Supporting information for

Six-coordinated nickel(II) complexes with benzothiadiazole Schiff-base ligands: synthesis, crystal structure, magnetic and HFEPR study

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Table S1. Shape measures calculation for six-coordinated nickel (II) ion of **1** and **2** obtained using SHAPE.

Structure [NiL_6]	Hexagon (D_{6h})	Pentagonal pyramid (C_{5v})	Octahedron (O_h)	Trigonal prism (D_{3h})	Johnson pentagonal pyramid J2 (C_{5v})
$Ni(L^1)_2$ **(1)**	31.110	25.415	0.880	12.280	28.919
$Ni(L^2)_2 \cdot CH_2Cl_2$ **(2)**	32.414	25.994	0.605	12.949	29.711

Table S2. Selected bond distances (Å) and angles (°) for **1**.

N(1)-Ni(1)	2.2207(16)	$N(1)^i$ -Ni(1)	2.2207(16)
N(3)-Ni(1)	2.0587(15)	$N(3)^i$ -Ni(1)	2.0587(15)
Ni(1)-O(1)	1.9977(13)	Ni(1)-$O(1)^i$	1.9977(13)
O(1)-Ni(1)-$O(1)^i$	97.64(8)	$O(1)^i$ -Ni(1)-N(1)	168.05(5)
O(1)-Ni(1)-$N(3)^i$	90.14(6)	$N(3)^i$ -Ni(1)-N(1)	97.87(6)
$O(1)^i$ -Ni(1)-$N(3)^i$	92.28(6)	N(3)-Ni(1)-N(1)	79.42(6)
O(1)-Ni(1)-N(3)	92.28(6)	O(1)-Ni(1)-$N(1)^i$	168.05(5)
$O(1)^i$ -Ni(1)-N(3)	90.14(6)	$O(1)^i$ -Ni(1)-$N(1)^i$	88.66(6)
$N(3)^i$ -Ni(1)-N(3)	176.32(8)	$N(3)^i$ -Ni(1)-$N(1)^i$	79.42(6)
O(1)-Ni(1)-N(1)	88.66(6)	N(3)-Ni(1)-$N(1)^i$	97.88(6)
N(1)-Ni(1)-$N(1)^i$	87.04(8)		

Symmetry code: i = -x+1,y,-z+1/2.

Table S3. Selected bond distances (Å) and angles (°) for **2**.

N(6)-Ni(1)	2.052(4)	N(2)-Ni(1)	2.159(5)
O(1)-Ni(1)	1.997(4)	N(3)-Ni(1)	2.060(4)
O(3)-Ni(1)	2.010(3)	N(5)-Ni(1)	2.181(4)
O(1)-Ni(1)-N(2)	170.94(16)	O(1)-Ni(1)-O(3)	95.89(16)
O(3)-Ni(1)-N(2)	87.69(16)	O(1)-Ni(1)-N(6)	98.18(17)
N(6)-Ni(1)-N(2)	90.10(18)	O(3)-Ni(1)-N(6)	90.41(16)
N(3)-Ni(1)-N(2)	80.97(18)	O(1)-Ni(1)-N(3)	90.30(17)
O(1)-Ni(1)-N(5)	87.64(16)	O(3)-Ni(1)-N(3)	97.33(16)
O(3)-Ni(1)-N(5)	170.35(16)	N(6)-Ni(1)-N(3)	167.90(17)
N(6)-Ni(1)-N(5)	80.19(16)	N(2)-Ni(1)-N(5)	90.16(17)
N(3)-Ni(1)-N(5)	91.62(16)		

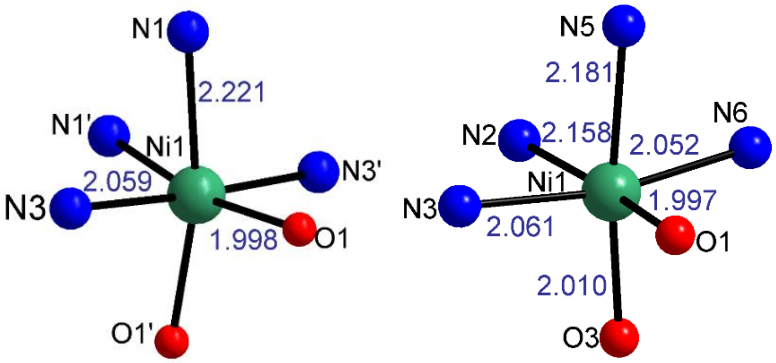

Fig. S1 The coordination enviroment of nickel(II) ion in complex **1** (left) and **2** (right).

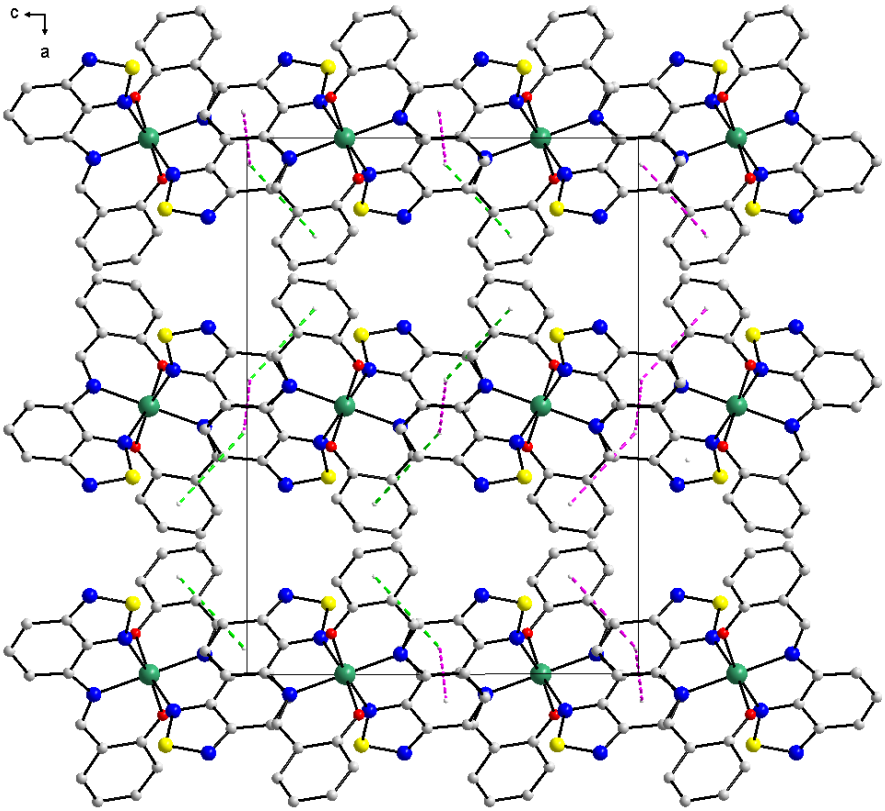

Fig. S2 Crystal packing of complex **1** along the *b* axis showing the π-π stacking interactions.

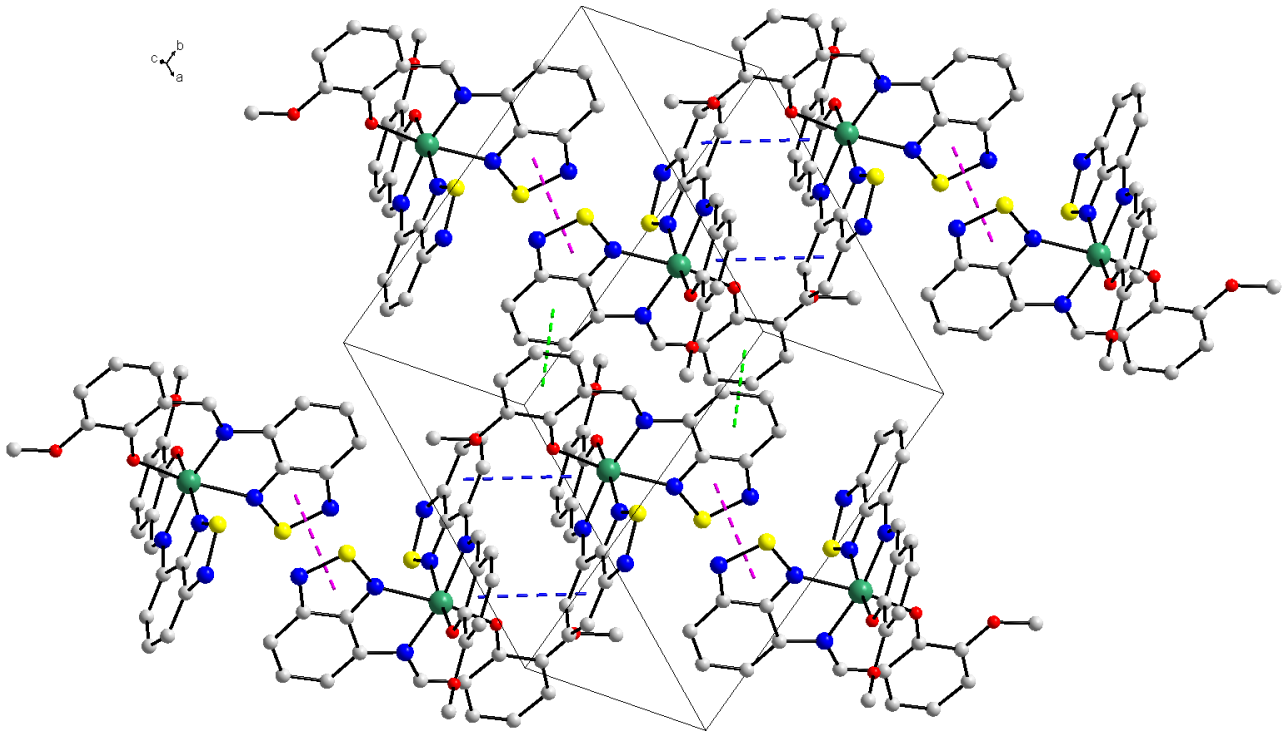

Fig. S3 Crystal structure of complex **2** showing π-π stacking interactions (solvent molecules are omitted for clarity).

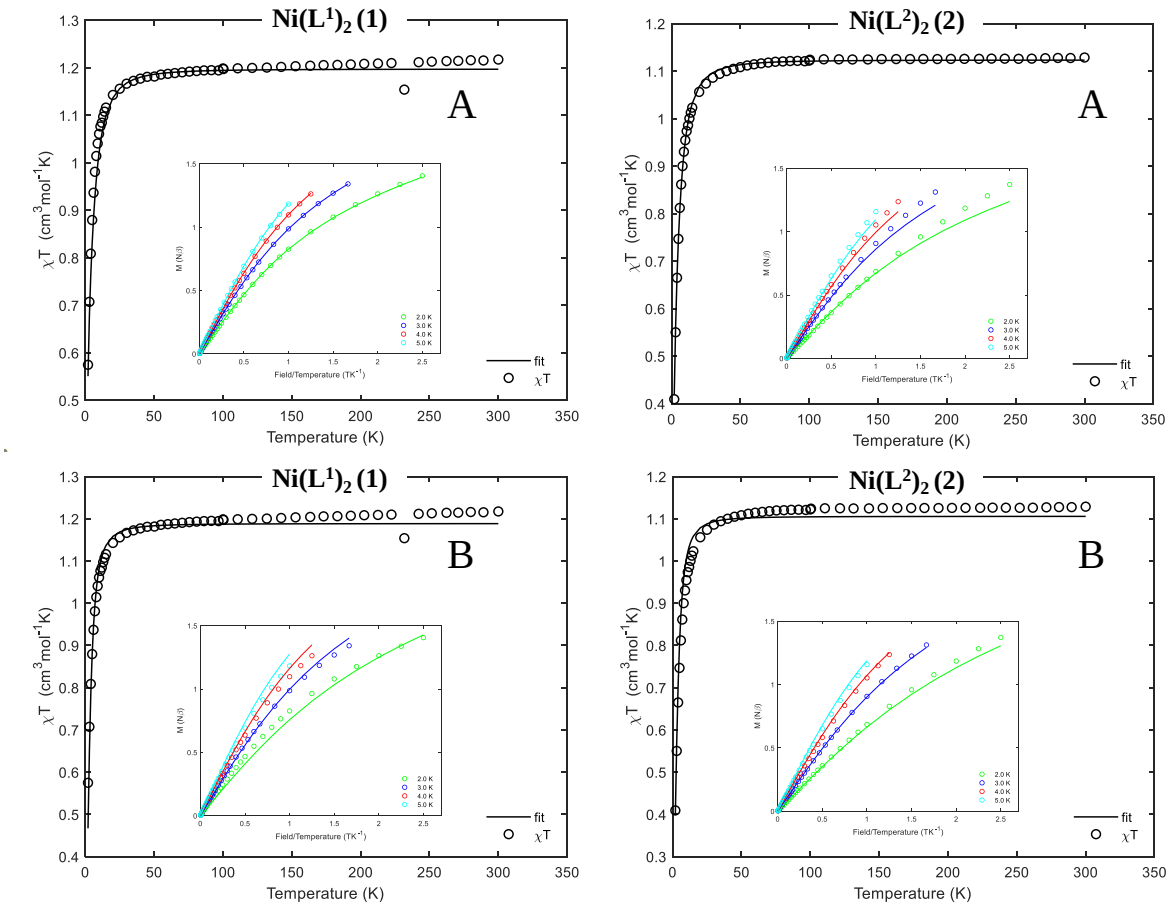

Fig. S4 Fits of Magnetic susceptibility (0.1 T) and magnetization at indicated temperatures for compounds **1** and **2** under conditions where D < 0 (A) and D > 0 (B).

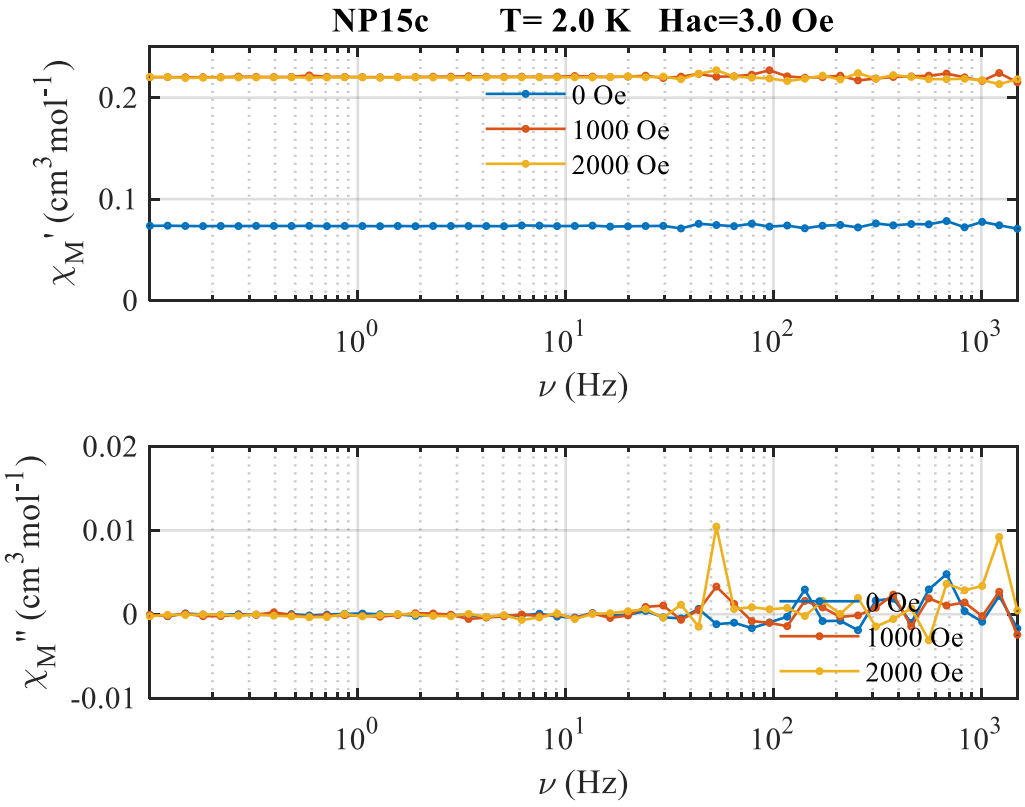

Fig. S5 The *ac* susceptibility (H_{ac}=3.0 Oe) for sample **2** at 0, 1000 and 2000 Oe.

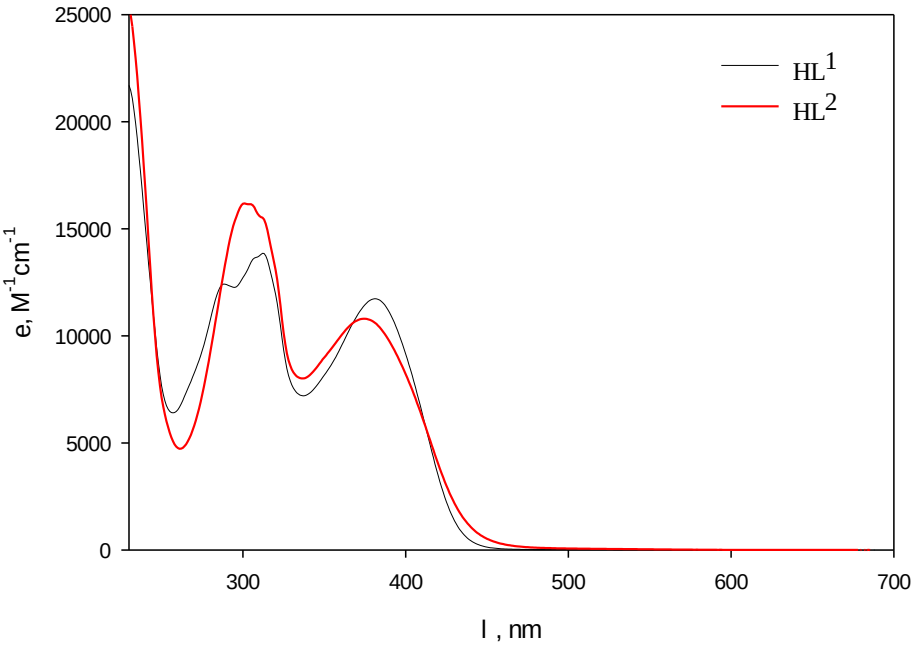

Fig. S6 UV-Vis spectra of the ligands HL^1 and HL^2 in dichloromethane ($C = 5 \times 10^{-5}$ M, room temperature).

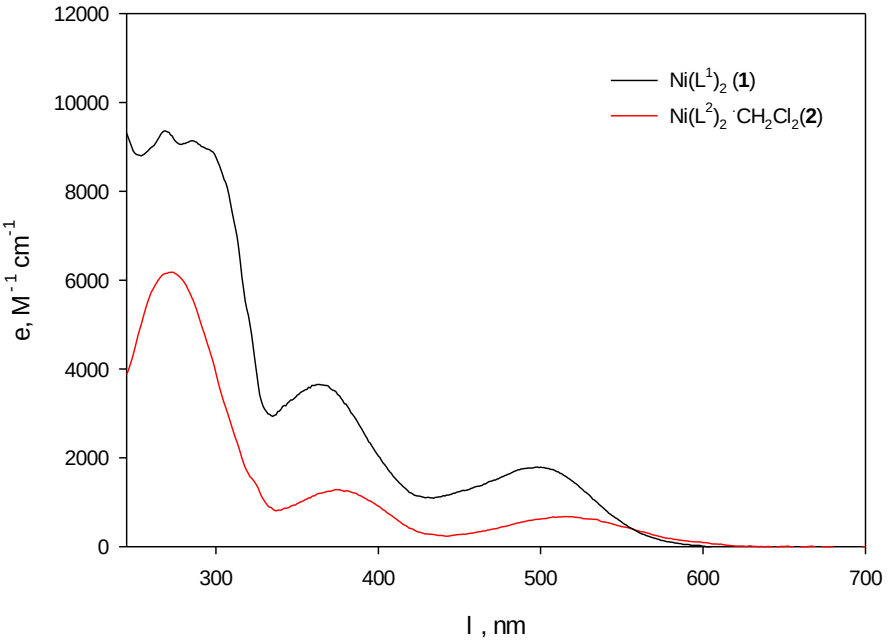

Fig. S7 UV-Vis spectra of complexes **1** and **2** in acetonitrile ($C = 1.5 \times 10^{-5}$ M, room temperature).

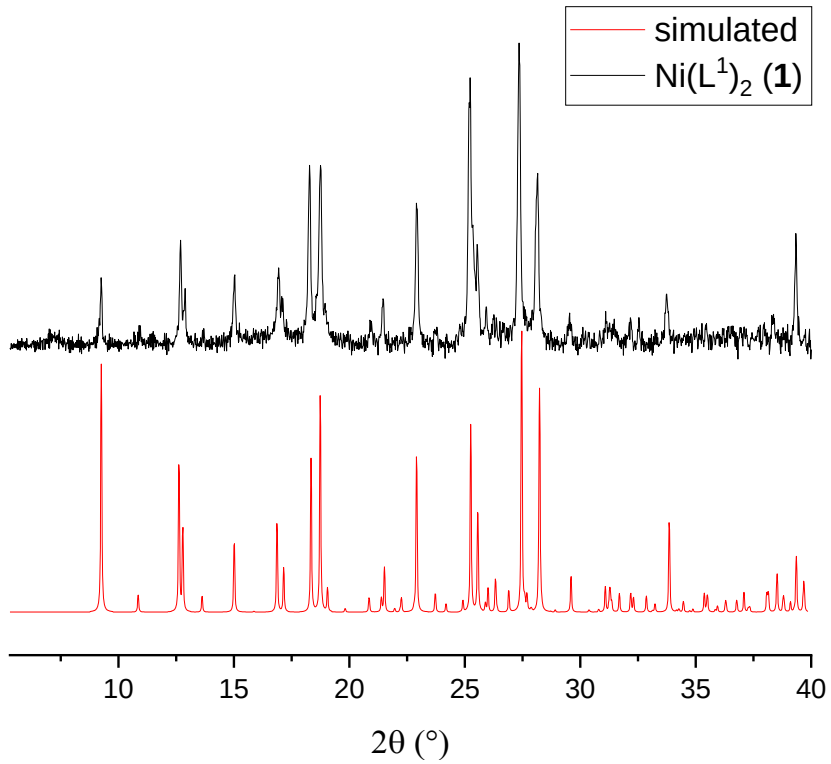

Fig. S8 Experimental powder X-ray diffraction (PXRD) diffractogram of complex **1** (top) and the simulated one from single crystal data (bottom).

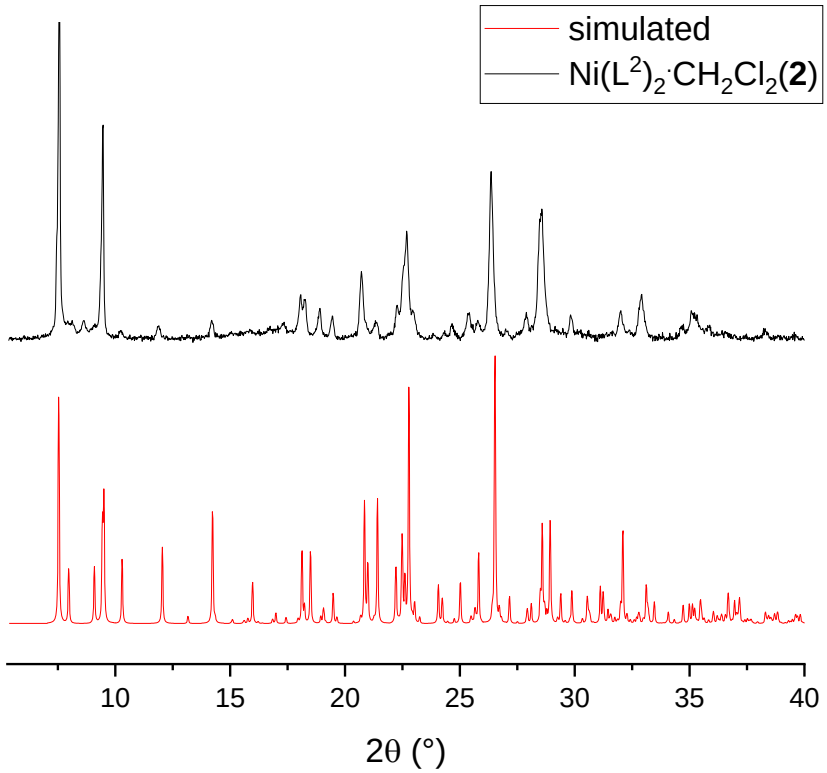

Fig. S9 Experimental powder X-ray diffraction (PXRD) diffractogram of complex **2** (top) and the simulated one from single crystal data (bottom).