Supporting Information

for

Co-Ligand and Solvent Effects on The Spin Crossover Behaviors of PtS-type Porous Coordination Polymers

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Crystallographic Data Collection and Squeeze Details for 2·*S* and 3·*S*

Single-crystal X-ray diffraction data of **2**·*S* and **3**·*S* were recorded on Agilent SuperNova diffractometer at relevant temperature. The structure was solved by direct method and refined by full-matrix least-squares techniques on F^2 with SHELXL-97.[2] Non-hydrogen atoms were refined anisotropically, hydrogen atoms were generated geometrically and refined isotropically. Attempts to define the highly disordered solvent molecules were unsuccessful, so the structure was refined with the PLATON [3] "SQUEEZE" procedure. Void channels are calculated by Mercury [4] "Void" command.

Squeeze details for **2**·*S* at 100 K: Approximately 66.1% of the unit cell volume comprises a large region of disordered solvent that could not be modeled as discrete atomic sites. We employed PLATON SQUEEZE to calculate the contribution to the diffraction from the solvent region and thereby produced a set of solvent-free diffraction intensities. SQUEEZE estimated a total count of 718 electrons per unit cell. According to the final formula which was calculated from TGA combined with elemental analysis data, these electrons were assigned to be 20 methanol and 8 dichloromethane molecules per unit cell. The F(000) value with solvent is 2720, Mu (mm^-1) value with solvent is 3.059, and crystal density with solvent is 0.822.

Squeeze details for **2**·*S* at 155 K: Approximately 69.4% of the unit cell volume comprises a large region of disordered solvent that could not be modeled as discrete atomic sites. We employed PLATON SQUEEZE to calculate the contribution to the diffraction from the solvent region and thereby produced a set of solvent-free diffraction intensities. SQUEEZE estimated a total count of 1495 electrons per unit cell. According to the final formula that was calculated from TGA combined with elemental analysis data, these electrons were assigned to be 40 methanol and 16 dichloromethane molecules per unit cell. The F(000) value with

solvent is 5440, Mu (mm^-1) value with solvent is 2.713, and crystal density with solvent is 0.729.

Squeeze details for **2**·*S* at 220 K: Approximately 66.1% of the unit cell volume comprises a large region of disordered solvent that could not be modeled as discrete atomic sites. We employed PLATON SQUEEZE to calculate the contribution to the diffraction from the solvent region and thereby produced a set of solvent-free diffraction intensities. SQUEEZE estimated a total count of 724 electrons per unit cell. According to the final formula that was calculated from TGA combined with elemental analysis data, these electrons were assigned to be 20 methanol and 8 dichloromethane molecules per unit cell. The F(000) value with solvent is 2720, Mu (mm^-1) value with solvent is 2.531, and crystal density with solvent is 0.680.

Squeeze details for **3**·*S* at 110 K: Approximately 66.2% of the unit cell volume comprises a large region of disordered solvent that could not be modeled as discrete atomic sites. We employed PLATON SQUEEZE to calculate the contribution to the diffraction from the solvent region and thereby produced a set of solvent-free diffraction intensities. SQUEEZE estimated a total count of 748 electrons per unit cell. According to the final formula that was calculated from TGA combined with elemental analysis data, these electrons were assigned to be 20 methanol and 8 dichloromethane molecules per unit cell. The F(000) value with solvent is 2512, Mu (mm^-1) value with solvent is 2.272, and crystal density with solvent is 0.739.

Squeeze details for **3**·*S* at 175 K: Approximately 68.9% of the unit cell volume comprises a large region of disordered solvent that could not be modeled as discrete atomic sites. We employed PLATON SQUEEZE to calculate the contribution to the diffraction from the solvent region and thereby produced a set of solvent-free diffraction intensities. SQUEEZE estimated a total count of 1514 electrons per unit cell. According to the final formula that was calculated from TGA combined with elemental analysis data, these electrons were assigned to be 40 methanol and 16 dichloromethane molecules per unit cell. The F(000) value with solvent is 5024, Mu (mm^-1) value with solvent is 2.013, and crystal density with solvent is 0.654.

Squeeze details for **3**·*S* at 220 K: Approximately 66.9% of the unit cell volume comprises a large region of disordered solvent that could not be modeled as discrete atomic sites. We employed PLATON SQUEEZE to calculate the contribution to the diffraction from the solvent region and thereby produced a set of solvent-free diffraction intensities. SQUEEZE estimated a total count of 848 electrons per unit cell. According to the final formula that was calculated from TGA combined with elemental analysis data, these electrons were assigned to be 32 ethanol molecules per unit cell. The F(000) value with solvent is 2648, Mu (mm^-1) value with solvent is 1.169, and crystal density with solvent is 0.632.

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Table S1. Elemental Analysis for 2-4·*G* with various exchanged solvent molecules

Formula		Content [%]	Calcd [%]	Formula		Content [%]	Calcd [%]
$[Fe(NCSe)_2(tppm)]$	N:	5.909	6.220	$[Fe(NCSe)_2(tppm)]$	N:	6.432	6.325
$\cdot 11CH_3OH$	C:	58.87	58.67	$\cdot 5MeOH\cdot 2CH_2Cl_2$	C:	56.36	56.04
	H:	6.364	6.266		H:	4.669	4.855
$[Fe(NCSe)_2(tppm)]$	N:	5.663	6.147	$[Fe(NCSe)_2(tppm)]$	N:	15.64	15.36
$\cdot 8C_2H_5OH$	C:	62.07	62.37	$\cdot 9CH_3CN$	C:	64.17	64.08
	H:	6.466	6.487		H:	4.721	4.936
$[Fe(NCSe)_2(tppm)]$	N:	6.351	6.485	$[Fe(NCSe)_2(tppm)]$	N:	6.785	6.498
$\cdot 3.5CH_2Cl_2$	C:	54.24	54.216	$\cdot 3C_6H_{12}$	C:	70.55	70.58
	H:	3.334	3.655		H:	6.456	6.391
$[Fe(NCSe)_2(tppm)]$	N:	6.324	6.194	$[Fe(NCSe)_2(tppm)]$	N:	6.336	6.238
$\cdot 3CHCl_3$	C:	51.46	51.34	$\cdot 6CH_3COCH_3$	C:	65.13	65.08
	H:	3.456	3.194		H:	5.917	5.686
$[Fe(NCBH_3)_2(tppm)]$	N:	6.935	6.883	$[Fe(NCBH_3)_2(tppm)]$	N:	6.642	7.012
$\cdot 11CH_3OH$	C:	62.91	64.93	$\cdot 5MeOH\cdot 2CH_2Cl_2$	C:	61.77	62.13
	H:	6.857	7.430		H:	5.549	5.887
$[Fe(NCBH_3)_2(tppm)]$	N:	6.524	6.794	$[Fe(NCBH_3)_2(tppm)]$	N:	16.94	16.97
$\cdot 8C_2H_5OH$	C:	66.86	68.94	$\cdot 9CH_3CN$	C:	71.17	70.83
	H:	6.864	7.659		H:	5.721	5.944
$[Fe(NCBH_3)_2(tppm)]$	N:	7.251	6.956	$[Fe(NCBH_3)_2(tppm)]$	N:	6.965	6.974
$\cdot 4CH_2Cl_2$	C:	58.25	58.65	$\cdot 4C_6H_{12}$	C:	78.55	78.74
	H:	4.234	4.505		H:	7.465	7.862
$[Fe(NCBH_3)_2(tppm)]$	N:	6.435	6.852	$[Fe(NCBH_3)_2(tppm)]$	N:	7.146	6.906
$\cdot 3CHCl_3$	C:	56.46	56.79	$\cdot 6CH_3COCH_3$	C:	72.13	72.05
	H:	3.864	4.026		H:	6.707	6.792
$\{Fe[N(CN)_2]_2(tppm)\}$	N:	10.77	11.00	$\{Fe[N(CN)_2]_2(tppm)\}$	N:	11.03	11.20
$\cdot 11CH_3OH$	C:	63.81	64.14	$\cdot 5MeOH\cdot 2CH_2Cl_2$	C:	60.86	61.45

	H:	6.346	6.695		H:	5.469	5.157
$\{Fe[N(CN)_2]_2(tppm)\}$	N:	10.49	10.86	$\{Fe[N(CN)_2]_2(tppm)\}$	N:	20.94	20.63
$\cdot 8C_2H_5OH$	C:	67.56	68.00	$\cdot 9CH_3CN$	C:	69.57	69.81
	H:	7.109	6.879		H:	5.321	5.234
$\{Fe[N(CN)_2]_2(tppm)\}$	N:	11.35	11.11	$\{Fe[N(CN)_2]_2(tppm)\}$	N:	10.98	11.14
$\cdot 4CH_2Cl_2$	C:	58.23	58.12	$\cdot 4C_6H_{12}$	C:	77.55	77.37
	H:	4.234	3.838		H:	6.756	7.054
$\{Fe[N(CN)_2]_2(tppm)\}$	N:	10.52	10.95	$\{Fe[N(CN)_2]_2(tppm)\}$	N:	11.36	11.03
$\cdot 3CHCl_3$	C:	56.46	56.35	$\cdot 6CH_3COCH_3$	C:	70.50	70.97
	H:	3.656	3.389		H:	6.007	6.035

Table S2. Selected Bond Angles [deg] for 2·*S* and 3·*S*.

2·*S* at 100 K.

$N(1)^{\#2}$-Fe(1)-N(1)	84.6(3)	$N(2)^{\#4}$-Fe(2)-$N(2)^{\#6}$	176.1(12)
$N(1)^{\#1}$-Fe(1)-$N(1)^{\#2}$	179.9(3)	$N(2)^{\#5}$-Fe(2)-N(2)	176.1(12)
$N(1)^{\#3}$-Fe(1)-$N(1)^{\#2}$	95.4(18)	$N(2)^{\#5}$-Fe(2)-$N(2)^{\#4}$	83.9(11)
$N(1)^{\#3}$-Fe(1)-$N(1)^{\#1}$	84.6(3)	$N(2)^{\#5}$-Fe(2)-$N(2)^{\#6}$	96.2(6)
$N(1)^{\#1}$-Fe(1)-N(1)	95.4(18)	N(2)-Fe(2)-$N(2)^{\#4}$	96.2(10)
$N(1)^{\#3}$-Fe(1)-N(1)	179.9(3)	N(2)-Fe(2)-$N(2)^{\#6}$	83.9(5)
$N(3)^{\#1}$-Fe(1)-N(1)	89.97(17)	$N(4)^{\#4}$-Fe(2)-N(2)	91.9(3)
$N(3)^{\#1}$-Fe(1)-$N(1)^{\#1}$	90.04(17)	$N(4)^{\#4}$-Fe(2)-$N(2)^{\#4}$	88.1(7)
$N(3)^{\#1}$-Fe(1)-$N(1)^{\#2}$	90.04(17)	$N(4)^{\#4}$-Fe(2)-$N(2)^{\#5}$	91.9(9)
$N(3)^{\#1}$-Fe(1)-$N(1)^{\#3}$	89.96(17)	$N(4)^{\#4}$-Fe(2)-$N(2)^{\#6}$	88.1(7)
N(3)-Fe(1)-N(1)	90.04(17)	N(4)-Fe(2)-N(2)	88.1(3)
N(3)-Fe(1)-$N(1)^{\#1}$	89.96(17)	N(4)-Fe(2)-$N(2)^{\#4}$	91.9(7)
N(3)-Fe(1)-$N(1)^{\#2}$	89.96(17)	N(4)-Fe(2)-$N(2)^{\#5}$	88.1(9)
N(3)-Fe(1)-$N(1)^{\#3}$	90.03(17)	N(4)-Fe(2)-$N(2)^{\#6}$	91.9(7)
N(3)-Fe(1)-$N(3)^{\#1}$	180.0	N(4)-Fe(2)-$N(4)^{\#4}$	180.0

Symmetry codes: #1) $x, -y + 1/2, -z + 1$; #2) $-x + 1/2, y, -z + 1$; #3) $-x + 1/2, -y + 1/2, z$; #4) $-x + 3/2, -y + 3/2, z$; #5) $x, -y + 3/2, -z + 2$; #6) $-x + 3/2, y, -z + 2$.

2·*S* at 155 K.

$N(1)^{\#1}$-Fe(1)-N(1)	90.1(2)	$N(2)^{\#5}$-Fe(2)-$N(2)^{\#6}$	90.2(4)
$N(3)^{\#2}$-Fe(1)-N(1)	178.90(19)	$N(4)^{\#4}$-Fe(2)-$N(2)^{\#5}$	89.6(3)
$N(3)^{\#2}$-Fe(1)-$N(1)^{\#1}$	88.82(15)	$N(4)^{\#4}$-Fe(2)-$N(2)^{\#6}$	179.7(4)
$N(3)^{\#2}$-Fe(1)-$N(3)^{\#3}$	92.2(2)	$N(4)^{\#4}$-Fe(2)-N(4)	90.7(4)
$N(3)^{\#3}$-Fe(1)-N(1)	88.82(15)	$N(4)^{\#6}$-Fe(2)-N(2)	89.6(3)
$N(3)^{\#3}$-Fe(1)-$N(1)^{\#1}$	178.90(19)	$N(4)^{\#4}$-Fe(2)-N(2)	179.7(4)
$N(5)^{\#1}$-Fe(1)-N(1)	91.2(3)	$N(6)^{\#4}$-Fe(2)-$N(2)^{\#5}$	89.2(5)
$N(5)^{\#1}$-Fe(1)-$N(1)^{\#1}$	93.1(3)	$N(6)^{\#4}$-Fe(2)-$N(2)^{\#6}$	90.2(5)
$N(5)^{\#1}$-Fe(1)-$N(3)^{\#2}$	88.6(3)	$N(6)^{\#4}$-Fe(2)-N(4)	90.5(4)
$N(5)^{\#1}$-Fe(1)-$N(3)^{\#3}$	87.2(3)	$N(6)^{\#4}$-Fe(2)-$N(4)^{\#4}$	89.9(5)

N(5)$^{\#1}$-Fe(1)-N(5)	174.0(5)	N(6)-Fe(2)-N(2)$^{\#5}$	90.2(5)
N(5)-Fe(1)-N(1)	93.1(3)	N(6)-Fe(2)-N(2)$^{\#6}$	89.2(5)
N(5)-Fe(1)-N(1)$^{\#1}$	91.2(3)	N(6)-Fe(2)-N(4)	89.9(5)
N(5)-Fe(1)-N(3)$^{\#2}$	87.2(3)	N(6)-Fe(2)-N(4)$^{\#4}$	90.5(4)
N(5)-Fe(1)-N(3)$^{\#3}$	88.6(3)	N(6)-Fe(2)-N(6)$^{\#4}$	179.1(6)

Symmetry codes: #1) $x, -y + 1/2, -z + 1/2$; #2) $x - 1, -y + 1/2, -z + 1/2$; #3) $x - 1, y, z$; #4) $-x + 3/2, -y, z$; #5) $-x + 3/2, y - 1/2, -z + 3/2$; #6) $x, -y + 1/2, -z + 3/2$.

2·*S* at 220 K.

N(1)$^{\#2}$-Fe(1)-N(1)	91.74(12)	N(2)$^{\#4}$-Fe(2)-N(2)$^{\#6}$	177.8(9)
N(1)$^{\#2}$-Fe(1)-N(1)$^{\#1}$	179.1(3)	N(2)$^{\#5}$-Fe(2)-N(2)	177.8(9)
N(1)$^{\#2}$-Fe(1)-N(1)$^{\#3}$	88.27(12)	N(2)$^{\#5}$-Fe(2)-N(2)$^{\#4}$	90.5(8)
N(1)$^{\#3}$-Fe(1)-N(1)$^{\#1}$	91.74(12)	N(2)$^{\#5}$-Fe(2)-N(2)$^{\#6}$	89.5(8)
N(1)-Fe(1)-N(1)$^{\#1}$	88.27(12)	N(2)-Fe(2)-N(2)$^{\#4}$	89.5(4)
N(1)-Fe(1)-N(1)$^{\#3}$	179.1(3)	N(2)-Fe(2)-N(2)$^{\#6}$	90.5(4)
N(3)$^{\#1}$-Fe(1)-N(1)	90.46(13)	N(4)$^{\#4}$-Fe(2)-N(2)	91.0(2)
N(3)$^{\#1}$-Fe(1)-N(1)$^{\#1}$	89.55(13)	N(4)$^{\#4}$-Fe(2)-N(2)$^{\#4}$	88.9 (5)
N(3)$^{\#1}$-Fe(1)-N(1)$^{\#2}$	89.55(13)	N(4)$^{\#4}$-Fe(2)-N(2)$^{\#5}$	1.0(7)
N(3)$^{\#1}$-Fe(1)-N(1)$^{\#3}$	90.46(13)	N(4)$^{\#4}$-Fe(2)-N(2)$^{\#6}$	88.9 (5)
N(3)-Fe(1)-N(1)	89.55(13)	N(4)-Fe(2)-N(2)	88.9(2)
N(3)-Fe(1)-N(1)$^{\#1}$	90.46(13)	N(4)-Fe(2)-N(2)$^{\#4}$	91.0(5)
N(3)-Fe(1)-N(1)$^{\#2}$	90.46(13)	N(4)-Fe(2)-N(2)$^{\#5}$	88.9(7)
N(3)-Fe(1)-N(1)$^{\#3}$	89.55(13)	N(4)-Fe(2)-N(2)$^{\#6}$	91.0(5)
N(3)-Fe(1)-N(3)$^{\#1}$	180.0	N(4)-Fe(2)-N(4)$^{\#4}$	180.0

Symmetry codes: #1) $x, -y + 1/2, -z + 1$; #2) $-x + 1/2, y, -z + 1$; #3) $-x + 1/2, -y + 1/2, z$; #4) $-x + 3/2, -y + 3/2, z$; #5) $x, -y + 3/2, -z + 2$; #6) $-x + 3/2, y, -z + 2$.

3·*S* at 110 K.

N(1)$^{\#2}$-Fe(1)-N(1)	84.6(3)	N(2)$^{\#4}$-Fe(2)-N(2)$^{\#6}$	176.1(12)
N(1)$^{\#1}$-Fe(1)-N(1)$^{\#2}$	179.9(3)	N(2)$^{\#5}$-Fe(2)-N(2)	176.1(12)
N(1)$^{\#3}$-Fe(1)-N(1)$^{\#2}$	95.4(18)	N(2)$^{\#4}$-Fe(2)-N(2)$^{\#5}$	83.9(10)
N(1)$^{\#3}$-Fe(1)-N(1)$^{\#1}$	84.6(3)	N(2)$^{\#5}$-Fe(2)-N(2)$^{\#6}$	96.2(6)
N(1) $^{\#1}$-Fe(1)-N(1)	95.4(18)	N(2)-Fe(2)-N(2)$^{\#4}$	96.3(10)
N(1) $^{\#3}$-Fe(1)-N(1)	179.9(3)	N(2)-Fe(2)-N(2)$^{\#6}$	83.9(5)
N(3)$^{\#1}$-Fe(1)-N(1)	89.96(17)	N(4)$^{\#4}$-Fe(2)-N(2)	92.0(3)
N(3)$^{\#1}$-Fe(1)-N(1)$^{\#1}$	90.04(17)	N(4)$^{\#4}$-Fe(2)-N(2)$^{\#4}$	88.0(7)
N(3)$^{\#1}$-Fe(1)-N(1)$^{\#2}$	90.04(17)	N(4)$^{\#4}$-Fe(2)-N(2)$^{\#5}$	92.0(9)
N(3)$^{\#1}$-Fe(1)-N(1)$^{\#3}$	89.96(17)	N(4)$^{\#4}$-Fe(2)-N(2)$^{\#6}$	88.0(6)
N(3)-Fe(1)-N(1)	90.04(17)	N(4)-Fe(2)-N(2)	88.0(3)
N(3)-Fe(1)-N(1)$^{\#1}$	89.96(17)	N(4)-Fe(2)-N(2)$^{\#4}$	92.0(7)
N(3)-Fe(1)-N(1)$^{\#2}$	89.96(17)	N(4)-Fe(2)-N(2)$^{\#5}$	88.0(9)
N(3)-Fe(1)-N(1)$^{\#3}$	90.04(17)	N(4)-Fe(2)-N(2)$^{\#6}$	92.0(7)
N(3)-Fe(1)-N(3)$^{\#1}$	180.0	N(4)-Fe(2)-N(4)$^{\#4}$	180.0

Symmetry codes: #1) $x, -y + 1/2, -z + 1$; #2) $-x + 1/2, y, -z + 1$; #3) $-x + 1/2, -y + 1/2, z$; #4) $-x + 3/2, -y + 3/2, z$; #5) $x, -y + 3/2, -z + 2$; #6) $-x + 3/2, y, -z + 2$.

3·*S* at 175 K.

N(1)-Fe(1)-N(1)$^{\#1}$	90.2(2)	N(2)$^{\#5}$-Fe(2)-N(2)$^{\#6}$	89.8(4)
N(3)$^{\#2}$-Fe(1)-N(1)	178.90(19)	N(4)$^{\#4}$-Fe(2)-N(2)$^{\#5}$	89.9(3)
N(3)$^{\#2}$-Fe(1)-N(1)$^{\#1}$	88.75(15)	N(4)$^{\#4}$-Fe(2)-N(2)$^{\#6}$	179.4(4)
N(3)$^{\#3}$-Fe(1)-N(3)$^{\#2}$	92.3(2)	N(4)$^{\#6}$-Fe(2)-N(2)	89.9(3)
N(3)$^{\#3}$-Fe(1)-N(1)	88.75(15)	N(4)$^{\#4}$-Fe(2)-N(2)	179.4(4)
N(3)$^{\#3}$-Fe(1)-N(1)$^{\#1}$	178.90(19)	N(4)-Fe(2)-N(4)$^{\#4}$	90.5(4)
N(5)$^{\#1}$-Fe(1)-N(1)	91.1(3)	N(6)$^{\#4}$-Fe(2)-N(2)$^{\#5}$	89.0(5)
N(5)$^{\#1}$-Fe(1)-N(1)$^{\#1}$	93.1(3)	N(6)$^{\#4}$-Fe(2)-N(2)$^{\#6}$	90.4(5)
N(5)$^{\#1}$-Fe(1)-N(3)$^{\#2}$	88.6(3)	N(6)$^{\#4}$-Fe(2)-N(4)	90.6(5)
N(5)$^{\#1}$-Fe(1)-N(3)$^{\#3}$	87.2(3)	N(6)$^{\#4}$-Fe(2)-N(4)$^{\#4}$	90.0(6)
N(5)$^{\#1}$-Fe(1)-N(5)	174.0(5)	N(6)-Fe(2)-N(2)$^{\#5}$	90.4(5)
N(5)-Fe(1)-N(1)	93.1(3)	N(6)-Fe(2)-N(2)$^{\#6}$	89.0(5)
N(5)-Fe(1)-N(1)$^{\#1}$	91.1(3)	N(6)-Fe(2)-N(4)	90.0(6)
N(5)-Fe(1)-N(3)$^{\#2}$	87.2(3)	N(6)-Fe(2)-N(4)$^{\#4}$	90.6(5)
N(5)-Fe(1)-N(3)$^{\#3}$	88.6(3)	N(6)-Fe(2)-N(6)$^{\#4}$	179.1(6)

Symmetry codes: #1) $x, -y + 1/2, -z + 1/2$; #2) $x - 1, -y + 1/2, -z + 1/2$; #3) $x - 1, y, z$; #4) $-x + 3/2, -y, z$; #5) $-x + 3/2, y - 1/2, -z + 3/2$; #6) $x, -y + 1/2, -z + 3/2$.

3·*S* at 220 K.

N(1)$^{\#2}$-Fe(1)-N(1)	91.85(18)	N(2)$^{\#4}$-Fe(2)-N(2)$^{\#6}$	177.8(9)
N(1)$^{\#2}$-Fe(1)-N(1)$^{\#1}$	179.1(3)	N(2)$^{\#5}$-Fe(2)-N(2)	177.8(9)
N(1)$^{\#3}$-Fe(1)-N(1)$^{\#2}$	88.16(18)	N(2)$^{\#4}$-Fe(2)-N(2)$^{\#5}$	90.7(8)
N(1)$^{\#3}$-Fe(1)-N(1)$^{\#1}$	91.85(18)	N(2)$^{\#5}$-Fe(2)-N(2)$^{\#6}$	89.4(8)
N(1)-Fe(1)-N(1)$^{\#1}$	88.16(18)	N(2)-Fe(2)-N(2)$^{\#4}$	89.4(4)
N(1)-Fe(1)-N(1)$^{\#3}$	179.1(3)	N(2)-Fe(2)-N(2)$^{\#6}$	90.7(4)
N(3)$^{\#1}$-Fe(1)-N(1)	90.43(13)	N(4)$^{\#4}$-Fe(2)-N(2)	91.1(2)
N(3)$^{\#1}$-Fe(1)-N(1)$^{\#1}$	89.57(13)	N(4)$^{\#4}$-Fe(2)-N(2)$^{\#4}$	88.9 (5)
N(3)$^{\#1}$-Fe(1)-N(1)$^{\#2}$	89.57(13)	N(4)$^{\#4}$-Fe(2)-N(2)$^{\#5}$	91.1(7)
N(3)$^{\#1}$-Fe(1)-N(1)$^{\#3}$	90.43(13)	N(4)$^{\#4}$-Fe(2)-N(2)$^{\#6}$	88.9 (5)
N(3)-Fe(1)-N(1)	89.57(13)	N(4)-Fe(2)-N(2)	88.9(2)
N(3)-Fe(1)-N(1)$^{\#1}$	90.43(13)	N(4)-Fe(2)-N(2)$^{\#4}$	91.1(6)
N(3)-Fe(1)-N(1)$^{\#2}$	90.43(13)	N(4)-Fe(2)-N(2)$^{\#5}$	88.9(7)
N(3)-Fe(1)-N(1)$^{\#3}$	89.57(13)	N(4)-Fe(2)-N(2)$^{\#6}$	91.1(5)
N(3)-Fe(1)-N(3)$^{\#1}$	180.0	N(4)-Fe(2)-N(4)$^{\#4}$	180.0

Symmetry codes: #1) $x, -y + 1/2, -z + 1$; #2) $-x + 1/2, y, -z + 1$; #3) $-x + 1/2, -y + 1/2, z$; #4) $-x + 3/2, -y + 3/2, z$; #5) $x, -y + 3/2, -z + 2$; #6) $-x + 3/2, y, -z + 2$.

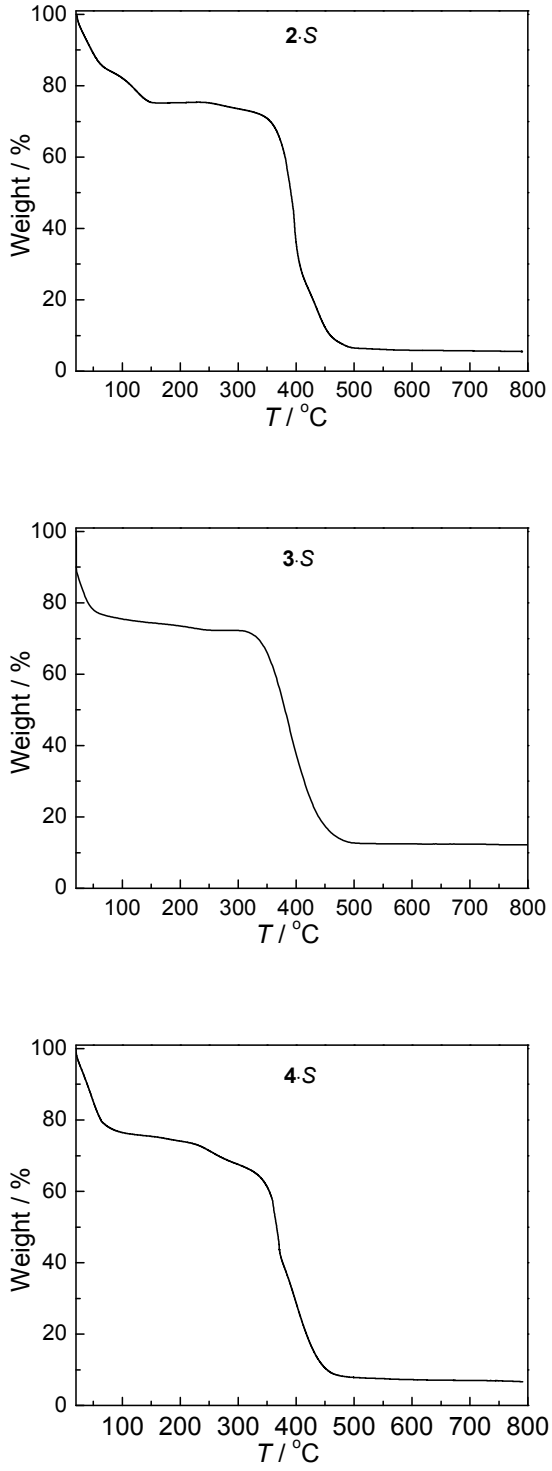

Figure S1. Thermogravimetric analysis of **2**-**4**·*S*.

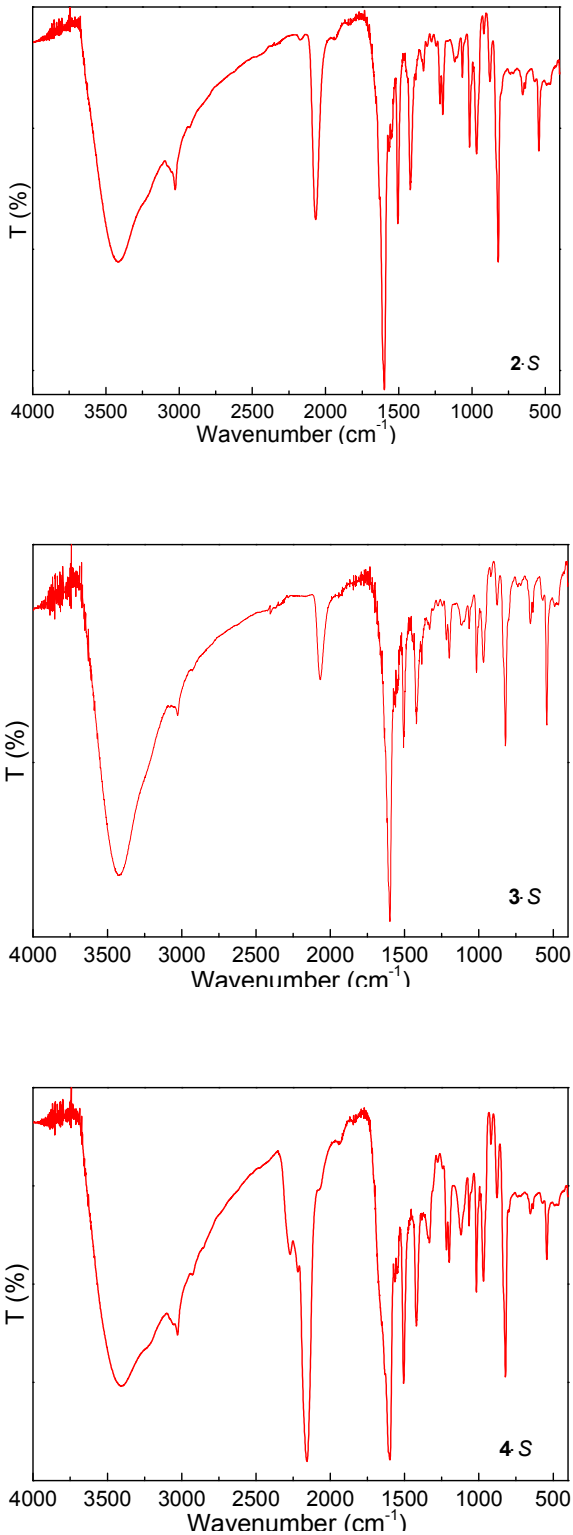

Figure S2. IR spectra of **2**-**4**·*S*.