Supplementary Information

Utilization of Mixtures of Aromatic N-Donor Ligands of Different Coordination Ability for the Solvothermal Synthesis of Thiostannate Containing Molecules

Jessica Hilbert, Christian Näther and Wolfgang Bensch

Content

Figure S1	Comparison of the experimental PXRD pattern of I and II with those simulated from single-crystal X-ray data.	2
Table S1	Selected angles (°) of the octahedral Ni ²⁺ environment of I and II.	3
Table S2	Dihedral angles between the phen moieties for compounds I and II.	3
Figure S2	IR spectra of I (top) and II (bottom).	3
Figure S3	Raman spectra of I (top) and II (bottom).	4
Figure S4	UV/vis spectra of compound I.	4
Figure S5	UV/Vis spectra of compound II.	5
Figure S6	DTA, TG and DTG curves for compound I.	5
Figure S7	DTA, TG and DTG curves for compound II.	6
Figure S8	Temperature dependence of the magnetic susceptibility for compound I in field of 100 Oe.	6
Figure S9	Temperature dependence of the magnetic susceptibility for compound II in field of 100 Oe.	7



Fig. S1: Comparison of the experimental PXRD pattern of I (top) and II (bottom) with those simulated from single-crystal X-ray data.

	I		II
N1 ^a – Ni1 – N1	165.69(1)	N21 – Ni1 – N1	162.82(12)
N2 – Ni1 – S1 ^a	173.19(9)	N22 – Ni1 – S2	172.28(9)
N2a – Ni1 – S1	173.19(9)	N2 – Ni1 – S3	172.36(8)
N1 ^a – Ni1 – N2	91.54(13)	N22 – Ni1 – N1	92.95(12)
N1 – Ni1 – N2 ^a	91.54(13)	N21 – Ni1 – N2	88.00(11)
N2 – Ni1 – N2 ^a	93.84(18)	N22 – Ni1 – N2	91.35(11)
N1 – Ni1 – N2	78.64(13)	N1 – Ni1 – N2	77.38(11)
N1 ^a – Ni1 – N2 ^a	78.64(13)	N22 – Ni1 – N22	78.25(12)
N1 ^a – Ni1 – S1 ^a	95.27(9)	N21 – Ni1 – S2	94.11(9)
N1 – Ni1 – S1ª	94.64(9)	N2 – Ni1 – S2	89.46(8)
N2 – Ni1 – S1ª	87.36(9)	N1 – Ni1 – S2	94.72(8)
N1a – Ni1 – S1	94.64(9)	N21 – Ni1 – S3	99.34(8)
N1 – Ni1 – S1	95.27(9)	N22 – Ni1 – S3	88.13(9)
N2 – Ni1 – S1	87.36(9)	N1 – Ni1 – S3	95.04(8)
S1 ^a – Ni1 – S1	92.23(5)	S2 – Ni1 – S3	92.08(3)

Table S1: Selected angles (°) of the octahedral Ni²⁺ environment of I and II.

Table S2: Dihedral angles between the phen moieties for compounds I and II.

			II
N2 ^a – Ni1 – N1 – C10	82.70(33)	N22 – Ni1 – N1 – C1	-88.73(33)
N2 ^a – Ni1 – N1 – C11	-96.72(26)	N22 – Ni1 – N1 – C12	92.57(24)
N2 ^a – Ni1 – N2 – C1	-90.95(33)	N22 – Ni1 – N2 – C10	88.26(32)
N2 ^a – Ni1 – N2 – C12	95.23(26)	N22 – Ni1 – N2 – C11	-95.65(24)



Fig. S2: IR spectra of I (top) and II (bottom).



Fig. S3: Raman spectra of I (top) and II (bottom).



Fig. S4: UV/vis spectra of compound I.



Fig. S5: UV/Vis spectra of compound II.



Fig. S6: DTA, TG and DTG curves for compound I.



Fig. S7: DTA, TG and DTG curves for compound II.



Fig. S8: Temperature dependence of the magnetic susceptibility for compound I in field of 100 Oe.



Fig. S9: Temperature dependence of the magnetic susceptibility for compound **II** in field of 100 Oe.