Supplementary Information

Neutron Diffraction Studies of the Molecular Compound $[Co_2(bta)]_n$ (H_4bta = 1,2,4,5-benzenetetracarboxylic acid): in the Quest of Canted Ferromagnetism.

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Single Crystal X-ray Structure Determination and Refinement

X-ray diffraction data on a small single crystal of **1** was collected at 100 K on a Nonius Kappa CCD diffractometer with graphite-monochromated Mo-K_α radiation (0.71073 Å). Data were indexed, integrated and scaled using the EVALCCD program.[1] The crystal of compound **1** was a non-merohedral twin. The reflections for both components of the twin were indexed using DIRAX[2] and integrated through the EVALCCD.[3] The equivalent reflexions were merged using the TWINABS,[4] program suite. The twin refinement was performed with SHELXL97[5] using the HKLF4 data for the solution and the HKLF5 format for the refinement, including the TWIN and BASF statements. All the reflections having at least one contribution from the major component have been used for the HKLF5 refinement. The BASF factor in the final refinement of **1** gives a value of 0.6224, leading to percentages of 62.2(1) and 37.8(1) for each one of the twin domains. The structures of **1** were solved by direct methods using the SHELXS97 program. All non-hydrogen atoms were refined anisotropically by full-matrix least-squares technique based on F^2 using SHELXL97. The hydrogen atoms were positioned geometrically and refined with a riding model. The final geometrical calculations and the graphical manipulations

were carried out with PARST97,[6] PLATON[7] and DIAMOND[8] programs. Crystallographic data for the structure **1** has been deposited at the Cambridge Crystallographic Data Centre with CCDC reference number 952343.

Table S1. Crystal data and details of the structure determination for the complex **1**

Compound	**1**
Formula	$C_{10}H_2Co_2O_{10}$
M	367.98
Crystal system	Monoclinic
Space group	$C2/m$
a, Å	6.1453(5)
b, Å	17.4650(5)
c, Å	4.5525(5)
α, deg	90.00
β, deg	115.763(5)
γ, deg	90.00
V, Å^3	440.04(6)
Z	2
T(K)	100(2)
ρ_{calc} (Mg m^{-3})	2.777
λ (Mo-K$_\alpha$ Å)	0.71073
μ(Mo-K$_\alpha$ mm^{-1})	3.816
R_1, $I > 2\sigma(I)$ (all)	0.0390 (0.0338)
wR_2, $I > 2\sigma(I)$ (all)	0.0909 (0.0869)
Absortion Correction	TWINABS
Independent reflections	928

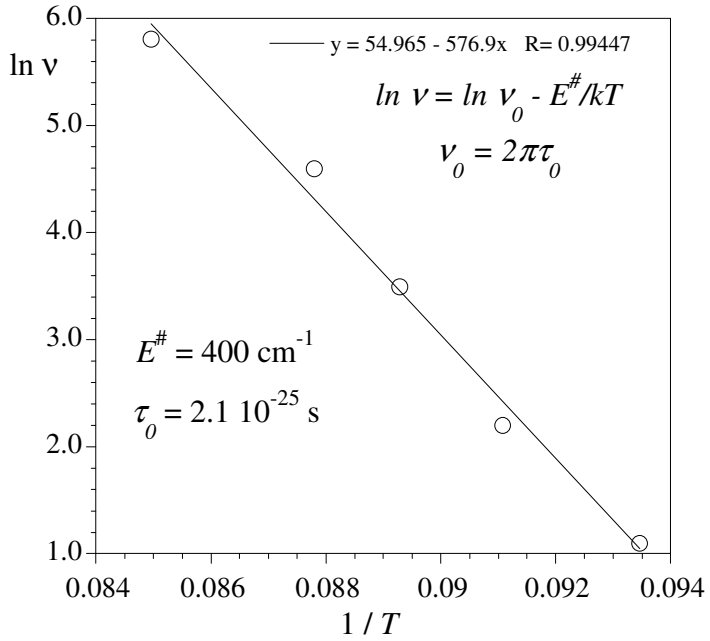

Figure S1: Arrhenius plot for **1**. The circles are experimental data from the AC-susceptibility (Figure 6). Solid line is least-squares fit to the Arrhenius law.

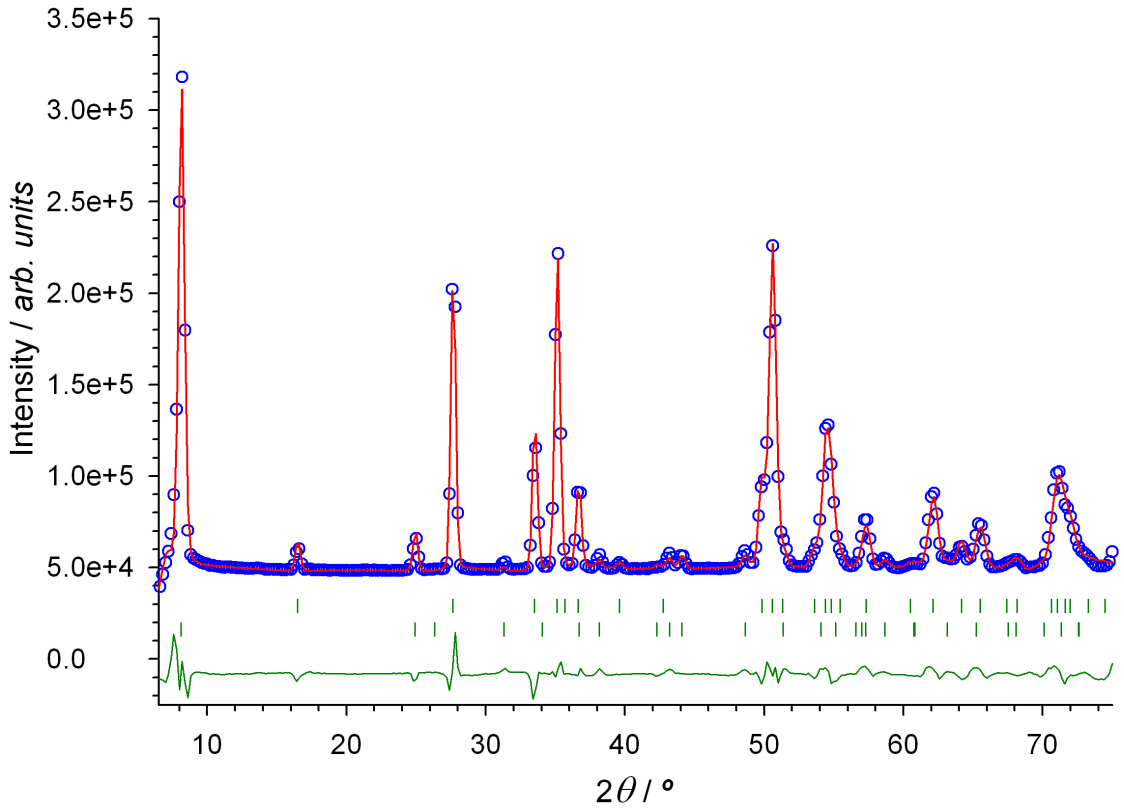

Figure S2. Neutron diffraction pattern of **1** at 2 K collected at D1B instrument: experimental data (o), calculated curve (—) and the difference between them (—). The green vertical lines represent the Bragg positions.

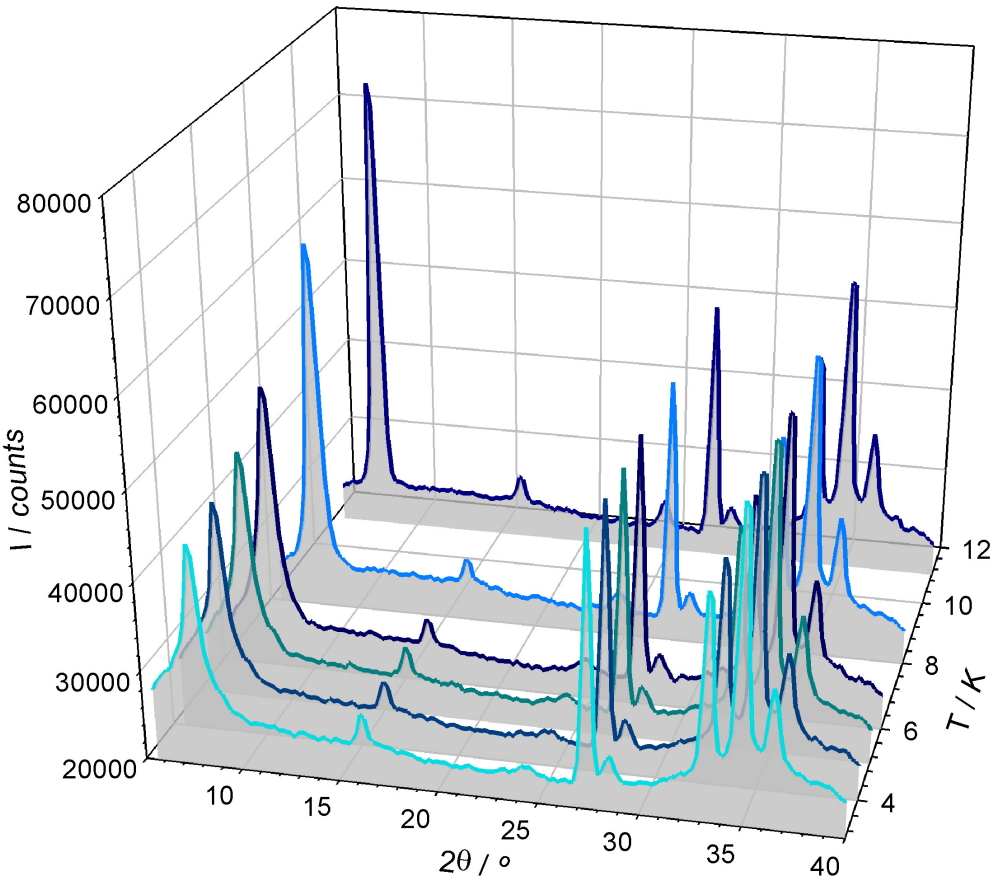

Figure S3: Neutron powder patterns of **1** collected at different temperatures after FC protocol (see text for details).

References:

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