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Supplementary Information

for the manuscript:

Influence of the coligand in the magnetic properties of a series of copper(II)-phenylmalonate complexes

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Table S1. Selected bond lengths (Å) and bond angles (º) for compound **2-4**[a,b]

		2	
Cu(1)–O(2)	1.955(3)	O(2)–Cu(1)–N(1)	102.88(14)
Cu(1)–O(4)	1.976(3)	O(4)–Cu(1)–O(1a)	89.89(14)
Cu(1)–O(1a)	1.954(3)	O(4)–Cu(1)–O(3b)	171.29(14)
Cu(1)–O(3b)	1.953(3)	O(4)–Cu(1)–N(1)	100.00(14)
Cu(1)–N(1)	2.242(4)	O(1a)–Cu(1)–O(3b)	91.64(14)
O(2)–Cu(1)–O(4)	87.59(14)	O(1a)–Cu(1)–N(1)	85.41(14)
O(2)–Cu(1)–O(1a)	171.64(14)	O(3b)–Cu(1)–N(1)	88.67(14)
O(2)–Cu(1)–O(3b)	89.68(14)		
		3	
Cu(1)–O(2)	1.977(2)	O(2)–Cu(1)–N(1)	97.38(10)
Cu(1)–O(4)	1.940(2)	O(4)–Cu(1)–O(1b)	90.55(10)
Cu(1)–O(1b)	1.968(2)	O(4)–Cu(1)–O(3a)	173.69(10)
Cu(1)–O(3a)	1.955(2)	O(4)–Cu(1)–N(1)	99.97(10)
Cu(1)–N(1)	2.249(3)	O(1b)–Cu(1)–O(3a)	90.94(10)
O(2)–Cu(1)–O(4)	88.18(10)	O(1b)–Cu(1)–N(1)	89.85(10)
O(2)–Cu(1)–O(1b)	172.77(10)	O(3a)–Cu(1)–N(1)	86.17(10)
O(2)–Cu(1)–O(3a)	89.57(10)		
		4	
Cu(1)–O(2)	1.9530(15)	O(2)–Cu(1)–N(1)	97.90(7)
Cu(1)–O(4)	1.9844(15)	O(4)–Cu(1)–O(1a)	89.43(6)
Cu(1)–O(1a)	1.9547(15)	O(4)–Cu(1)–O(3c)	173.42(6)
Cu(1)–O(3c)	1.9660(15)	O(4)–Cu(1)–N(1)	96.28(7)
Cu(1)–N(1)	2.2429(18)	O(1a)–Cu(1)–O(3c)	91.11(7)
O(2)–Cu(1)–O(4)	88.42(7)	O(1a)–Cu(1)–N(1)	87.80(7)
O(2)–Cu(1)–O(1a)	174.09(7)	O(3c)–Cu(1)–N(1)	90.29(7)
O(2)–Cu(1)–O(3c)	90.40(7)		

[a] Estimated standard deviations in the last significant digits are given in parentheses.
[b] Symmetry code: (a) x - 1/2, -y + 1/2, z - 1/2; (b) x + 1/2, -y + 1/2, z - 1/2; (c) x - 1/2, -y + 1/2, z + 1/2.

Table S2. Selected bond lengths (Å) and bond angles (º) for compound **6-8**[a,b]

		6	
Cu(1)–O(2)	1.948(5)	O(2)–Cu(1)–N(1)	99.9(2)
Cu(1)–O(4)	1.991(5)	O(4)–Cu(1)–O(1a)	89.3(2)
Cu(1)–O(1a)	1.958(4)	O(4)–Cu(1)–O(3c)	172.8(2)
Cu(1)–O(3c)	1.967(5)	O(4)–Cu(1)–N(1)	97.1(2)
Cu(1)–N(1)	2.239(6)	O(1a)–Cu(1)–O(3b)	91.58(19)
O(2)–Cu(1)–O(4)	88.1(2)	O(1a)–Cu(1)–N(1)	86.8(2)
O(2)–Cu(1)–O(1a)	173.0(2)	O(3c)–Cu(1)–N(1)	90.1(2)
O(2)–Cu(1)–O(3c)	90.1(2)		
		7	
Cu(1)–O(2)	1.940(3)	O(2)–Cu(1)–N(1)	99.40(13)
Cu(1)–O(4)	1.995(3)	O(4)–Cu(1)–O(1a)	89.23(12)
Cu(1)–O(1a)	1.958(3)	O(4)–Cu(1)–O(3c)	172.73(12)
Cu(1)–O(3c)	1.973(3)	O(4)–Cu(1)–N(1)	96.65(13)
Cu(1)–N(1)	2.241(3)	O(1a)–Cu(1)–O(3c)	91.88(12)
O(2)–Cu(1)–O(4)	88.13(13)	O(1a)–Cu(1)–N(1)	86.99(12)
O(2)–Cu(1)–O(1a)	173.33(12)	O(3c)–Cu(1)–N(1)	90.59(12)
O(2)–Cu(1)–O(3c)	89.99(12)		
		8	
Cu(1)–O(2)	1.947(4)	O(2)–Cu(1)–N(1)	99.07(16)
Cu(1)–O(4)	2.001(4)	O(4)–Cu(1)–O(1d)	89.01(15)
Cu(1)–O(1d)	1.963(3)	O(4)–Cu(1)–O(3b)	172.58(15)
Cu(1)–O(3b)	1.979(3)	O(4)–Cu(1)–N(1)	96.03(16)
Cu(1)–N(1)	2.244(4)	O(1d)–Cu(1)–O(3b)	92.03(15)
O(2)–Cu(1)–O(4)	88.17(15)	O(1d)–Cu(1)–N(1)	87.04(15)
O(2)–Cu(1)–O(1d)	173.51(15)	O(3b)–Cu(1)–N(1)	91.36(16)
O(2)–Cu(1)–O(3b)	90.03(15)		

[a] Estimated standard deviations in the last significant digits are given in parentheses.
[b] Symmetry code: (a) x - 1/2, -y + 1/2, z - 1/2; (b) x + 1/2, -y + 1/2, z - 1/2; (c) x - 1/2, -y + 1/2, z + ½; (d) x + 1/2, -y + 1/2, z + 1/2.

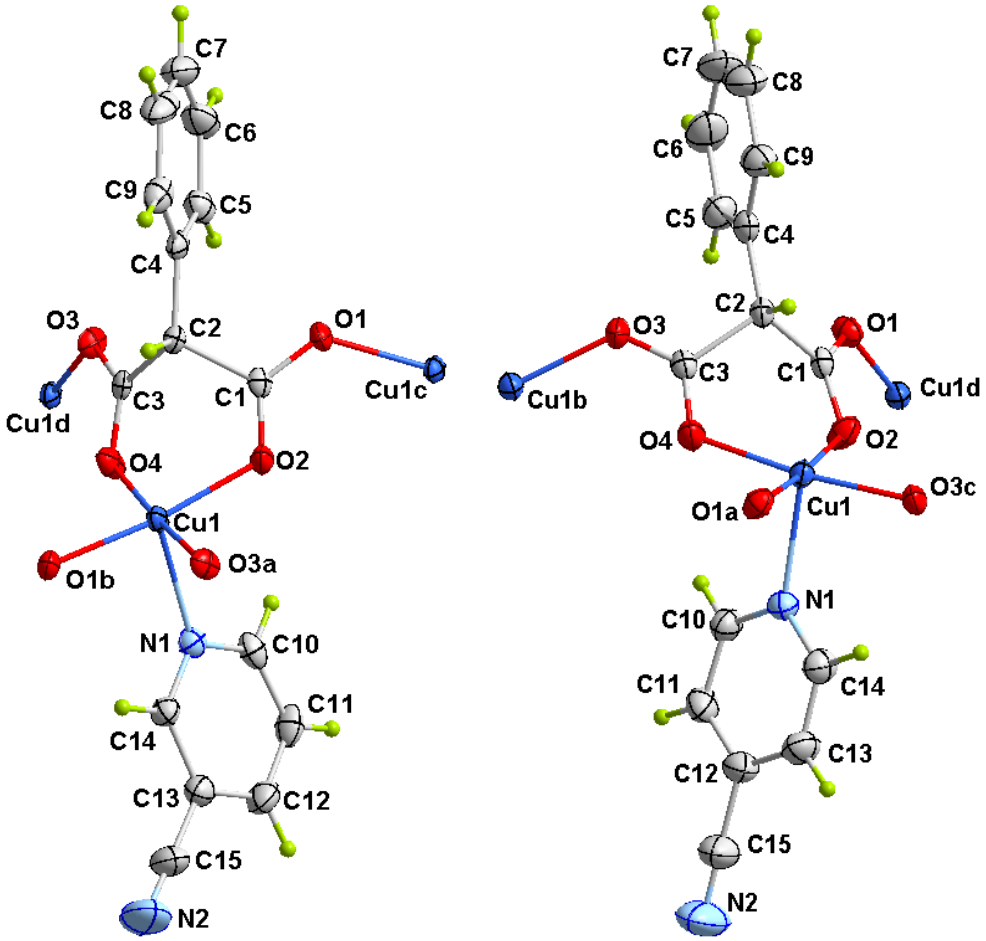

Figure S1. A view of a fragment of the crystal structure of **3** (left) and **4** (right) along with the atom numbering scheme. Ellipsoids are represented at 50% probability. Symmetry codes: (a) x - 1/2, -y + 1/2, z - 1/2; (b) x + 1/2, -y + 1/2, z - 1/2; (c) x - 1/2, -y + 1/2, z + 1/2 ; (d) = x + 1/2, -y + 1/2, z + 1/2.

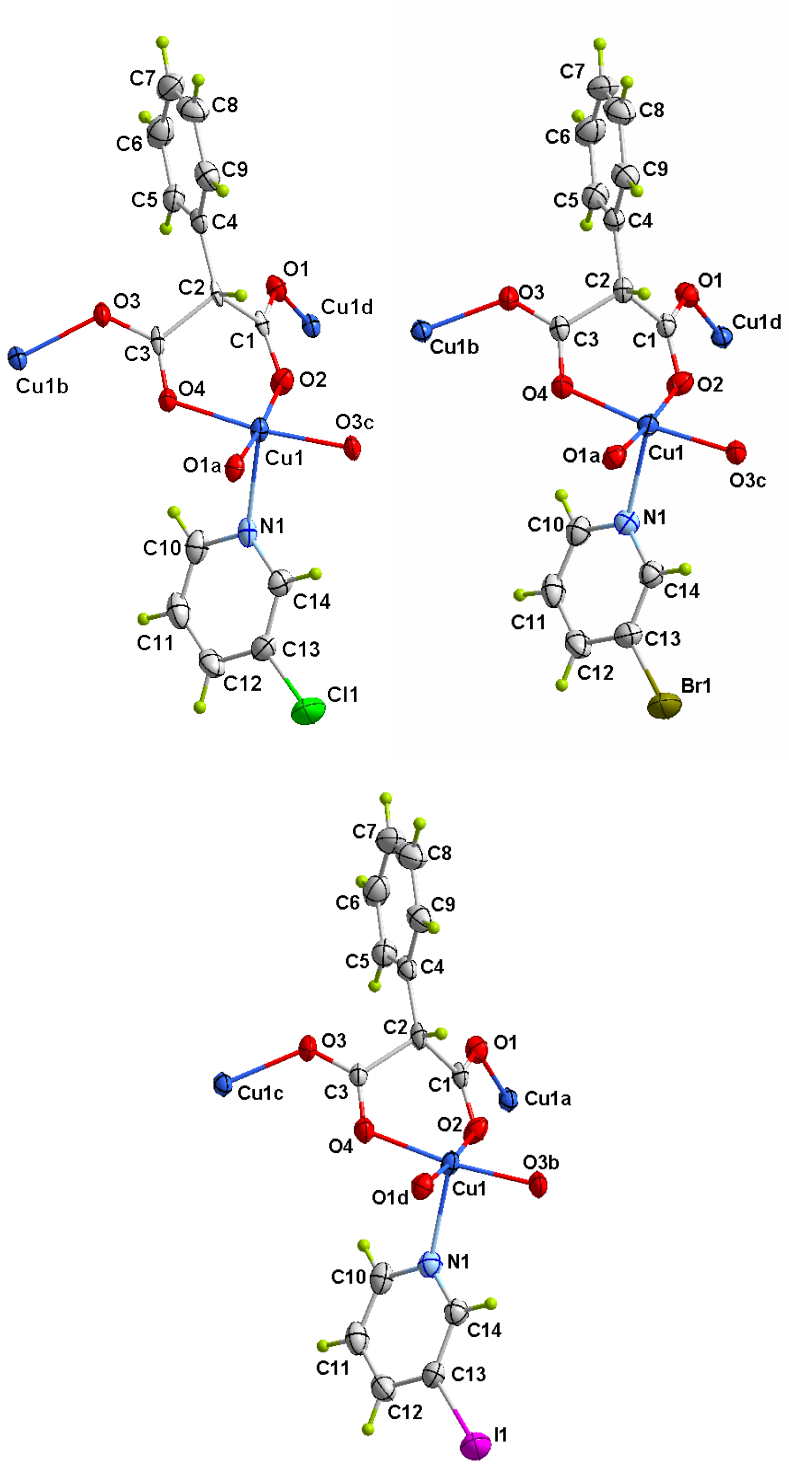

Figure S2. A view of a fragment of the crystal structure of **6**, **7** and **8** along with the atom numbering scheme. Ellipsoids are represented at 50% probability. Symmetry codes: (a) *x* - 1/2, -*y* + 1/2, *z* - 1/2; (b) *x* + 1/2, -*y* + 1/2, *z* - 1/2; (c) *x* - 1/2, -*y* + 1/2, *z* + 1/2 ; (d) = *x* + 1/2, -*y* + 1/2, *z* + 1/2.

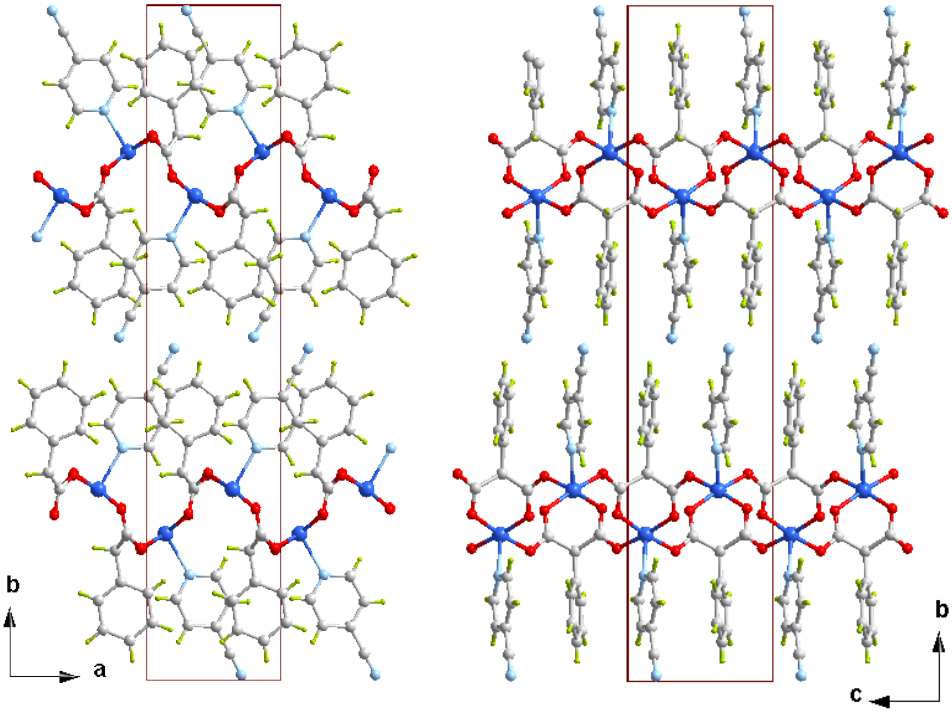

Figure S3. The crystal packing of compound **4** along the crystallographic *c* (left) and *a* directions (right). The unit cell edges are presented in dark red colour. The layers are twisted following an *ABABAB* sequence along the *b* axis.

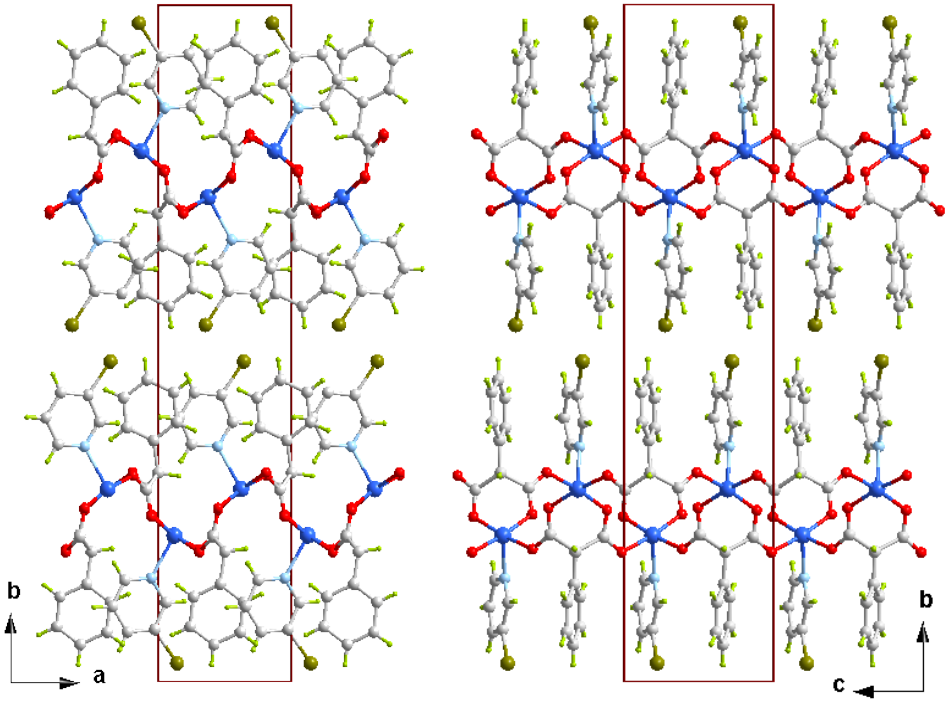

Figure S4. The crystal packing of compound **7** along the crystallographic *c* (left) and *a* directions (right). The unit cell edges are presented in dark red colour. The layers are twisted following an *ABABAB* sequence along the *b* axis.

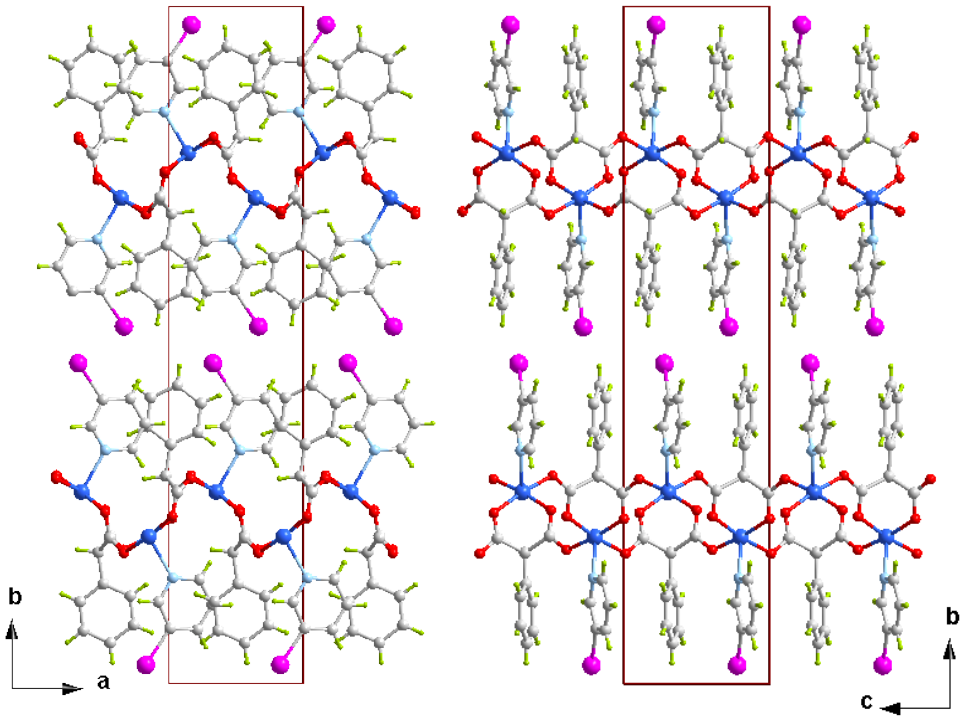

Figure S5. The crystal packing of compound **8** along the crystallographic *c* (left) and *a* directions (right). The unit cell edges are presented in dark red colour. The layers are twisted following an *ABABAB* sequence along the *b* axis.

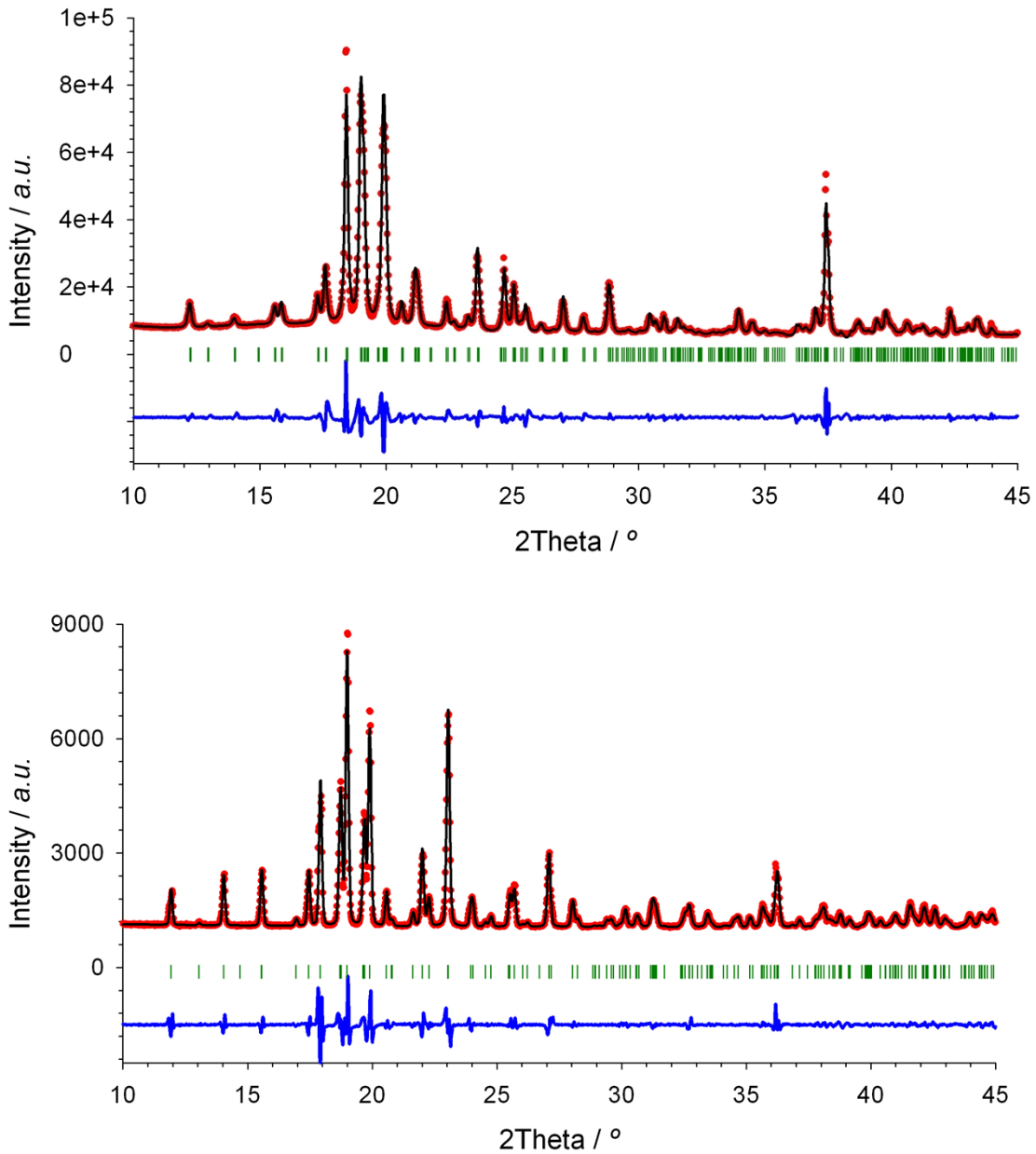

Figure S6. Up) Le-Bail fit of the powder diffraction pattern of compound **2**. The cell parameters are a = 7.02048 Å, b = 28.80420 Å, c = 6.04391 Å and β = 91.9745º. Bottom) Le-Bail fit of the powder diffraction pattern of compound **5**. The cell parameters are a = 6.178678 Å, b = 29.752108 Å, c = 6.994833 Å and β = 92.731514º, with the following statistics χ^2 = 8.34 and R_B = 0.78 %.The experimental and calculated data are represented as red circles and a black solid line respectively, whereas the blue line is the difference between them and the green vertical lines correspond to the Bragg positions.

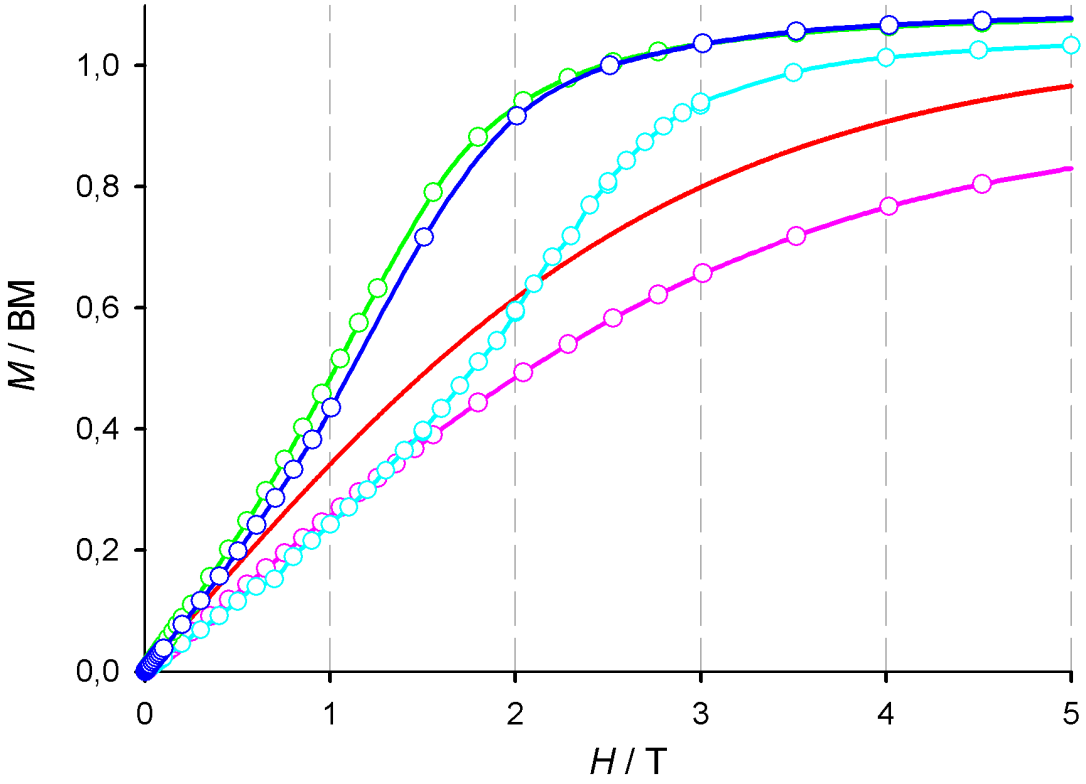

Figure S7. Magnetization vs. magnetic applied field plots at 2 K for **5** (light blue), **6** (pink), **7** (green) and **8** (dark blue). The lines are only an eye-guide, except for the red line which represents the Brillouin function for a S = 1/2 at 2 K.