Electronic Supplementary Material (ESI) for CrystEngComm

Supplementary Information

Synthesis, X-ray crystal structures and inclusion properties of a hydrogen-bonded coordination polymer $[Ni(SCN)_2(pppeH)_2]\cdot(guest)_x$

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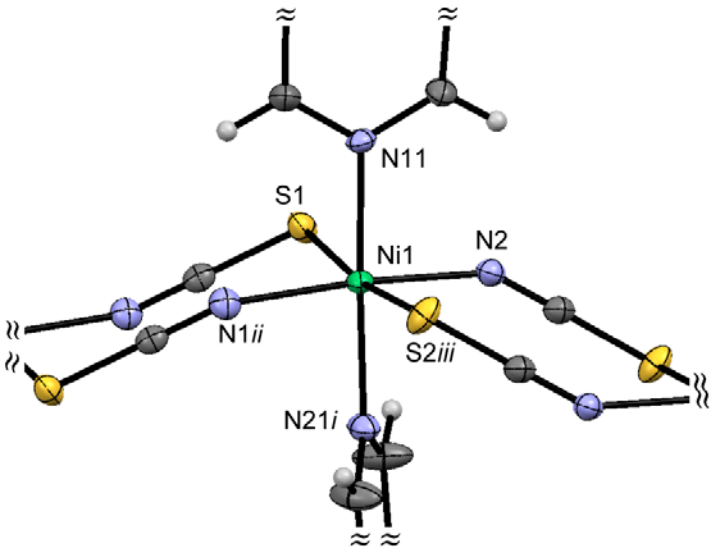

Figure S1. ORTEP drawing (50 % probability ellipsoids) of the coordination environment around the Ni^{2+} center of **2** with atomic numbering scheme. Symmetry codes: ^{i} $x, y, z - 1$; ^{ii} $-x, -y + 2, -z$; ^{iii} $-x, -y + 1, -z$.

Table S1. Selected bond lengths (Å) and angles (°) for **2**.

Ni1 – $N1^{ii}$	2.039(3)	$N1^{ii}$ – Ni1 – N2	171.8(1)
Ni1 – N2	2.038(3)	N11 – Ni1 –	176.2(2)
Ni1 – N11	2.138(3)	S1 – Ni1 – $S2^{iii}$	173.11(4)
Ni1 – $N21^{i}$	2.104(3)	$N1^{ii}$ – Ni1 – N11	86.7(1)
Ni1 – S1	2.514(1)	$N1^{ii}$ – Ni1 – S1	92.9(1)
Ni1 – $S2^{iii}$	2.561(1)	N11 – Ni1 – S1	91.5(1)

Symmetry codes: ^{i} $x, y, z - 1$; ^{ii} $-x, -y + 2, -z$; ^{iii} $-x, -y + 1, -z$.

Table S2. Hydrogen bond distances (Å) for **2**.

O11A	···	2.672(8)	O11B ··· O31B	2.48(4)
O12A	···	2.657(9)	O12B ··· O32B	2.51(4)

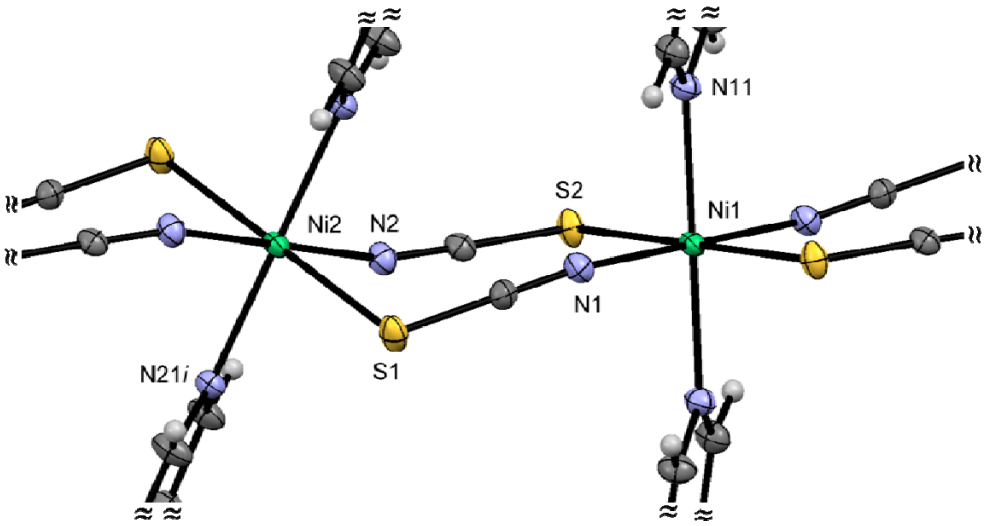

Figure S2. ORTEP drawing (50 % probability ellipsoids) of the coordination environments around the Ni^{2+} centers of **3** with atomic numbering scheme. Symmetry codes: ^{i} $x, y, z - 1$.

Table S3. Selected bond lengths (Å) and angles (°) for **3**.

Ni1 – N1	2.053(3)	N1 – Ni1 – N11	90.9(1)
Ni2 – N2	2.042(3)	N1 – Ni1 – S2	86.40(7)
Ni1 – N11	2.105(3)	N11 – Ni1 – S2	89.68(7)
Ni2 – N21^{i}	2.105(2)	N2 – Ni2 – N21^{i}	91.2(1)
Ni1 – S2	2.533(1)	N2 – Ni2 – S1	91.23(7)
Ni2 – S1	2.559(1)	N21^{i} – Ni1 – S1	89.50(7)

Symmetry codes: ^{i} $x, y, z - 1$.

Table S4. Hydrogen bond distances (Å) for **3**.

O11 ··· O31	2.619(3)	O12 ··· O32	2.628(3)

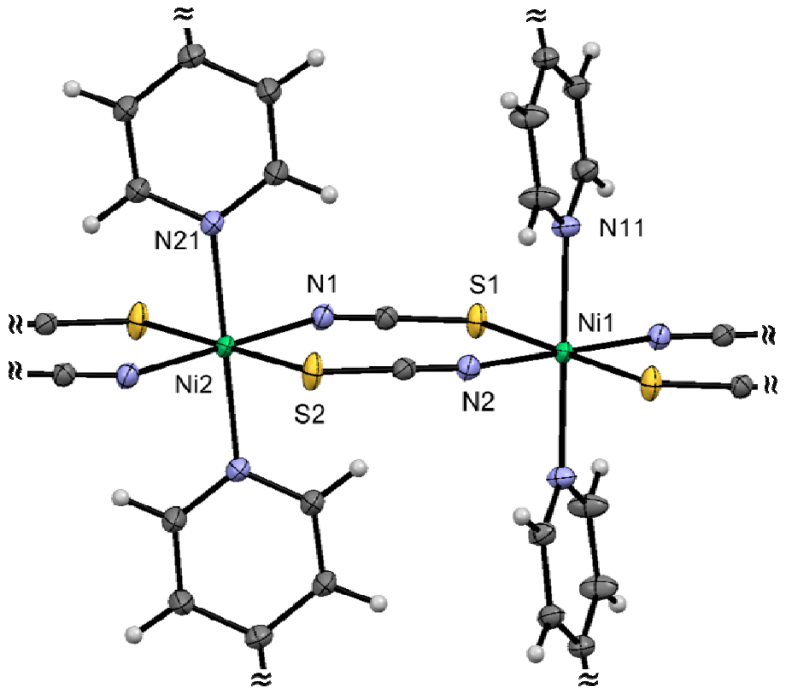

Figure S3. ORTEP drawing (50 % probability ellipsoids) of the coordination environments around the Ni^{2+} centers of **4** with atomic numbering scheme.

Table S5. Selected bond lengths (Å) and angles (°) for **4**.

Ni1 – N1	2.023(2)	N1 – Ni1 – N11	89.89(7)
Ni2 – N2	2.026(2)	N1 – Ni1 – S2	94.62(7)
Ni1 – N11	2.119(2)	N11 – Ni1 – S2	89.25(5)
Ni2 – N21	2.120(2)	N2 – Ni2 – N21	90.30(7)
Ni1 – S2	2.5185(9)	N2 – Ni2 – S1	92.59(7)
Ni2 – S1	2.5250(9)	N21 – Ni1 – S1	89.71(5)

Table S6. Hydrogen bond distances (Å) for **4**.

O11 ··· O12	2.633(2)	O31 ··· O32	2.634(2)