Supporting Material for “Zero Thermal Expansion in a Prussian Blue Analogue”

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Table S1. Refined structural parameters for $\text{Fe}^{\text{III}}[\text{Co}^{\text{III}}(\text{CN})_6]$ at 300 K. Estimated errors in the last digits are given in parentheses. The synchrotron X-ray wavelength is 0.42956 Å. The refined lattice constants for the majority phase is $a = 10.19240(6)$ Å, while for the minority phase is 10.2264(3) Å. The two phases are isostructural and adopt the space group $Fm-3m$. The fraction of the minority phase refined to a value of 35.8(3)%. Refinement of the fractional occupancies of the interstitial oxygen atoms resulted in values for the number of H_2O molecules per formula unit of 0.4 and 1.8 for the majority and minority phases, respectively. In the course of the refinement, the fractional coordinates of C and N together with the isotropic temperature factors of all the atoms were constrained to be equal in the two phases. The agreement factors are $R_{\text{F2}} = 4.90\%$, $R_{\text{wp}} = 5.66\%$ and $R_{\text{exp}} = 1.39\%$.

Majority phase	n	x	y	z	Position	B_{iso} (Å ²)
Co	1	0	0	0	$4a$	1.43(2)
Fe	1.000(10)	1/2	1/2	1/2	$4b$	1.43(2)
C	1	0.1972(10)	0	0	$24e$	2.03(5)
N	1	0.3037(8)	0	0	$24e$	2.03(5)
O	0.053(4)	0.2134(15)	0.2134(15)	0.2134(15)	$32f$	34.0(1)
Minority phase						
Co	1	0	0	0	$4a$	1.43(2)
Fe	0.940(14)	1/2	1/2	1/2	$4b$	1.43(2)
C	1	0.1972(10)	0	0	$24e$	2.03(5)
N	1	0.3037(8)	0	0	$24e$	2.03(5)
O	0.222(6)	0.2134(15)	0.2134(15)	0.2134(15)	$32f$	34.0(1)
Selected Bond Distances						
Fe-N	2.000(8) Å					
Co-C	2.010(11) Å					
C-N	1.086(4) Å

Fig. S1. Temperature dependence of the magnetic susceptibility ($H = 1$ Tesla) of the $\text{Fe}[\text{Co}(\text{CN})_6]$ sample.