

Supporting Information

Targeted construction of azido-bridged Ni₄
complexes with decisive effect of μ -1,3 azide
torsion on the spin ground state

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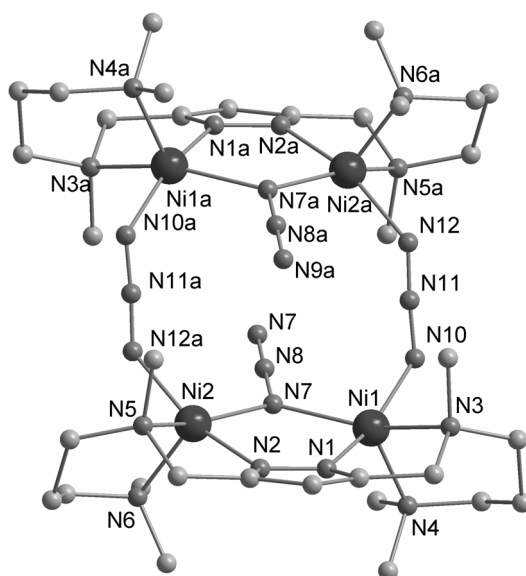


Figure S1: View of the molecular structure of **4b**. In the interest of clarity all hydrogen atoms have been omitted. Selected atom distances (Å) and angles (°): Ni(1)–N(1) 1.938(3), Ni(1)–N(10) 2.036(3), Ni(1)–N(4) 2.051(3), Ni(1)–N(7) 2.123(3), Ni(1)–N(3) 2.139(3), Ni(2)–N(2) 1.941(3), Ni(2)–N(12) 2.021(3), Ni(2)–N(6) 2.049(4), Ni(2)–N(7) 2.120(4), Ni(2)–N(5) 2.165(4), Ni1⋯Ni2 3.6141(8), Ni1⋯Ni2a 5.4797(7) (1), Ni1⋯Ni1a 6.707(1), Ni2⋯Ni2a 6.418(1), N7–N8 1.218(4), N8–N9 1.148(4), N10–N11 1.177(4), N11–N12 1.165(4); Ni1–N7–Ni2 116.8(2), N10–N11–N12 176.2(4). Symmetry transformation used to generate equivalent atoms: (a) $1/2-x, 3/2-y, 1-z$.

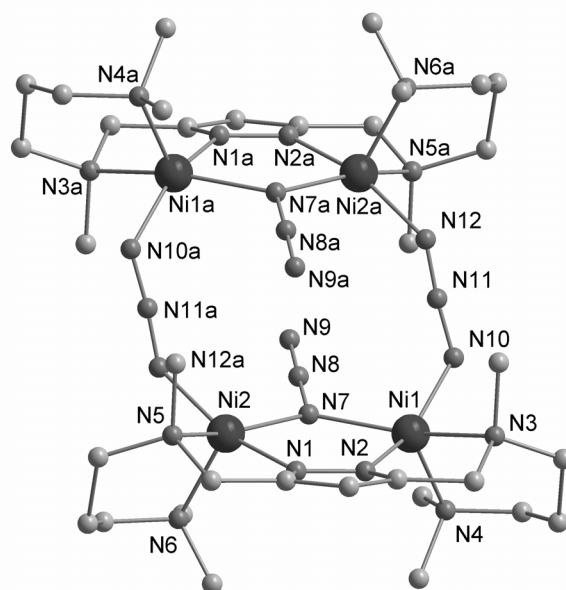


Figure S2: View of the molecular structure of **4c** (the non disordered molecule). In the interest of clarity all hydrogen atoms have been omitted. Selected atom distances (Å) and angles (°): Ni(1)–N(1) 1.925(6), Ni(1)–N(10) 2.013(6), Ni(1)–N(4) 2.047(7), Ni(1)–N(7) 2.132(6), Ni(1)–N(3) 2.169(7), Ni(2)–N(2) 1.922(6), Ni(2)–N(12) 2.033(7), Ni(2)–N(6) 2.044(6), Ni(2)–N(7) 2.133(6), Ni(2)–N(5) 2.161(6), Ni1⋯Ni2 3.645(1), Ni1⋯Ni2a 5.478(1) (1), Ni1⋯Ni1a 6.927(2), Ni2⋯Ni2a 6.214(2), N7–N8 1.212(9), N8–N9 1.152(10), N10–N11 1.185(9), N11–N12 1.167(9); Ni1–N7–Ni2 117.4(3), N10–N11–N12 175.1(7). Symmetry transformation used to generate equivalent atoms: (a) 1–*x*, 1–*y*, 1–*z*.

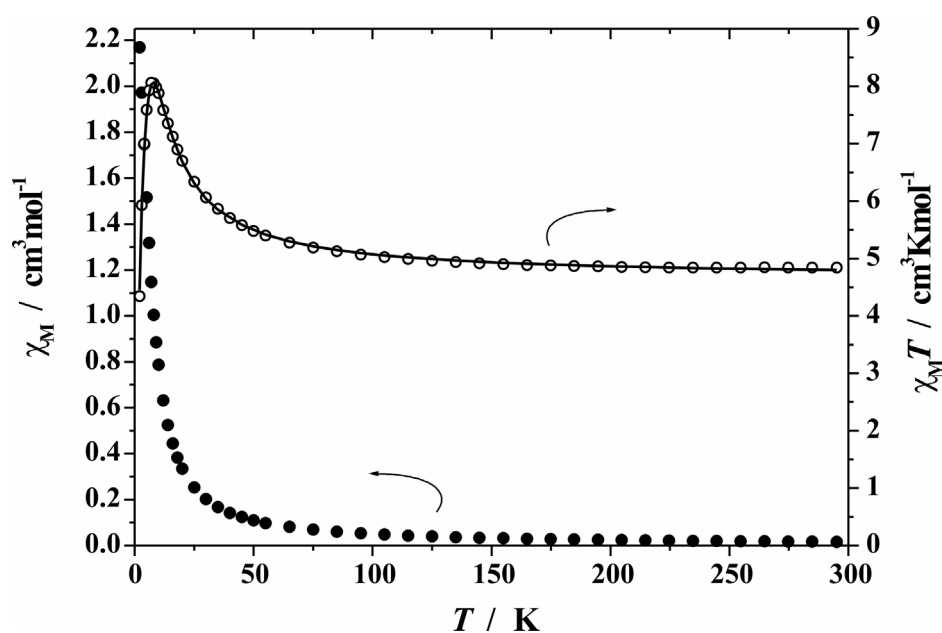


Figure S3: χ_M (solid circles) and $\chi_M T$ (open circles) vs. T plot for **4b** at 5000 G; the solid line represents the calculated curve fit.