ELECTRONIC SUPPORTING INFORMATION

Tailoring the physical properties of hybrid magnetic quinuclidine-based plastic compounds via weak interactions

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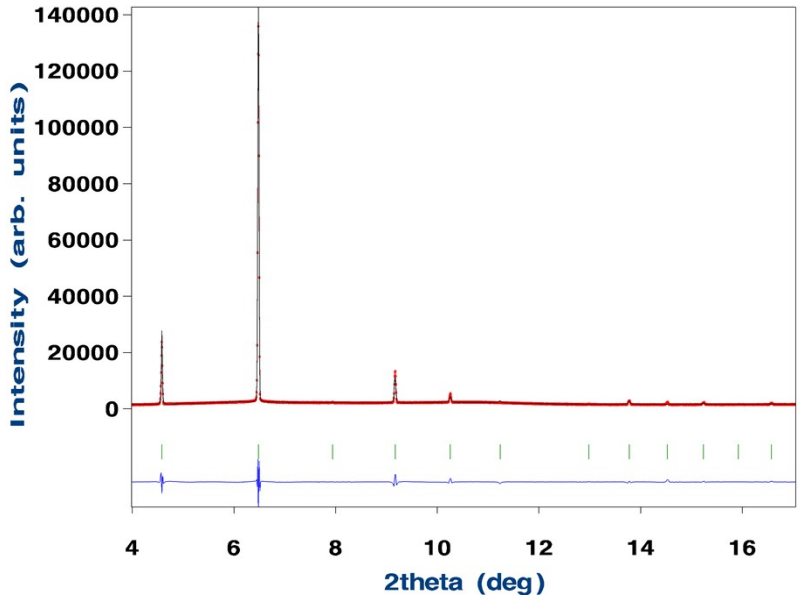

Figure S1: Rietveld refinement to the SXPD data at 420 K of compound **A** using the spherical shell model. Observed (red points) and calculated (black solid line) powder diffraction patterns for positions of the Bragg reflections are represented by green vertical bars. The observed-calculated difference patterns are depicted as a blue line. $R_{Bragg} = 4.76$.

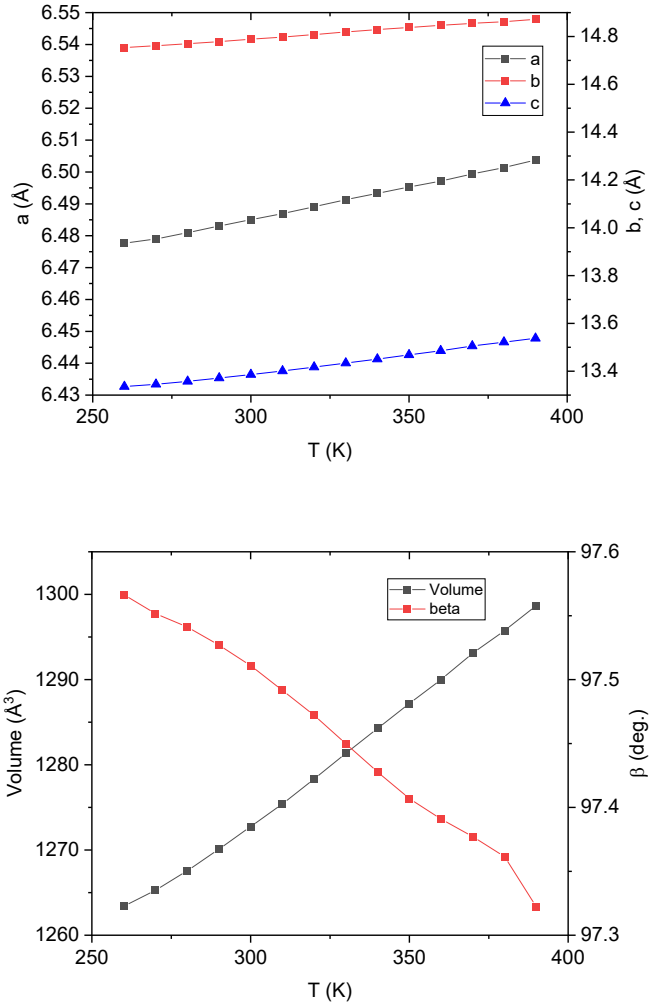

Figure S2: Evolution of the volume and cell parameters of compound **A** from 260 to 390 K obtained from pattern matching to the SXPD data.

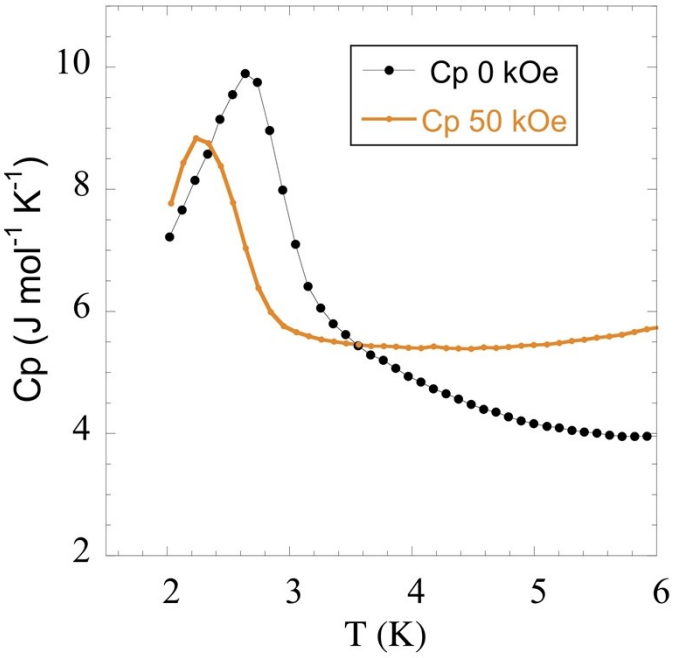

Figure S3:. The solid lines are guide for the eye.

Table S1: Relevant distances of compound **A** at 300 K obtained from single-crystal X-Ray data.

(3-oxoquinuclidinium)	**Length (Å)**	**FeCl4**	**Length (Å)**
C1-N1	1.472(7)	Fe1-Cl1	2.1736(16)
C1-C4	1.504(7)	Fe1-Cl3	2.189(2)
C2-N1	1.490(7)	Fe1-Cl2	2.207(2)
C2-C5	1.520(8)	Fe2-Cl6	2.1858(15)
C6-N1	1.492(6)	Fe2-Cl4	2.1947(17)
C3-C6	1.503(6)	Fe2-Cl5	2.1972(15)
C4-C7	1.534(8)		
C5-C7	1.510(7)		
C7-C3	1.470(7)		
C3-O1	1.208(5)		

Table S2: Relevant distances of compound **B** at 100 K obtained from single-crystal X-Ray data.

(3-oxoquinuclidinium)	Length (Å)	FeCl4	Length (Å)
C2-N1	1.4926(19)	Fe1-Cl3	2.1871(5)
C2-C3	1.512(2)	Fe1-Cl1	2.1990(6)
C8-C7	1.530(3)	Fe1-Cl2	2.2007(7)
C8-C4	1.542(3)	Fe2-Cl4	2.1868(7)
C4-C3	1.498(2)	Fe2-Cl5	2.1977(5)
C4-C5	1.537(3)	Fe2-Cl6	2.2182(6)
C7-N1	1.505(2)		
C6-N1	1.507(2)		
C6-C5	1.530(3)		
C3-O2	1.209(2)		

Table S3: Crystallographic data and single-crystal refinement details of compound **A** at 13 K from the refinement of the neutron single-crystal data.

	A_{II} @ 13 K
Empirical formula	C_{28} H_{48} Cl_{16} Fe_4 N_4 O_4
Formula weight	1295.34
Crystal system	monoclinic
Space group	*P* 1 2_1/*m* 1
a (Å)	6.445
b (Å)	14.509
c (Å)	13.037
β (°)	97.96
V (Å^3)	1207.3
Z	4
ρ (g·cm^{-3})	1.782
wavelength (Å $^{-1}$)	1.45567
Reflections [I>2σ(I)]	1909
Reflections [all data]	1911
parameters	244
Goodness of fit (S)[a]	1.293
R_1[b]/wR^2 [c] [I>2σ(I)]	0.0422 / 0.1011
R_1[b]/wR^2 [c] [all data]	0.0422 / 0.1011

Table S4: Relevant distances of compound **A** at 13 K obtained from single-crystal neutron diffraction measured at D19.

(3-oxoquinuclidinium)	Length (Å)	FeCl4	Length (Å)
C1-N1	1.5045(23)	Fe1-Cl1	2.1780(15)
C1-C4	1.5375(26)	Fe1-Cl3	2.1971(18)
C2-N1	1.5071(21)	Fe1-Cl2	2.2104(24)

C2-C5	1.5367(25)	Fe2-Cl6	2.1899(18)
C6-N1	1.4961(23)	Fe2-Cl4	2.1984(23)
C3-C6	1.5201(23)	Fe2-Cl5	2.2009(15)
C4-C7	1.5375(27)		
C5-C7	1.5406(24)		
C7-C3	1.5065(24)		
C3-O1	1.2035(25)		
X-H···Cl[a]	**Length (Å)**	**Angle (°)**	**a (symm. op.)**
N1-H1···Cl4	2.712(4)	128.3(3)	-1+*x, y, z*
N1-H1···Cl5	2.733(4)	120.1(3)	-1+*x*, 0.5-*y, z*
C2-H2A···Cl5	2.835(4)	131.6(3)	1-*x*, 0.5+*y, -z*
C2-H2B···Cl5	2.936(4)	118.3(3)	-1+*x*, 0.5-*y, z*
C3-H6A···Cl5	2.793(4)	124.9(3)	-1+*x*, 0.5-*y, z*
C4-H4A···Cl1	2.647(4)	152.3(3)	1+*x, y, z*
C4-H4B···Cl3	2.777(4)	175.4(3)	-*x*, 0.5+*y*, 1-*z*
C5-H5A···Cl5	2.698(4)	145.7(3)	2-*x*, 0.5+*y, -z*
C5-H5B···Cl2	2.765(5)	142.9(3)	-*x*, 0.5+*y*, 1-*z*
C7-H7···Cl2	2.818(4)	150.8(3)	1-*x*, 0.5+*y*, 1-*z*
C7-H7···Cl1	2.867(4)	127.7(3)	1-*x*, 1-*y*, 1-*z*
Fe···Fe[b]	**Length (Å)**		**b (symm. op.)**
Fe1···Fe2	6.340(2)		-1+*x, y, z*
Fe1···Fe1	6.4450(19)	Intra-plane	-1+*x, y, z*
Fe1···Fe2	6.879(2)		-1+*x, y*, 1+*z*
Fe1···Fe2	7.527(2)		-2+*x, y, z*
Fe1···Fe1	7.5402(6)	Inter-plane	-*x*, 0.5+*y*, 1-*z*
Fe2···Fe2	7.4048(5)		2-*x*, -0.5+*y*, -*z*