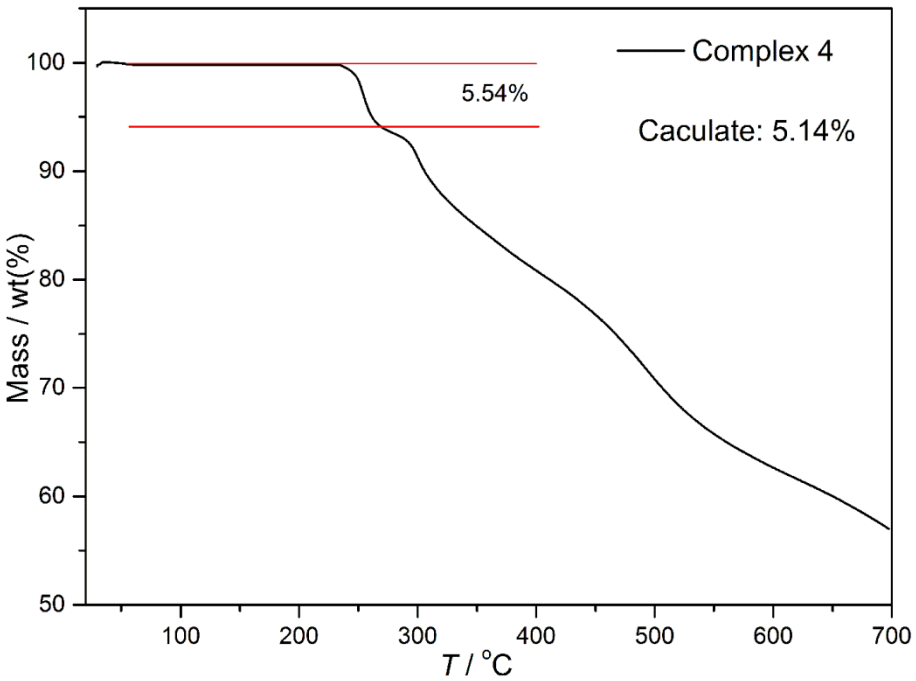

Figure S8. TG curve of compound $\mathbf{4}_{\mathbf{DNDS}}$ at a rate of 10 K·min^{-1} under at N_2 atmosphere.

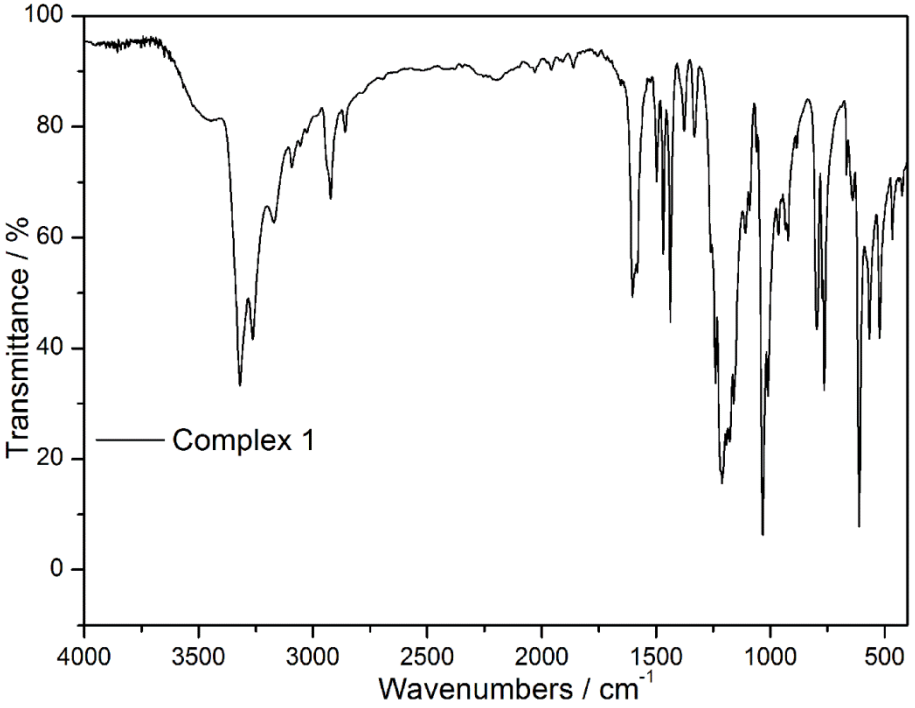

Figure S9. Infrared spectra of complex $\mathbf{1}_{\mathbf{NDS}}$ at room temperature

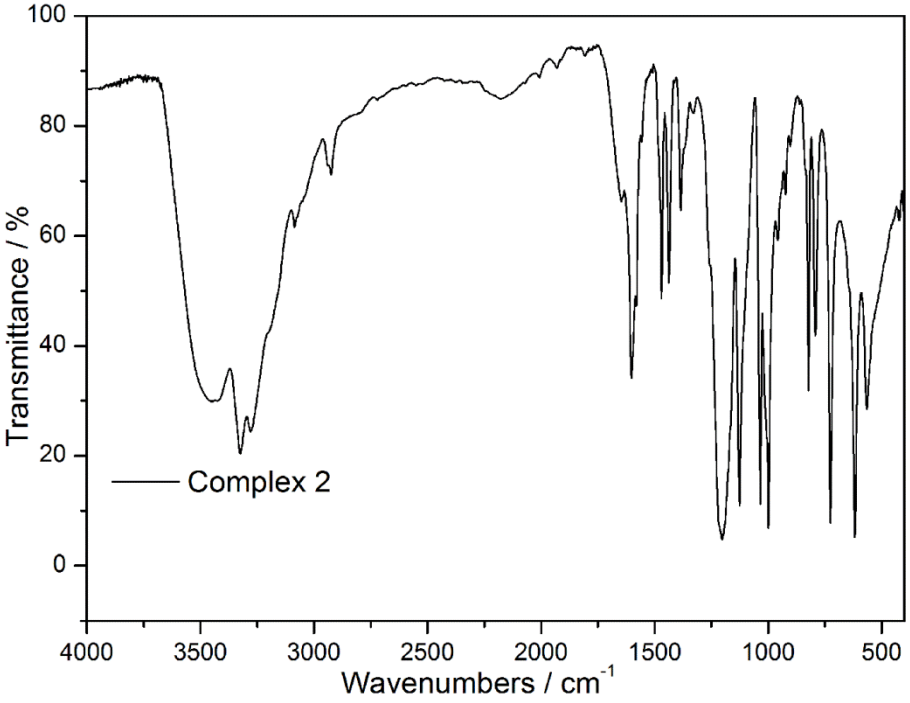

Figure S10. Infrared spectra of complex $\mathbf{2}_{\mathbf{BPDS}}$ at room temperature

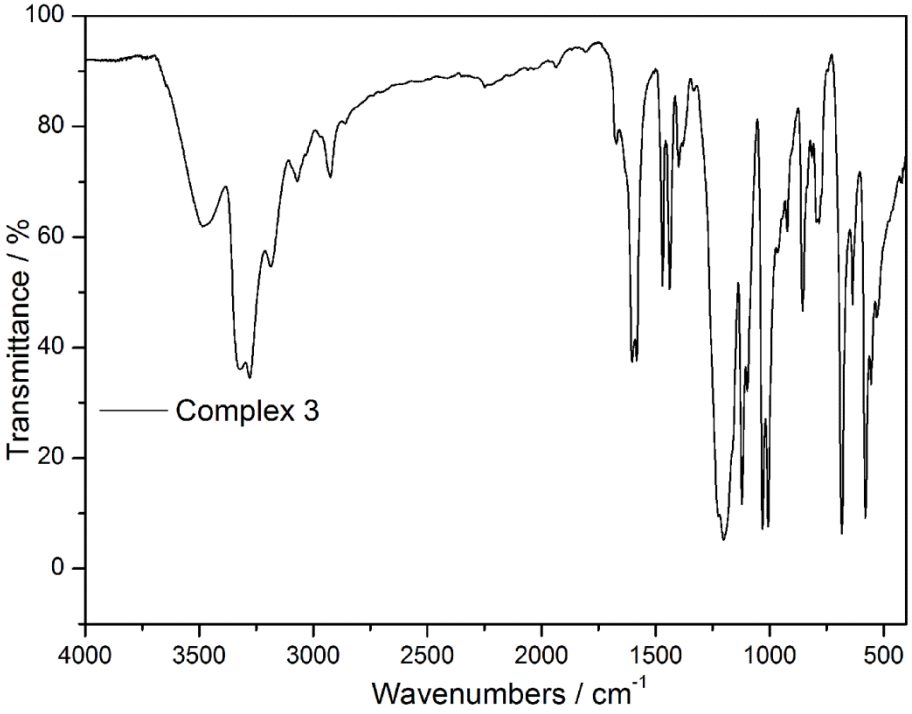

Figure S11. Infrared spectra of complex $\mathbf{3}_{\mathbf{ABDS}}$ at room temperature.

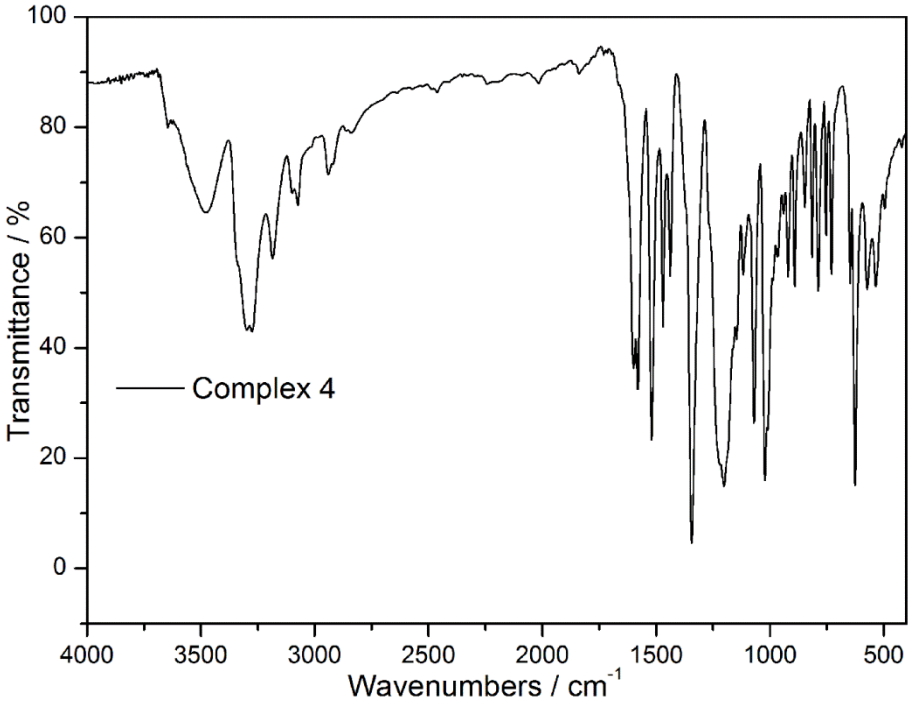

Figure S12. Infrared spectra of complex $\mathbf{4}_{\mathbf{DNDS}}$ at room temperature.

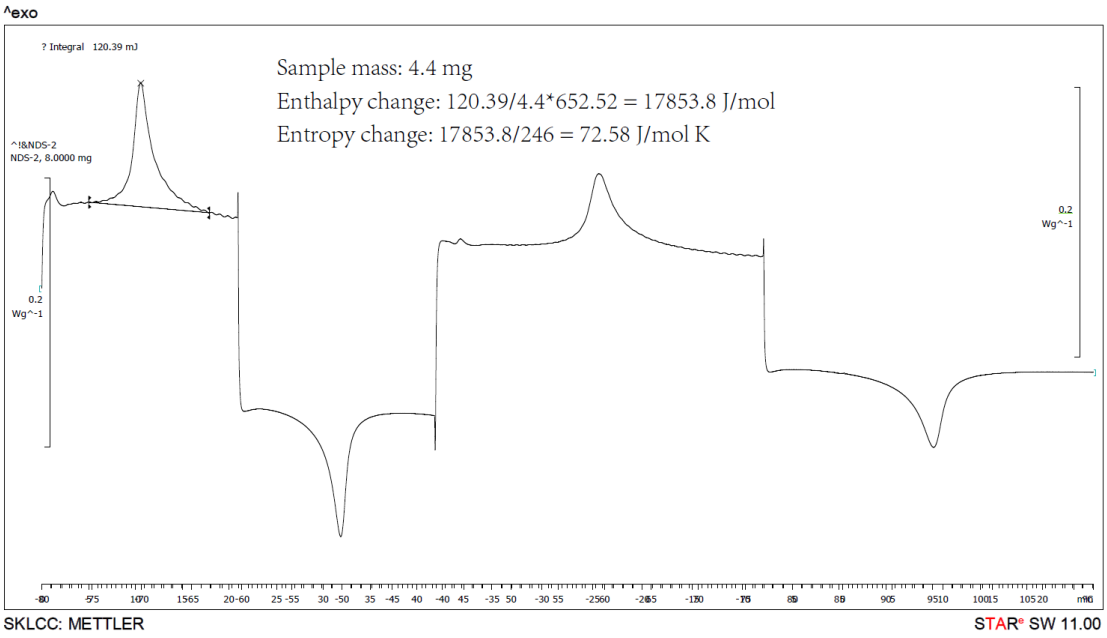

Figure S13. DSC data processing of complex $\mathbf{1}_{\mathbf{NDS}}$ (the first cooling process)

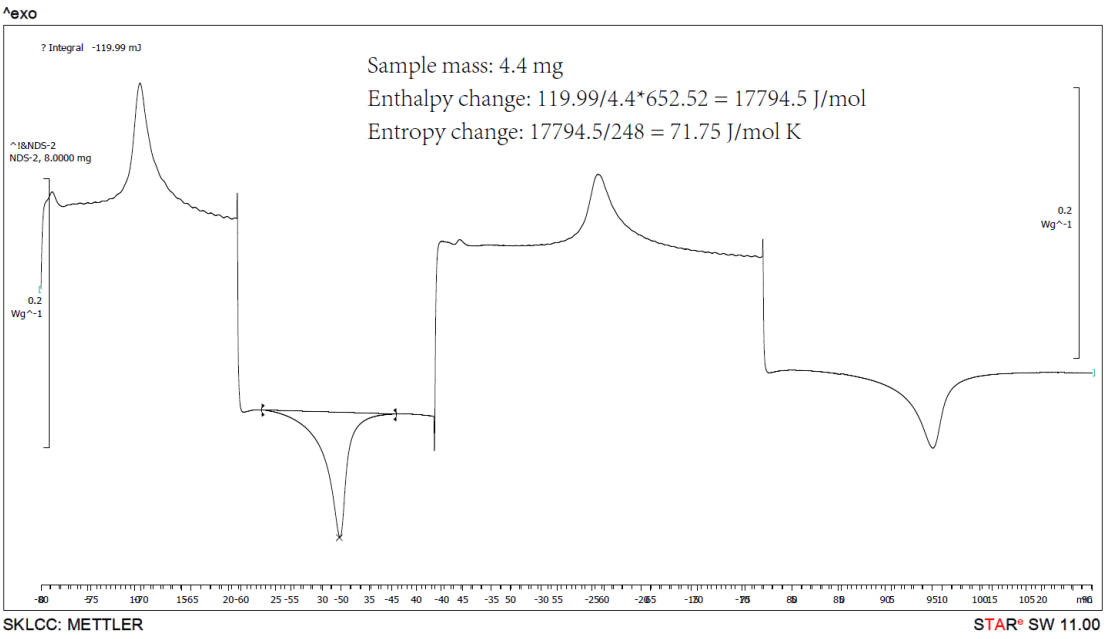

Figure S14. DSC data processing of complex $\mathbf{1}_{\mathbf{NDS}}$ (the first warming process)

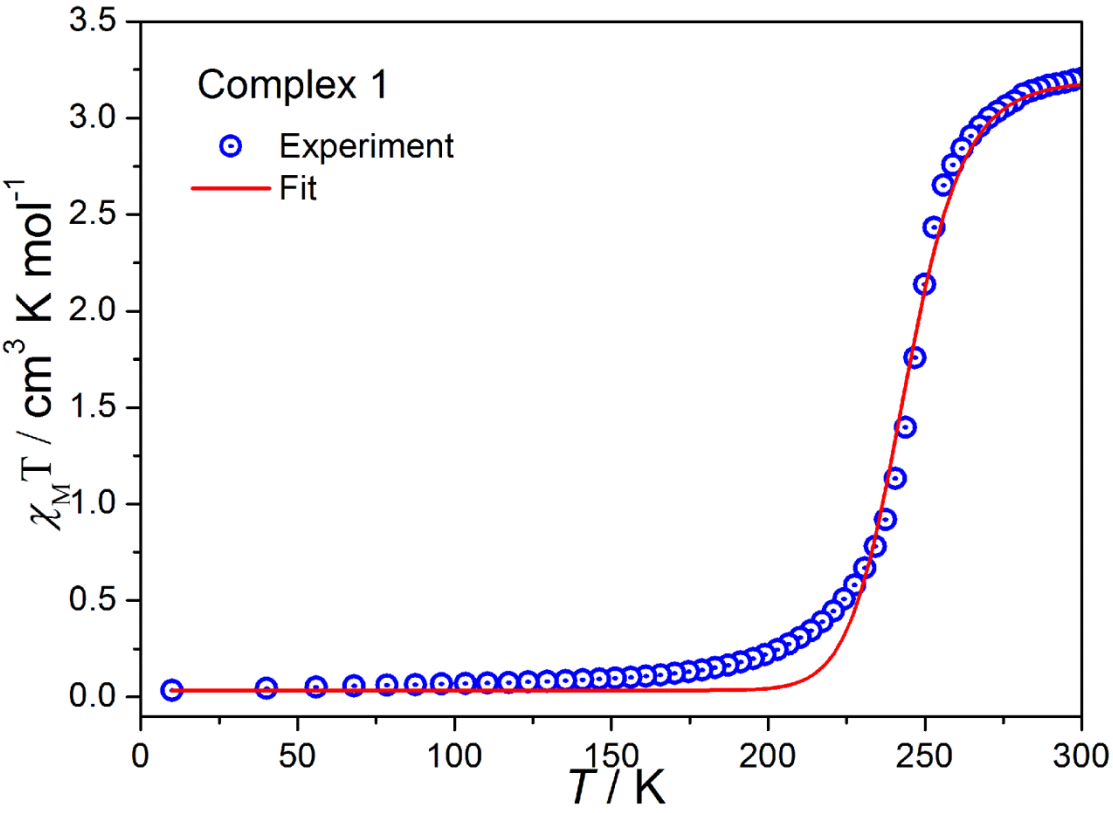

Figure S15. Temperature Plot of $\chi_M T$ vs. T for $\mathbf{1}_{\mathbf{NDS}}$ under an applied external magnetic field of 1 kOe. The red solid line corresponds to the domain model

Table S1. SHAPE analysis of the Fe(II) ion in complexes $\mathbf{1_{NDS}}$–$\mathbf{4_{DNDS}}$.

Lable		HP-6	PPY-6	OC-6	TPR-6	JPPY-5
Shape		Hexagon	Pentagonal pyramid	Octahedron	Trigonal prism	Johnson pentagonal pyramid (J2)
Symmertry		D_{6h}	C_{5v}	O_h	D_{3h}	C_{5v}
$\mathbf{1_{NDS}}$	123 K	33.388	24.729	***1.408***	12.291	28.774
	298 K	34.220	19.872	***4.358***	8.644	23.929
$\mathbf{2_{BPDS}}$	123 K	34.361	24.502	***1.787***	12.654	28.566
	298 K	34.989	22.047	***3.968***	11.617	26.020
$\mathbf{3_{ABDS}}$	123 K	33.561	25.398	***1.275***	12.925	29.505
	298 K	34.612	21.046	***4.097***	10.905	25.030
$\mathbf{4_{DNDS}}$	123 K	34.501	23.121	***2.425***	11.835	27.273
	298 K	33.928	20.368	***4.090***	10.590	24.104

Table S2. Selected bond lengths (Å) and angles (°) for complex $\mathbf{1_{NDS}}$

Bond lengths (Å)			
123 K		**298 K**	
Fe(1)-N(2)	1.890(4)	Fe(1)-N(2)	2.108(2)
Fe(1)-N(2)#1	1.890(4)	Fe(1)-N(2)#1	2.108(2)
Fe(1)-N(3)#1	2.023(5)	Fe(1)-N(3)	2.208(2)
Fe(1)-N(3)	2.023(5)	Fe(1)-N(3)#1	2.208(2)
Fe(1)-N(1)#1	2.028(5)	Fe(1)-N(1)	2.226(3)
Fe(1)-N(1)	2.028(5)	Fe(1)-N(1)#1	2.226(3)
Bond angles (°)			
123 K		**298 K**	
N(2)#1-Fe(1)-N(1)	81.29(19)	N(2)-Fe(1)-N(3)	110.22(9)
N(2)-Fe(1)-N(1)	99.72(19)	N(2)#1-Fe(1)-N(3)	76.11(9)
N(2)#1-Fe(1)-N(1)#1	99.72(19)	N(2)-Fe(1)-N(3)#1	76.11(9)
N(2)-Fe(1)-N(1)#1	81.29(19)	N(2)#1-Fe(1)-N(3)#1	110.22(9)
N(1)-Fe(1)-N(1)#1	90.60(4)	N(3)-Fe(1)-N(3)#1	91.44(15)
N(2)#1-Fe(1)-N(3)	83.03(19)	N(2)-Fe(1)-N(1)	97.85(10)
N(2)-Fe(1)-N(3)	95.99(19)	N(2)#1-Fe(1)-N(1)	76.30(10)
N(1)#1-Fe(1)-N(3)	90.60(3)	N(3)#1-Fe(1)-N(1)	92.59(12)
N(2)#1-Fe(1)-N(3)#1	95.99(19)	N(2)-Fe(1)-N(1)#1	76.30(10)
N(2)-Fe(1)-N(3)#1	83.03(19)	N(2)#1-Fe(1)-N(1)#1	97.85(10)
N(1)-Fe(1)-N(3)#1	90.60(3)	N(3)-Fe(1)-N(1)#1	92.59(12)
N(3)-Fe(1)-N(3)#1	92.50(4)	N(1)-Fe(1)-N(1)#1	96.90(2)

Table S3. Selected bond lengths (Å) and angles (°) for complex $\mathbf{2_{BPDS}}$

Bond lengths (Å)			
123 K		**298 K**	
Fe(1)-N(5)	1.952(3)	Fe(1)-N(2)	2.113(2)
Fe(1)-N(2)	1.953(3)	Fe(1)-N(5)	2.108(2)
Fe(1)-N(1)	2.073(3)	Fe(1)-N(1)	2.211(2)
Fe(1)-N(3)	2.074(3)	Fe(1)-N(3)	2.217(2)
Fe(1)-N(6)	2.077(3)	Fe(1)-N(6)	2.226(2)
Fe(1)-N(4)	2.088(3)	Fe(1)-N(4)	2.247(2)
Bond angles (°)			
123 K		**298 K**	
N(5)-Fe(1)-N(1)	98.76(10)	N(2)-Fe(1)-N(1)	76.05(8)
N(2)-Fe(1)-N(1)	80.48(11)	N(5)-Fe(1)-N(1)	102.79(8)
N(5)-Fe(1)-N(3)	99.07(11)	N(2)-Fe(1)-N(3)	76.56(9)
N(2)-Fe(1)-N(3)	81.68(11)	N(5)-Fe(1)-N(3)	104.60(9)
N(5)-Fe(1)-N(6)	80.81(11)	N(2)-Fe(1)-N(6)	103.87(13)
N(2)-Fe(1)-N(6)	99.36(11)	N(5)-Fe(1)-N(6)	76.23(8)
N(1)-Fe(1)-N(6)	92.13(11)	N(1)-Fe(1)-N(6)	93.43(9)
N(3)-Fe(1)-N(6)	92.08(11)	N(3)-Fe(1)-N(6)	94.72(9)
N(5)-Fe(1)-N(4)	80.67(11)	N(2)-Fe(1)-N(4)	104.31(8)
N(2)-Fe(1)-N(4)	99.15(11)	N(5)-Fe(1)-N(4)	75.81(8)
N(1)-Fe(1)-N(4)	90.40(11)	N(1)-Fe(1)-N(4)	92.06(9)
N(3)-Fe(1)-N(4)	91.11(11)	N(3)-Fe(1)-N(4)	92.90(10)

Table S4. Selected bond lengths (Å) and angles (°) for complex $\mathbf{3_{ABDS}}$

Bond lengths (Å)			
123 K		**298 K**	
Fe(1)-N(5)	1.900(3)	Fe(1)-N(2)	2.110(3)
Fe(1)-N(2)	1.905(2)	Fe(1)-N(5)	2.112(3)
Fe(1)-N(4)	2.039(3)	Fe(1)-N(1)	2.212(3)
Fe(1)-N(3)	2.045(2)	Fe(1)-N(3)	2.216(3)
Fe(1)-N(6)	2.051(3)	Fe(1)-N(6)	2.223(4)
Fe(1)-N(1)	2.057(2)	Fe(1)-N(4)	2.228(4)
Bond angles (°)			
123 K		**298 K**	
N(5)-Fe(1)-N(4)	83.25(11)	N(2)-Fe(1)-N(1)	75.73(11)
N(2)-Fe(1)-N(4)	99.09(10)	N(5)-Fe(1)-N(1)	105.10(12)
N(5)-Fe(1)-N(3)	96.69(10)	N(2)-Fe(1)-N(3)	75.72(10)
N(2)-Fe(1)-N(3)	82.34(10)	N(5)-Fe(1)-N(3)	103.57(12)
N(4)-Fe(1)-N(3)	90.75(11)	N(2)-Fe(1)-N(6)	106.36(13)
N(5)-Fe(1)-N(6)	82.22(11)	N(5)-Fe(1)-N(6)	76.05(17)
N(2)-Fe(1)-N(6)	95.44(10)	N(1)-Fe(1)-N(6)	92.78(15)
N(3)-Fe(1)-N(6)	91.43(11)	N(3)-Fe(1)-N(6)	91.85(13)
N(5)-Fe(1)-N(1)	98.31(10)	N(2)-Fe(1)-N(4)	101.03(13)
N(2)-Fe(1)-N(1)	82.59(10)	N(5)-Fe(1)-N(4)	76.54(17)
N(4)-Fe(1)-N(1)	93.17(10)	N(1)-Fe(1)-N(4)	95.92(14)
N(6)-Fe(1)-N(1)	88.44(10)	N(3)-Fe(1)-N(4)	92.91(13)

Table S5. Selected bond lengths (Å) and angles (°) for complex $\mathbf{4_{DNDS}}$

Bond lengths (Å)			
123 K		**298 K**	
Fe(1)-N(2)	1.990(3)	Fe(1)-N(5)	2.1137(19)
Fe(1)-N(5)	1.990(2)	Fe(1)-N(2)	2.1152(19)
Fe(1)-N(3)	2.089(3)	Fe(1)-N(3)	2.227(2)
Fe(1)-N(4)	2.114(2)	Fe(1)-N(4)	2.230(2)
Fe(1)-N(6)	2.117(3)	Fe(1)-N(6)	2.231(2)
Fe(1)-N(1)	2.118(3)	Fe(1)-N(1)	2.235(2)
Bond angles (°)			
123 K		**298 K**	
N(2)-Fe(1)-N(3)	80.10(13)	N(5)-Fe(1)-N(3)	108.34(8)
N(5)-Fe(1)-N(3)	103.16(13)	N(2)-Fe(1)-N(3)	76.05(8)
N(2)-Fe(1)-N(4)	99.77(10)	N(5)-Fe(1)-N(4)	75.51(8)
N(5)-Fe(1)-N(4)	79.09(10)	N(2)-Fe(1)-N(4)	103.65(8)
N(3)-Fe(1)-N(4)	90.01(10)	N(3)-Fe(1)-N(4)	91.34(8)
N(2)-Fe(1)-N(6)	101.96(10)	N(5)-Fe(1)-N(6)	75.76(8)
N(5)-Fe(1)-N(6)	79.23(10)	N(2)-Fe(1)-N(6)	105.20(8)
N(3)-Fe(1)-N(6)	93.51(12)	N(3)-Fe(1)-N(6)	95.18(10)
N(2)-Fe(1)-N(1)	79.08(10)	N(5)-Fe(1)-N(1)	99.55(7)
N(5)-Fe(1)-N(1)	97.62(9)	N(2)-Fe(1)-N(1)	76.01(7)
N(4)-Fe(1)-N(1)	91.59(10)	N(4)-Fe(1)-N(1)	92.41(8)
N(6)-Fe(1)-N(1)	92.68(11)	N(6)-Fe(1)-N(1)	94.85(10)

Table S6. The hydrogen bonds in complex $\mathbf{1}_{\mathbf{NDS}}$

	D-H···A	**D···A (Å)**	**∠D-H···A (deg)**
1-123 K	N1-H1D···O1#1	3.1790(7)	136.349(4)
	N1-H1C···O2#2	2.9147(8)	154.930(3)
	N3-H3B···O1WA#3	3.2078(1)	140.277(5)
	N3-H3B···O1WB#3	2.7617(1)	152.458(5)
	O1WA-H1WA···O1	2.8035(9)	154.899(6)
	O1WB-H1WC···O1	2.8631(1)	156.066(7)
	O1WA-H1WB···O3#4	2.9402(1)	134.415(7)
	O1WB-H1WD···O#4	3.0336(1)	149.755(8)
1-298 K	N1-H1C···O2#2	3.3655(4)	137.525(2)
	N3-H1D···O2#2	3.2376(3)	130.040(2)
	N1-H1D···O1WA#3	3.3327(8)	148.931(3)
	N1-H1D···O1WB#3	2.9159(9)	159.033(3)
	O1WA-H1WA···O1	2.9787(8)	138.207(5)
	O1WB-H1WC···O1	3.0650(9)	146.082(5)
	O1WA-H1WB···O3#4	2.7981(7)	153.423(4)
	O1WB-H1WD···O3#4	2.8486(7)	155.441(4)
Symmetry operator: #1 = -x, y, 0.5-z; #2 = -0.5+x, -0.5+y, z; #3 = 0.5-x, -0.5+y, 0.5-z; #4 = 1-x, y, 0.5-z			

Table S7. The hydrogen bonds in complex $\mathbf{2_{BPDS}}$

	D-H···A	**D···A (Å)**	**∠D-H···A (deg)**
2-123 K	N1-H1C···O2#1	2.9599(4)	154.690(2)
	N1-H1D···O6	2.9357(4)	147.031(2)
	N3-H3C···O1W	2.9420(4)	162.429(2)
	N3-H3B···O2W	3.0810(4)	164.259(2)
	N4-H4B···O2#1	3.1517(4)	140.572(2)
	N4-H4C···O1W	3.0344(4)	148.205(2)
	N6-H6A···O5#2	2.9937(4)	162.176(2)
	N6-H6B···O6	2.9436(4)	158.028(2)
	O1W-H1WA···O3#3	2.7406(4)	124.995(2)
	O1W-H1WB···O4	2.8027(4)	153.683(2)
	O2W-H2WA···O5#2	3.0153(4)	140.873(2)
	O3WB-H3WB···O4	2.8727(7)	123.790(5)
	O4W-H4WB···O1	3.1072(7)	116.047(4)
	O4W-H4WA···O5#4	3.1032(6)	134.715(4)
	O5WA-H5W···O1	2.9366(7)	157.123(6)
	O5WB-H5W'···O1	2.5277(7)	125.259(6)
	O5W'-H5WE···O3WA#5	2.9668(9)	130.417(6)
2-298 K	N1-H1C···O2#1	3.0340(3)	160.686(2)
	N1-H1D···O6	3.0229(2)	147.255(2)
	N3-H3C···O1W	3.0175(4)	166.077(2)
	N3-H3B···O2W	3.1805(4)	170.346(2)
	N4-H4B···O2#1	3.0997(3)	149.575(2)
	N4-H4C···O1W	3.1775(4)	150.028(2)
	N6-H6A···O5#2	3.0516(1)	170.574(3)
	N6-H6B···O6	2.9817(9)	162.009(3)
	O1W-H1WA···O3#3	2.7542(3)	123.842(2)
	O1W-H1WB···O4#4	2.8171(1)	152.745(3)
	O2W-H2WA···O5#2	3.0644(1)	142.044(3)
	O4W-H4WA···O5	3.0940(1)	157.792(5)
	O4W-H4WB···O1	3.2547(1)	123.328(5)
	O5W-H5WB···O1	2.8682(1)	177.804(6)
	O5WB-H5WF···O3WA#5	3.0899(1)	158.507(6)
Symmetry operator: #1 = 1-x, 1-y, 1-z; #2 = 0.5-x, -0.5+y, 1.5-z; #3 = 0.5+x, 0.5-y, 0.5+z; #4 = x, y, -1+z; #5 = 1-x, 1-y, 2-z			

Table S8. The hydrogen bonds in complex $\mathbf{3}_{\mathbf{ABDS}}$

	D-H···A	**D···A (Å)**	**∠D-H···A (deg)**
3-123 K	N1-H1C···O5#1	3.1259(4)	147.400(2)
	N1-H1D···O3#2	3.2162(3)	146.326(2)
	N3-H3B···O1	2.8910(3)	151.611(2)
	N3-H3C···O5#3	3.1271(3)	161.870(2)
	N4-H4B···O6#1	3.0095(4)	171.136(2)
	N4-H4C···O1W#4	3.1199(4)	166.712(2)
	N6-H6A···O3A#5	3.0134(4)	141.210(2)
	N6-H6B···O3#2	3.2239(3)	140.415(2)
	O1W-H1WB···O2	2.8792(4)	168.011(2)
3-298 K	N1-H1C···O5A#1	3.1709(8)	147.804(2)
	N1-H1D···O3#2	3.3488(4)	147.322(2)
	N3-H3B···O1	2.9879(4)	128.362(2)
	N3-H3C···O5B#3	3.0337(2)	160.886(7)
	N4-H4B···O6A#1	3.1646(9)	166.613(3)
	N4-H4C···O1W#4	3.3826(6)	148.414(3)
	N6-H6A···O3A#5	3.1509(5)	137.617(3)
	N6-H6B···O3#2	3.2017(5)	153.406(3)
	O1W-H1WB···O2	2.8913(5)	166.799(3)
Symmetry operator: #1 = 1-x, 1-y, 1-z; #2 = 1+x, y, z; #3 = -x, 1-y, 1-z; #4 = x, 1+y, z; #5 = 1-x, 1-y, -z			

Table S9. The hydrogen bonds in complex $\mathbf{4_{DNDS}}$

	D-H···A	**D···A (Å)**	**∠D-H···A (deg)**
4-123 K	N1-H1D···O1#1	3.0041(4)	165.009(2)
	N1-H1C···O6	2.9357(3)	157.484(2)
	N3-H3A···O2#2	2.8734(4)	163.426(2)
	N3-H3B···O5#3	3.3419(5)	145.011(2)
	N4-H4C···O3#1	2.9092(4)	167.146(2)
	N4-H4B···O5#3	3.0780(3)	176.093(2)
	N6-H6B···O2#2	3.3541(4)	129.459(2)
	C29- H29A···O5#5	3.1707(8)	136.838(4)
	C29- H29B···O8	3.1331(7)	127.152(4)
	C29- H29C···O9	3.1511(7)	144.344(4)
4-298 K	N1-H1D···O1#1	3.0427(4)	165.796(2)
	N1-H1C···O6	2.9852(3)	160.988(2)
	N3-H3A···O2#2	2.9243(3)	160.892(2)
	N3-H3B···O5#3	3.4026(4)	157.201(2)
	N4-H4C···O3#1	2.9604(3)	177.330(2)
	N4-H4B···O5#3	3.0851(3)	174.573(2)
	N6-H6B···O2#2	3.3549(4)	136.541(2)
	C29- H29A···O5#5	3.1887(7)	136.114(4)
	C29- H29B···O8	3.2505(7)	131.435(4)
	C29- H29C···O9	3.2205(8)	143.933(5)
Symmetry operator: #1 = 1-x, 1-y, 1-z; #2 = -x, 1-y, 1-z; #3 = x, 1+y, z; #4 = 1-x, -y, 1-z; #5 = -1+x, y, z			

Reference

[S1] O. Kahn, Molecular Magnetism, VCH, Weinheim, Germany, 1993.

[S2] (a) *SAINT Software Users Guide, Version 7.0*, Bruker Analytical X-Ray Systems, Madison, WI, 1999. (b) Sheldrick, G. M. *SADABS, Version 2.03*, Bruker Analytical X-Ray Systems, Madison, WI, 2000.

[S3] Sheldrick, G. M.; *SHELXTL, Version 6.14*, Bruker AXS, Inc., Madison, WI, 2000–2003.