Electronic Supplementary Material (ESI) for CrystEngComm.

Polynuclear coordination compounds: A magnetostructural study of ferromagnetically coupled Ni_4O_4 cubane core motif

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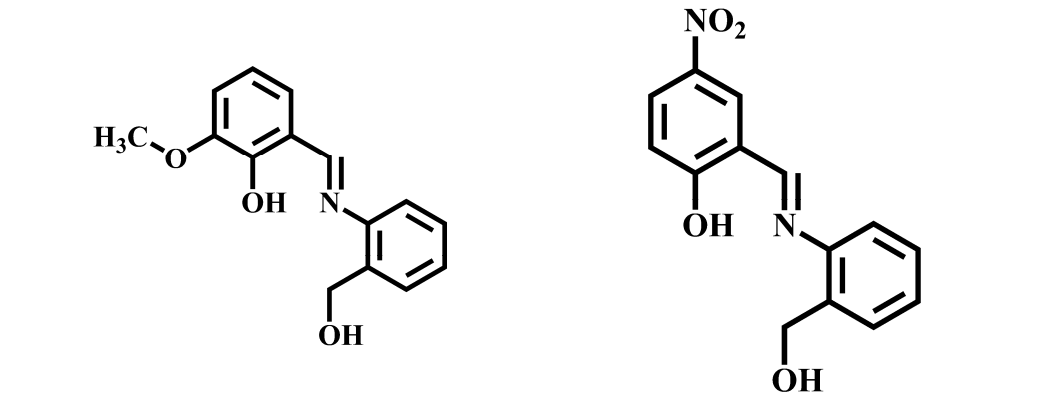
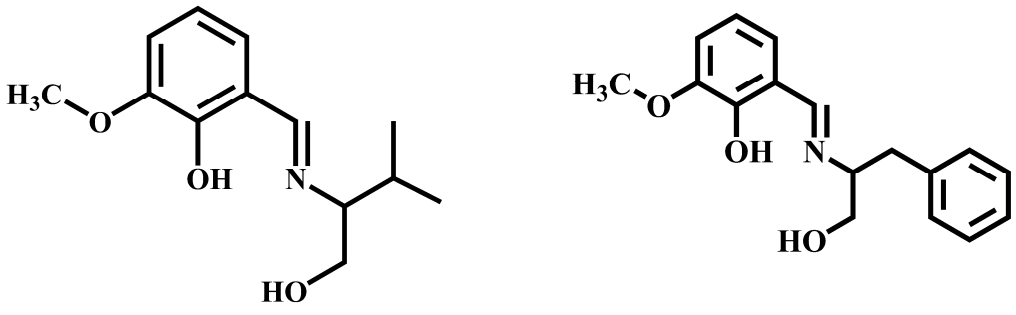


H_2L^1 H_2L^2



H_2L^3 H_2L^4

Fig S1 Representation of the ligands

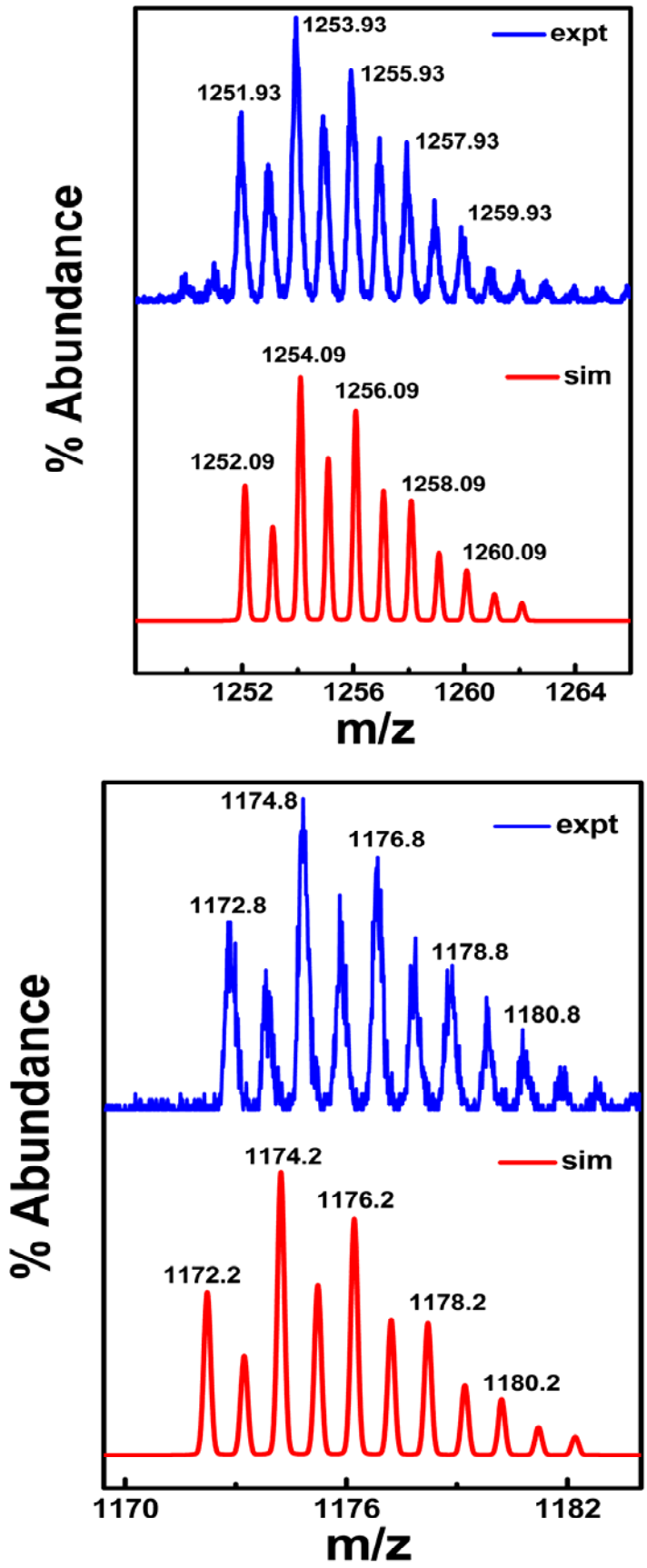


Fig S2 Molecular ion peak in the ESI-MS spectrum for **1**(top) and **4**(bottom) with simulated and observed isotopic distributions.

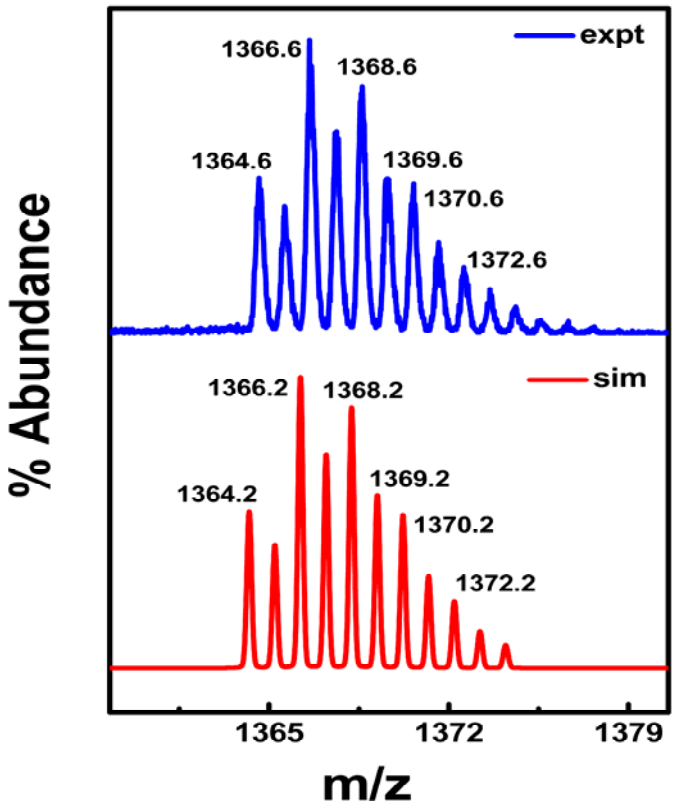


Fig S3 Molecular ion peak in the ESI-MS spectrum for **5** with simulated and observed isotopic distributions.

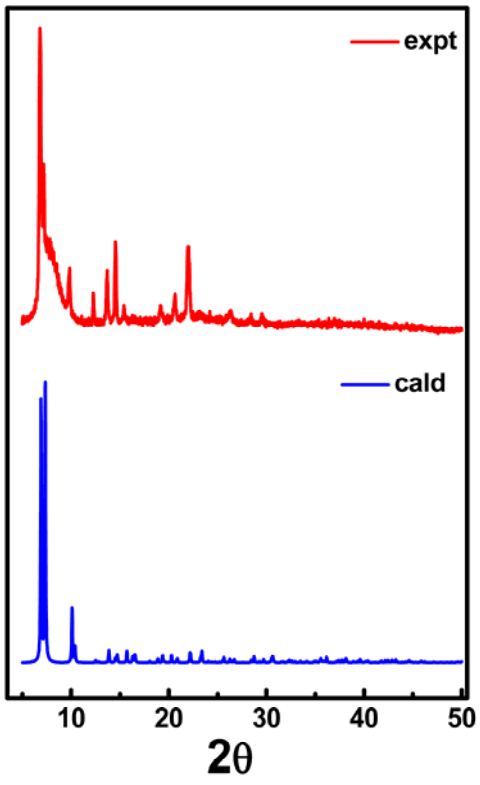


Fig S4: Experimental (red) and calculated (blue) powder XRD patterns of complex **1**.

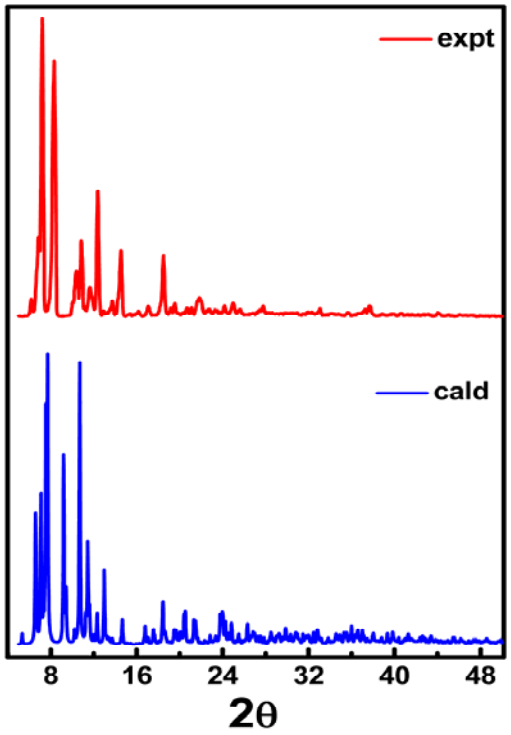


Fig S5: Experimental (red) and calculated (blue) powder XRD patterns of complex **2**.

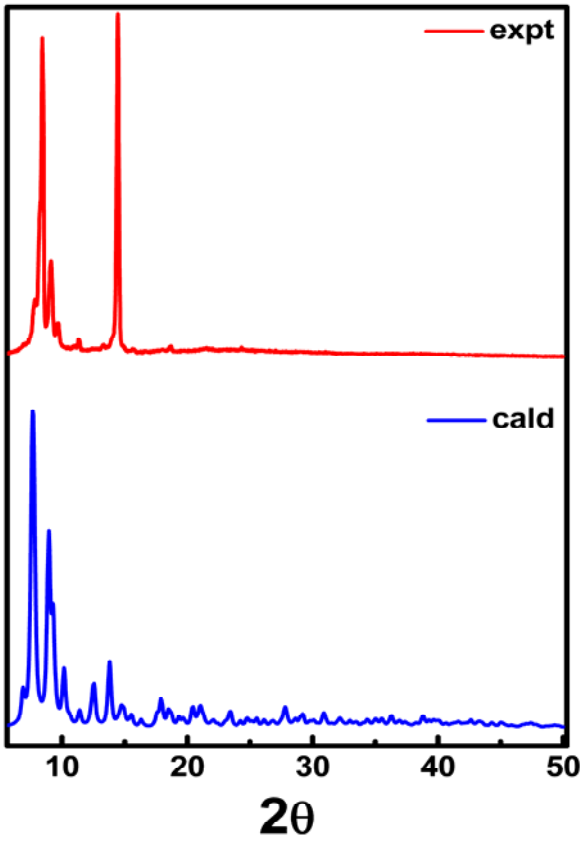


Fig S6: Experimental (red) and calculated (blue) powder XRD patterns of complex **3**.

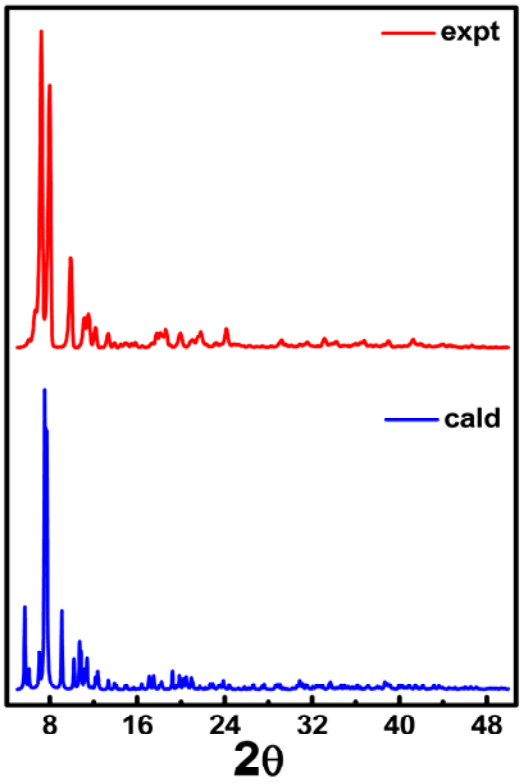


Fig S7: Experimental (red) and calculated (blue) powder XRD patterns of complex **4**.

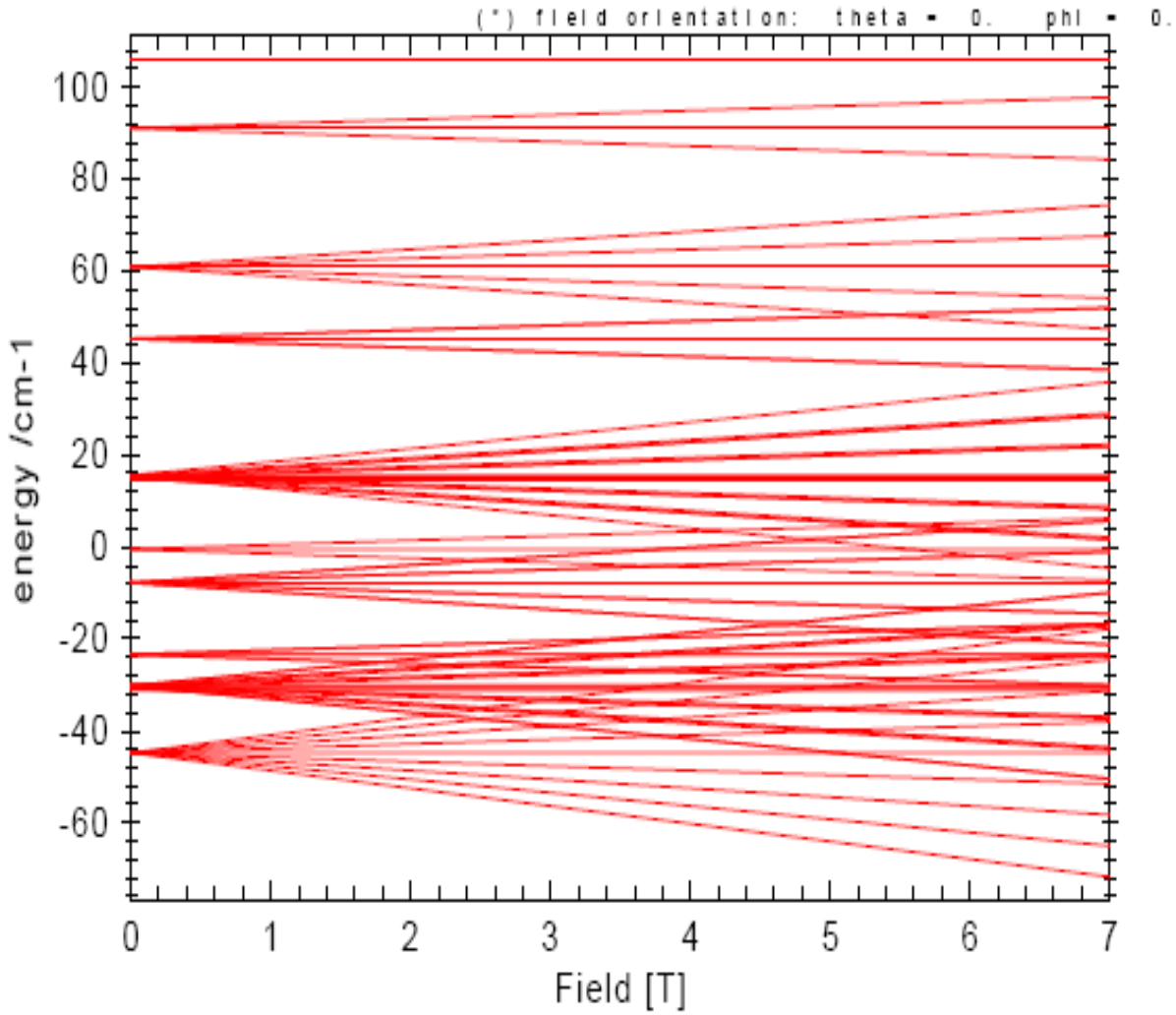


Fig S8 Energy level calculation for **1** with parameters $g = 2.06$, $J_1 = -3.9$ cm^{-1}, $J_2 = +7.55$ cm^{-1}.

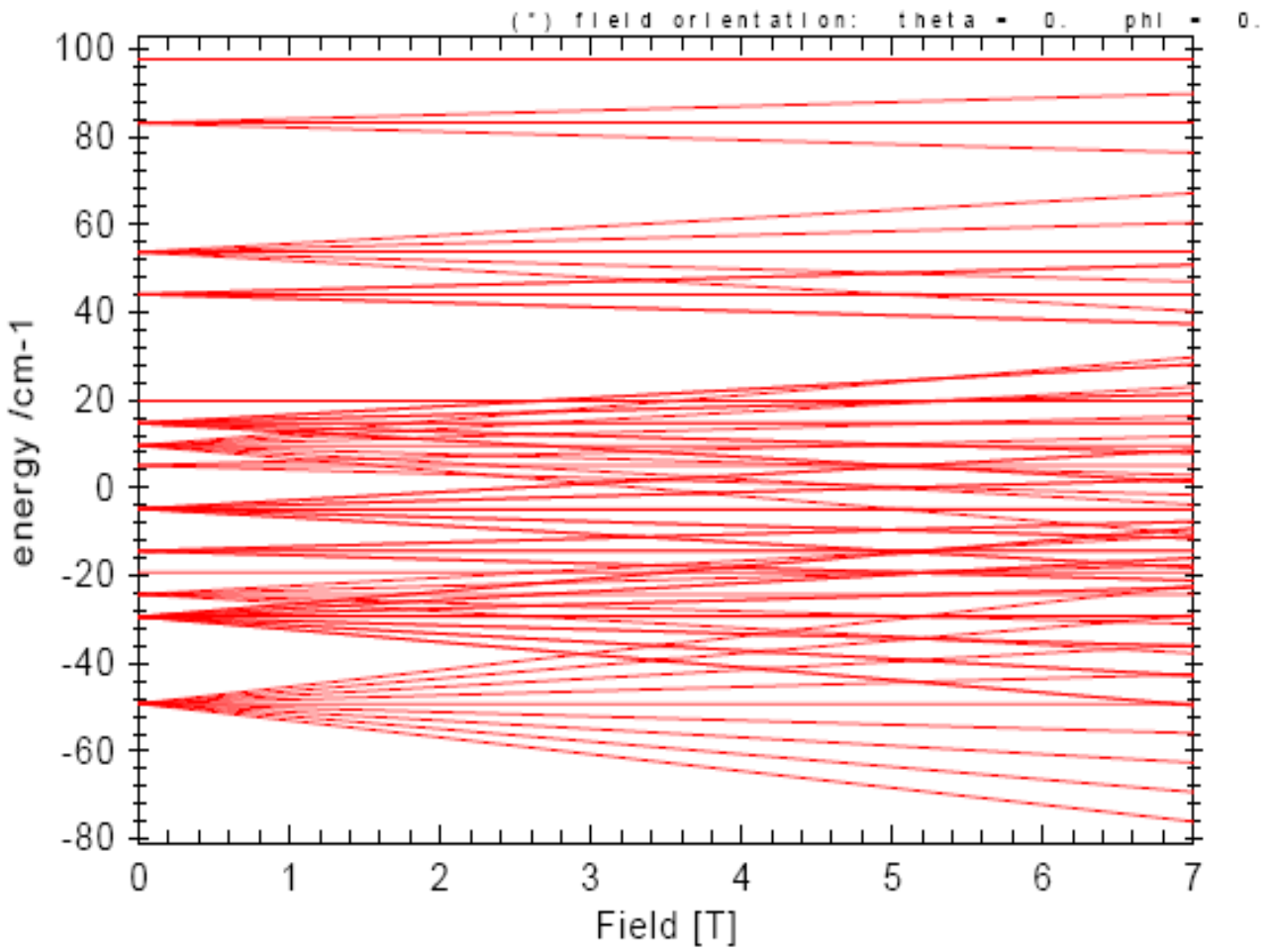


Fig S9 Energy level calculation for **2** with parameters $g = 2.055$, $J_1 = -2.45$ cm^{-1}, $J_2 = +7.3$ cm^{-1}.

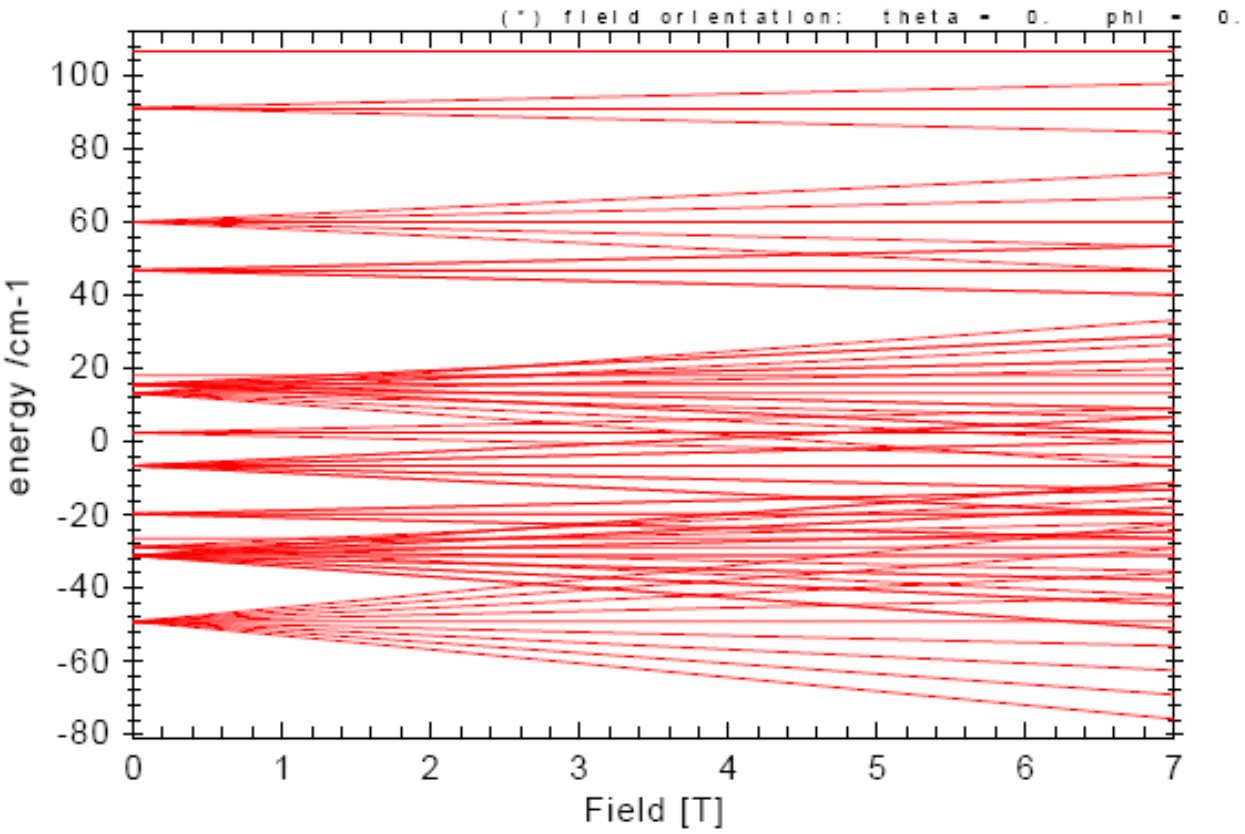


Fig S10 Energy level calculation for **3** with parameters $g = 2.045$, $J_1 = -3.2$ cm^{-1}, $J_2 = +7.8$ cm^{-1}.

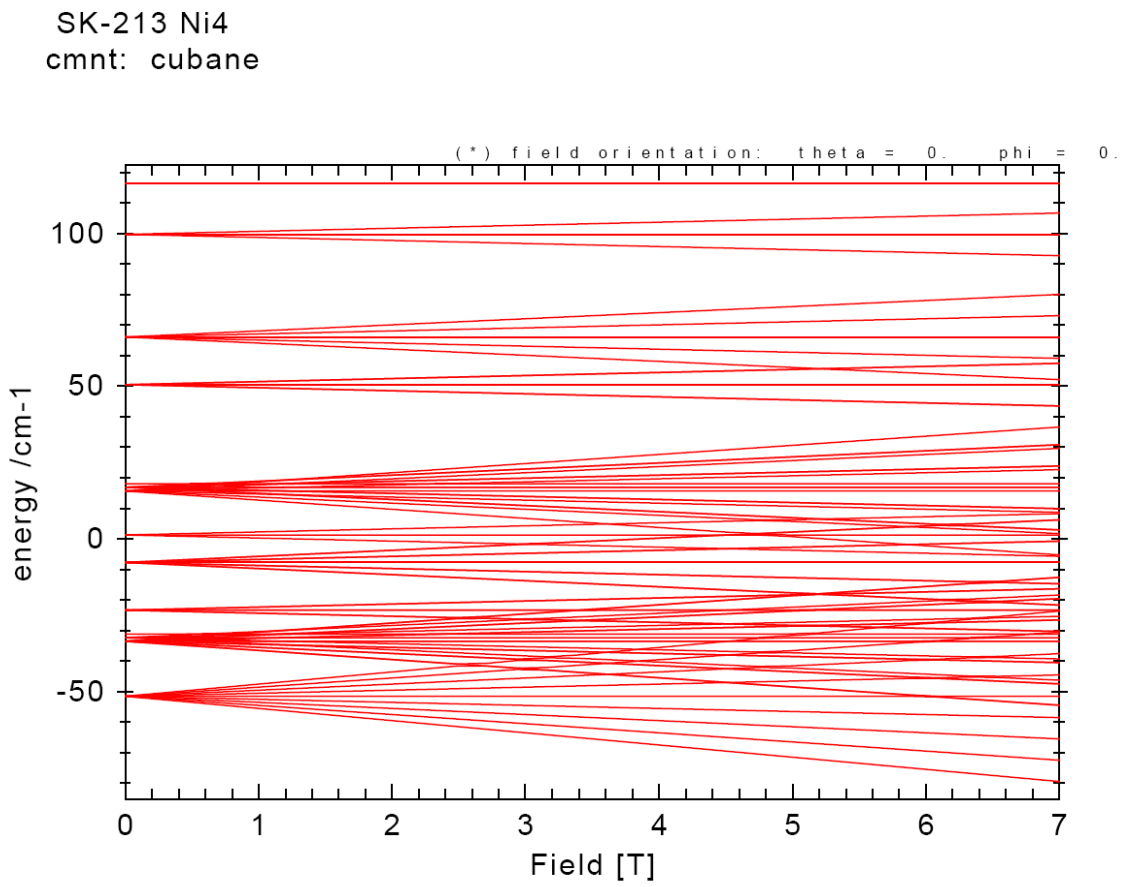


Fig S11 Energy level calculation for **4** with parameters $g = 2.13$, $J_1 = -3.9$ cm^{-1}, $J_2 = +8.4$ cm^{-1}.

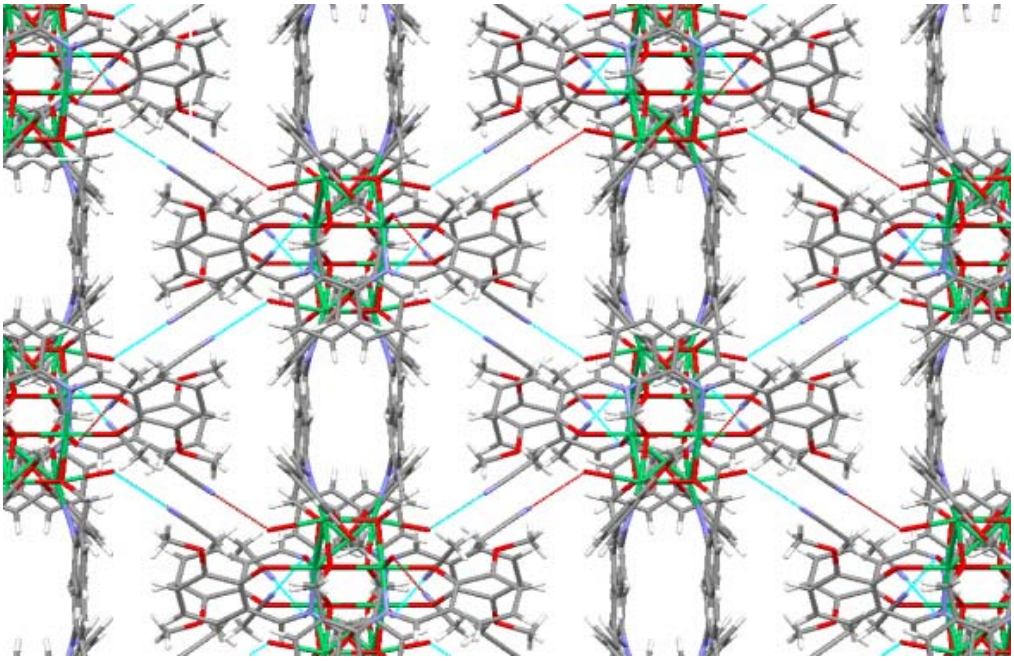


Fig. S12: A perspective view of the 3D packing of **1**; green lines represent hydrogen bonding.

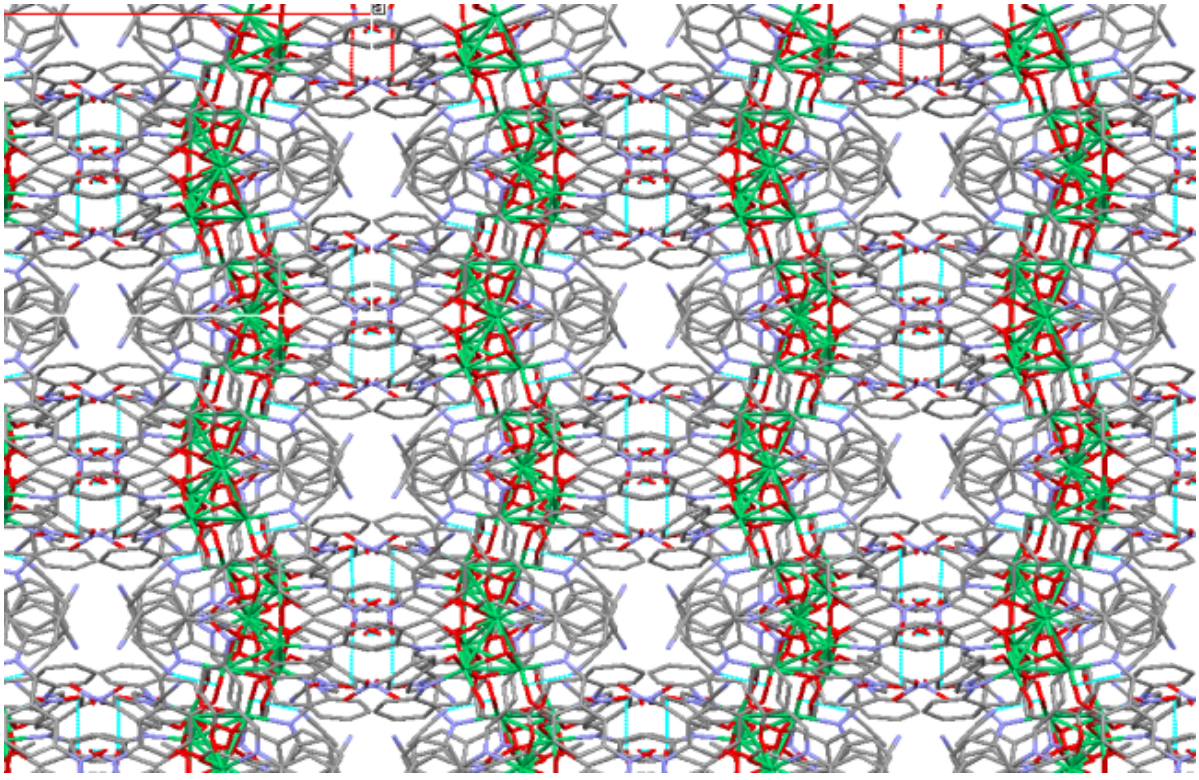


Fig. S13: A perspective view of the 3D packing of **2**; green lines represent hydrogen bonding.

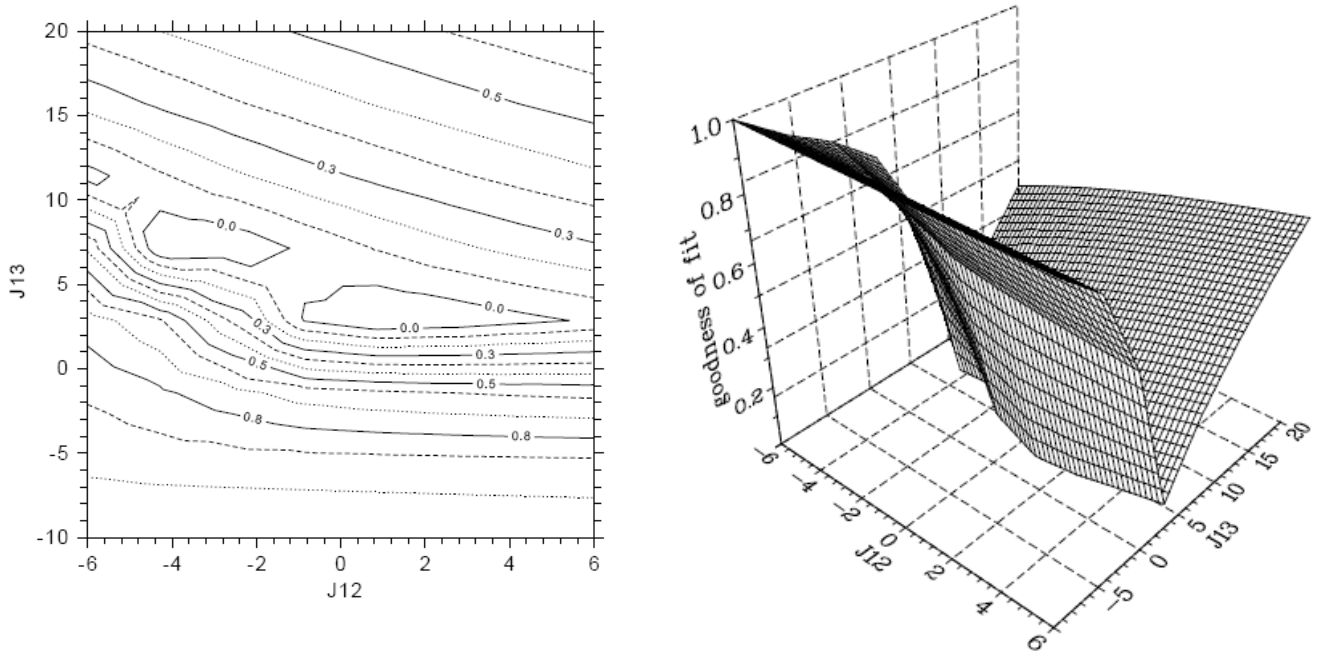


Fig. S14: 2D and 3D-contour projection of the relative error surface of fitting the magnetic data of **1**.

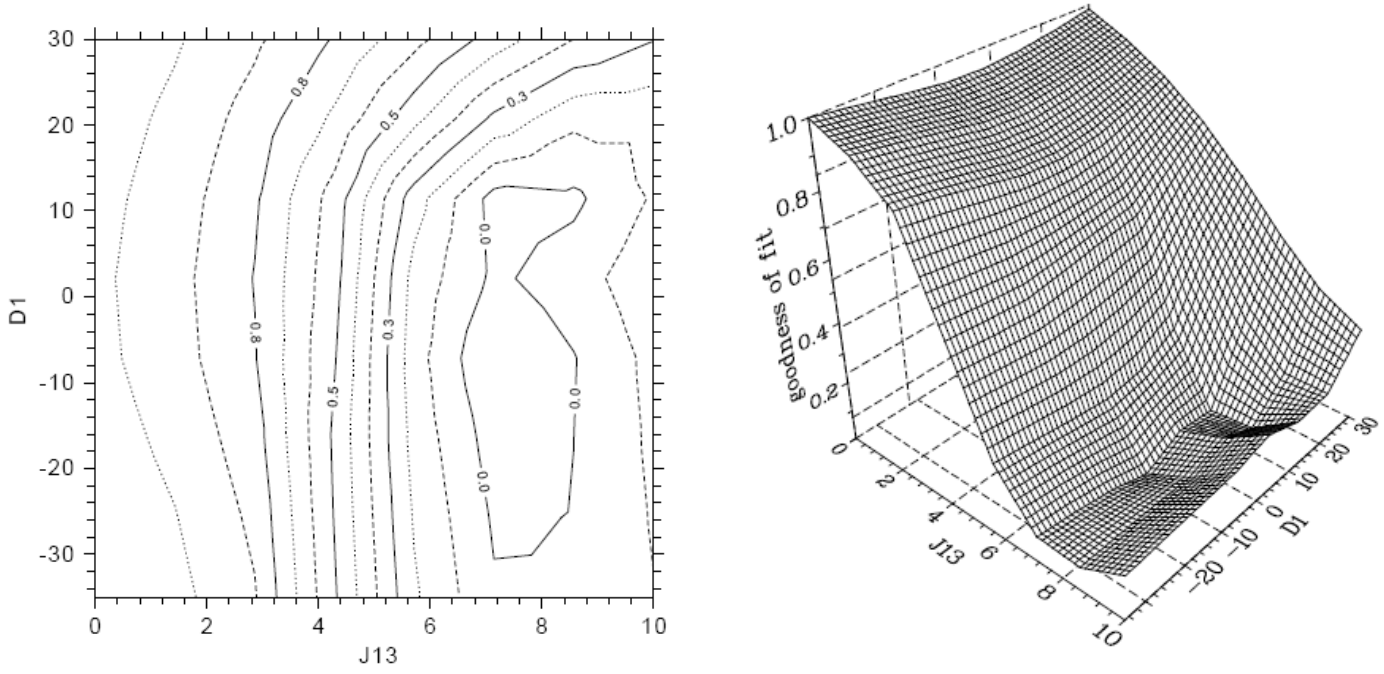


Fig. S15: 2D and 3D-contour projection of the relative error surface of fitting the magnetic data of **1**.

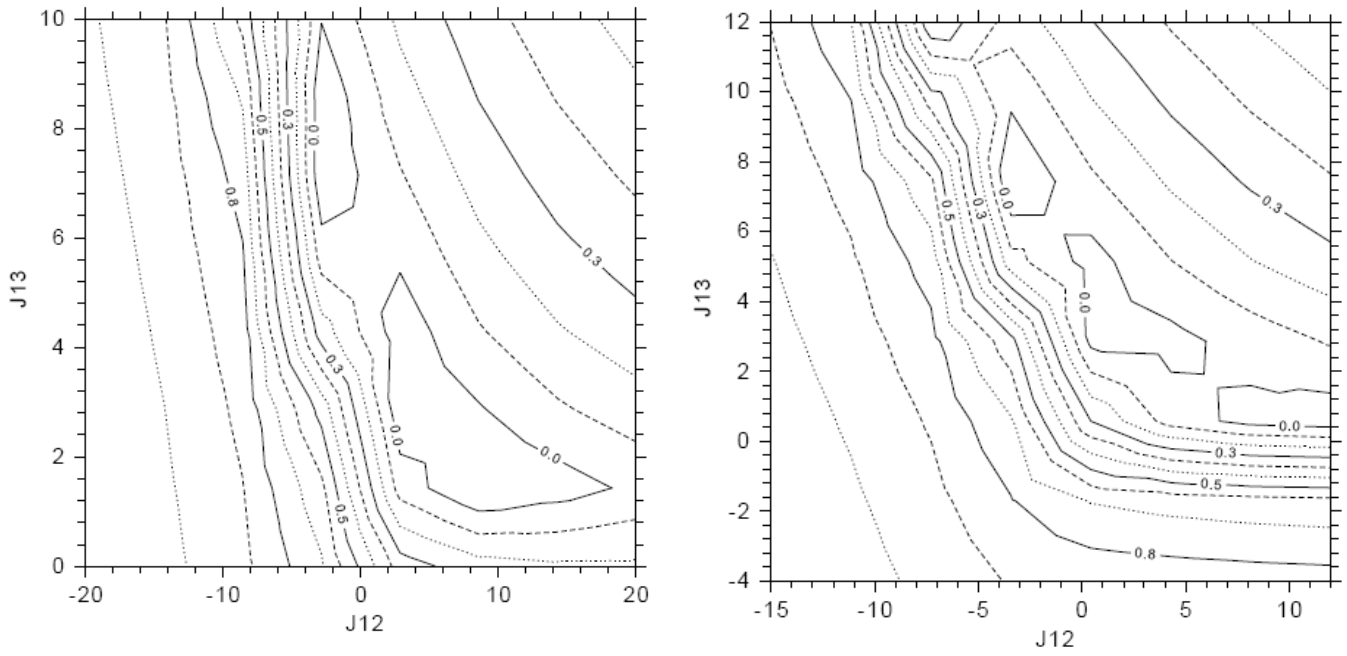


Fig. S16: 2D-contour projection of the relative error surface of fitting the magnetic data of **2** and **3**.

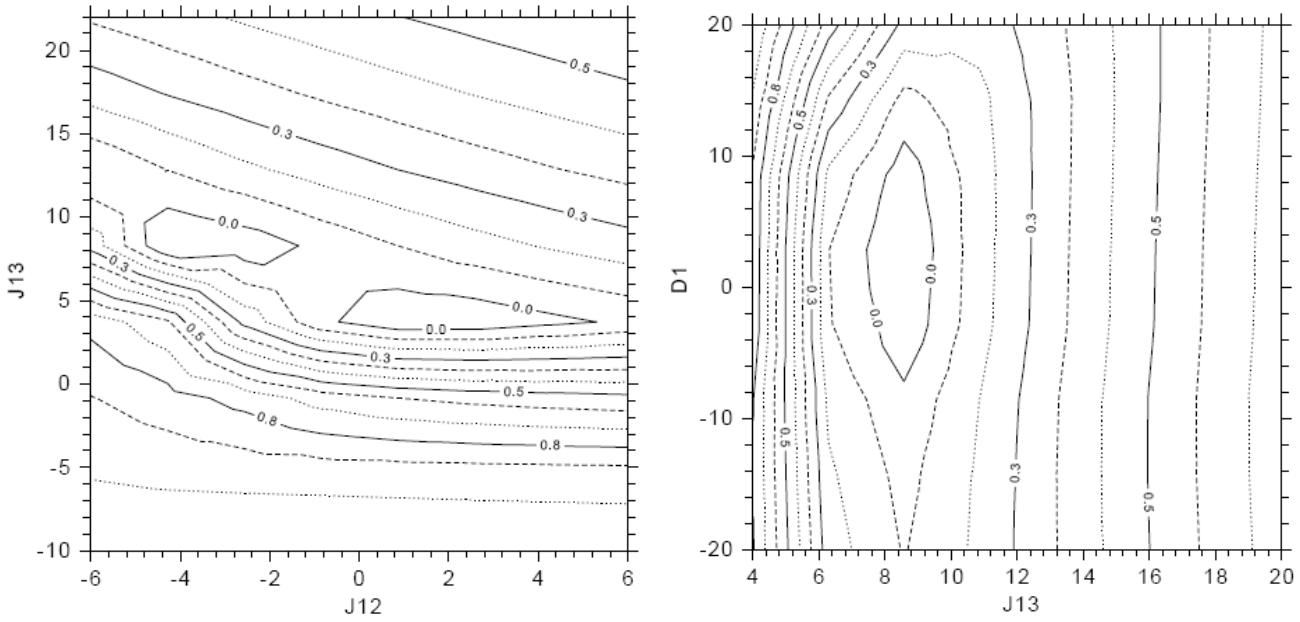


Fig. S17: 2D-contour projection of the relative error surface of fitting the magnetic data of **4**.

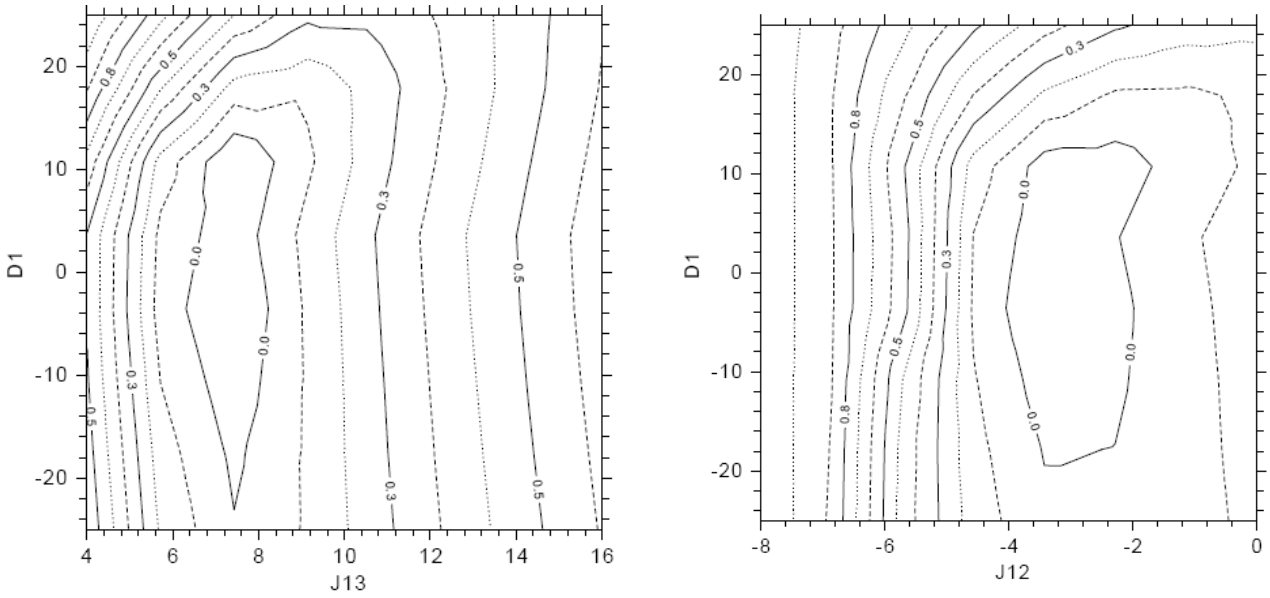


Fig. S18: 2D-contour projection of the relative error surface of fitting the magnetic data of **2**.

The magnetic data was also simulated by using additional parameter D based on the Hamiltonian noted below:

$H = -2J_1 (S_1 \bullet S_2 + S_3 \bullet S_4) - 2J_2 (S_1 \bullet S_3 + S_1 \bullet S_4 + S_2 \bullet S_3 + S_2 \bullet S_4) + \Sigma D_{Ni} S_{iz}^2$

The simulation yielded the parameters $J_1 = -3.75$ cm^{-1}, $J_2 = +7.66$ cm^{-1}, $D_{Ni} = |4|$ cm^{-1}, g = 2.06 for **1**; $J_1 = -2.27$ cm^{-1}, $J_2 = +7.45$ cm^{-1}, $D_{Ni} = |4|$ cm^{-1}, g = 2.06 for **2**; $J_1 = -3.06$ cm^{-1}, $J_2 = +7.88$ cm^{-1}, $D_{Ni} = |4|$ cm^{-1}, g = 2.05 for **3** and $J_1 = -3.72$ cm^{-1}, $J_2 = +8.53$ cm^{-1}, $D_{Ni} = |4|$ cm^{-1}, g = 2.13 for **4**.

Table S1 for selected Bond Lengths (**Å**) and Angles (deg) for complex **(5)**

Ni(1)●●●Ni(2)	3.038(1)	Ni(2)●●●Ni(3)	3.035(2)
Ni(1)●●●Ni(3)	3.159(2)	Ni(2)●●●Ni(4)	3.175(2)
Ni(1)●●● Ni(4)	3.037(1)	Ni(3)●●●Ni(4)	3.039(2)
Ni(1) - O(2)	1.979(6)	Ni(3) - O(3)	2.147(6)
Ni(1) - O(3)	1.996(6)	Ni(3) - O(6)	2.018(6)
Ni(1) - O(9)	2.143(6)	Ni(3) - O(8)	1.977(6)
Ni(1) - O(12)	2.032(6)	Ni(3) - O(9)	1.993(6)
Ni(1) - O(13)	2.172(7)	Ni(3) - O(15)	2.159(6)
Ni(1) - N(1)	1.988(8)	Ni(3) - N(3)	1.980(8)
Ni(2) - O(3)	2.065(6)	Ni(4) - O(6)	2.144(6)
Ni(2) - O(5)	1.959(6)	Ni(4) - O(9)	2.068(6)
Ni(2) - O(6)	1.993(6)	Ni(4) - O(11)	1.962(6)
Ni(2) - O(12)	2.136(6)	Ni(4) - O(12)	1.997(6)
Ni(2) - O(14)	2.165(6)	Ni(4) - O(16)	2.188(6)
Ni(2) - N(2)	1.999(8)	Ni(4) - N(4)	2.002(8)
Ni(1) - O(3) - Ni(2)	96.9(3)	Ni(2) - O(3) - Ni(3)	92.2(2)
Ni(1) - O(12) - Ni(2)	93.6(3)	Ni(2) - O(6) - Ni(3)	98.4(3)
Ni(1) - O(3) - Ni(3)	99.3(3)	Ni(2) - O(6) - Ni(4)	100.2(3)
Ni(1) - O(9) - Ni(3)	99.5(3)	Ni(2) - O(12) - Ni(4)	100.3(3)
Ni(1) - O(9) - Ni(4)	92.3(2)	Ni(3) - O(6) - Ni(4)	93.8(2)
Ni(1) - O(12) - Ni(4)	97.8(3)	Ni(3) - O(9) - Ni(4)	96.9(3)
O(2) - Ni(1) - O(3)	171.6(3)	O(8) - Ni(3) - O(9)	171.8(3)
O(5) - Ni(2) - O(6)	168.5(3)	O(11) - Ni(4) - O(12)	166.7(3)