Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Electronic Supplementary Information

Ferromagnetic Ising Chains in Frustrated *Ln*ODCO$_3$: The Influence of Magnetic Structure in Magnetocaloric Frameworks†

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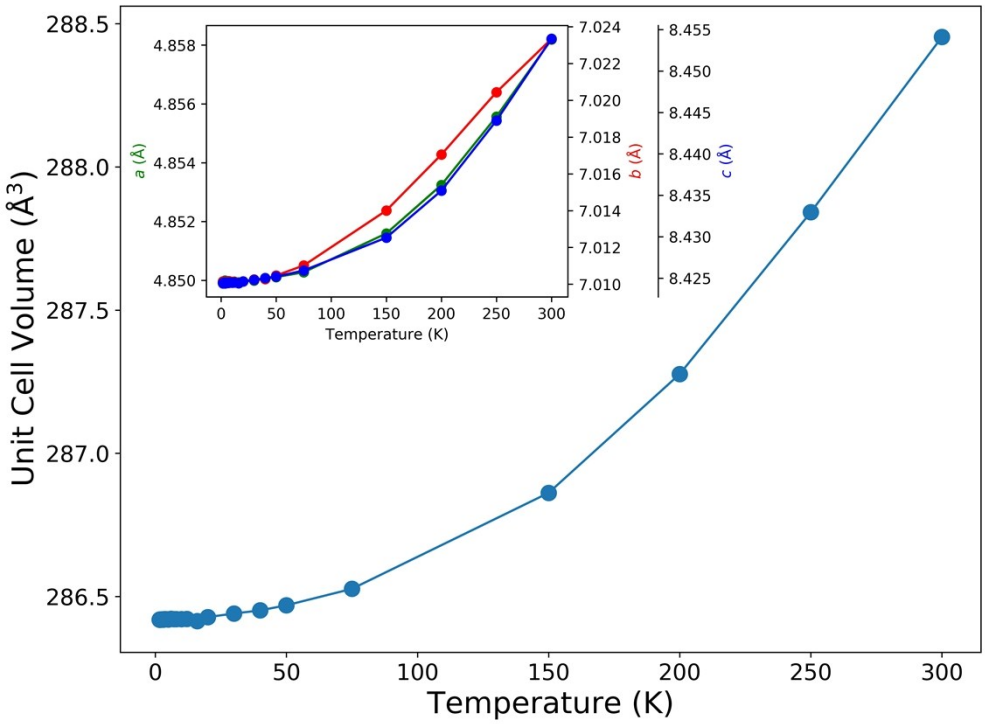

Figure S1: *Changes in the volume of the unit cell and lattice parameters of $TbODCO_3$ with respect to temperature.*

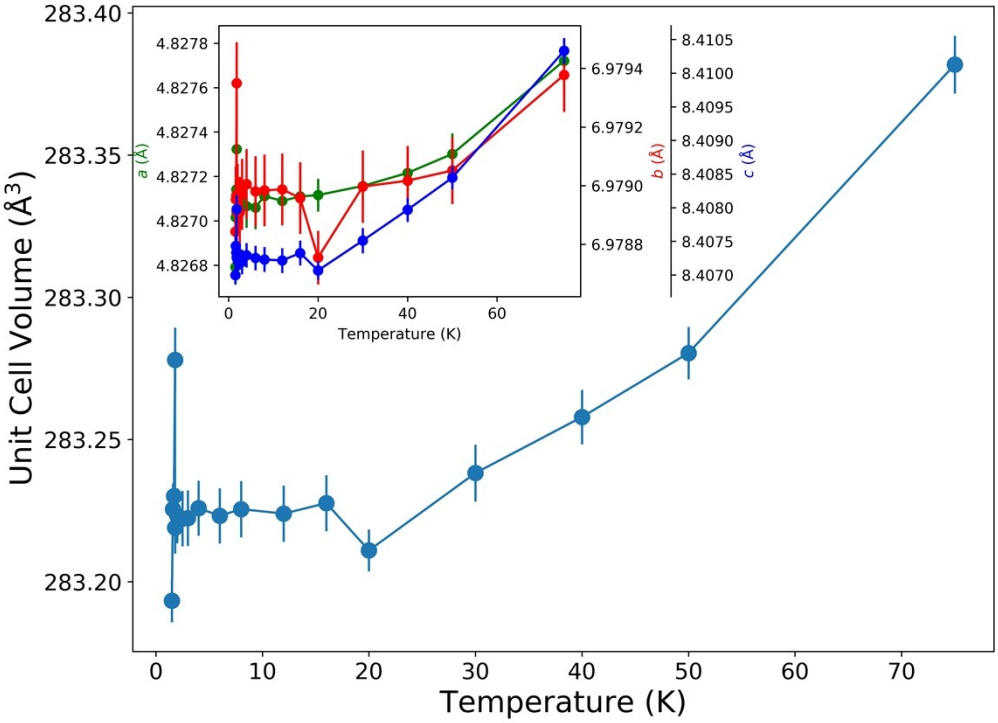

Figure S2*: Changes in the volume of the unit cell and lattice parameters of $DyODCO_3$ with respect to temperature.*

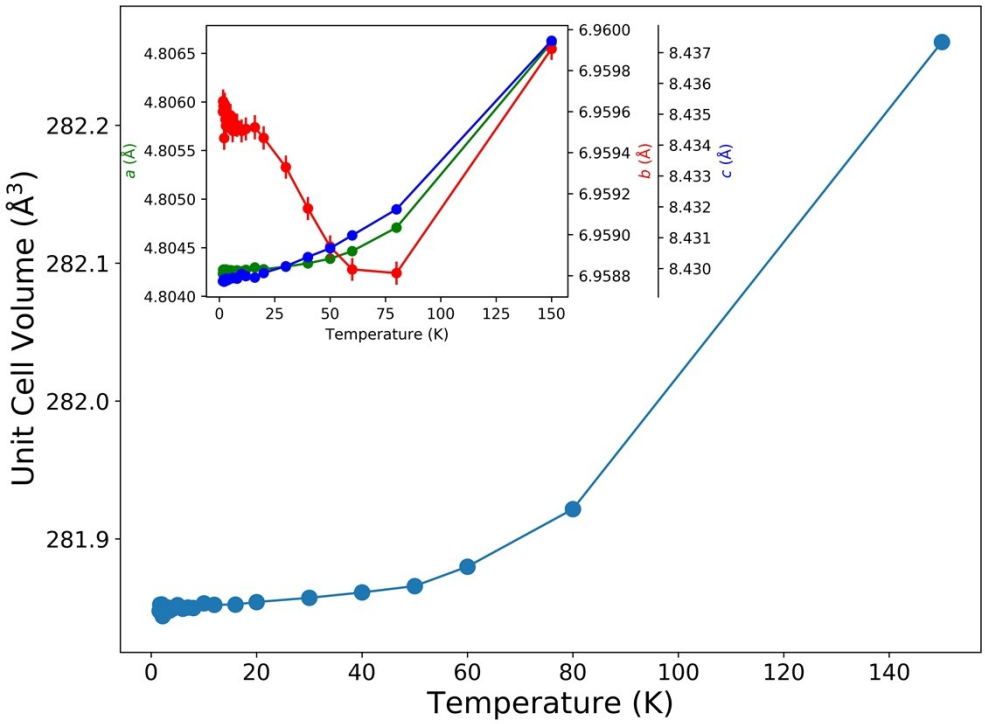

Figure S3: *Changes in the volume of the unit cell and lattice parameters of $HoODCO_3$ with respect to temperature.*

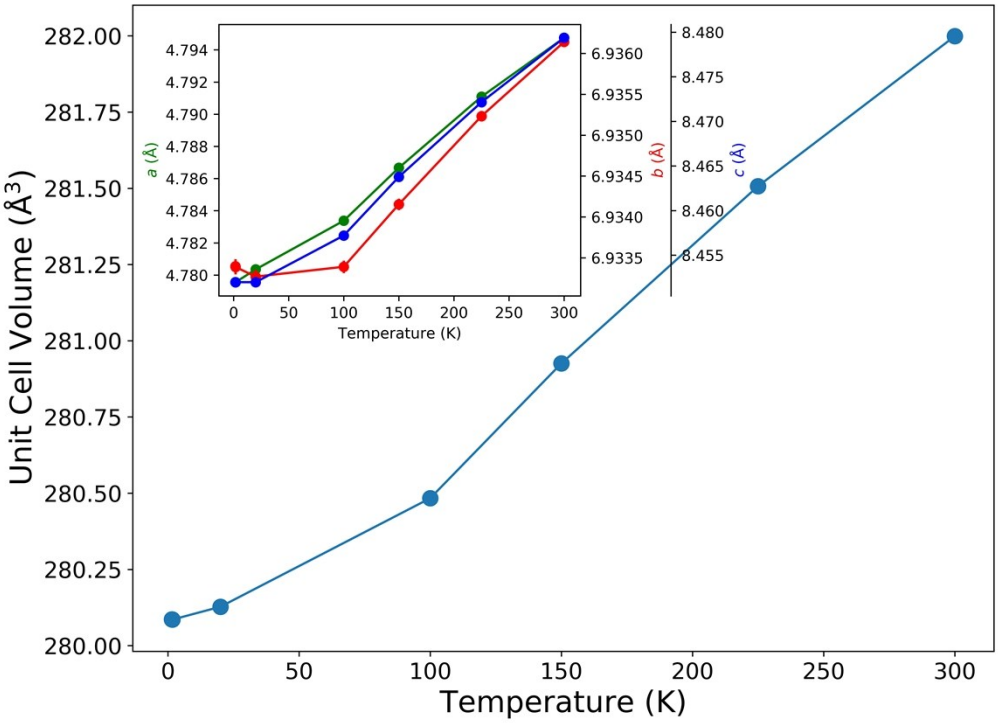

Figure S4*: Changes in the volume of the unit cell and lattice parameters of $ErODCO_3$ with respect to temperature.*

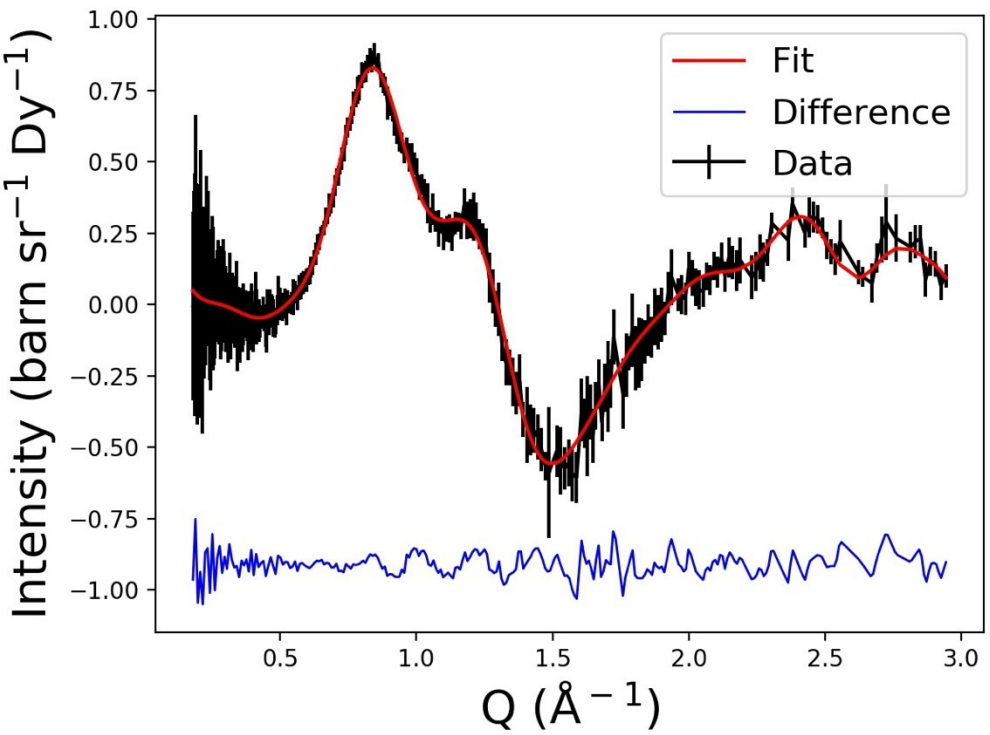

Figure S5: *Reverse Monte Carlo fit at 1.5 K for $DyODCO_3$ using a Heisenberg model.*

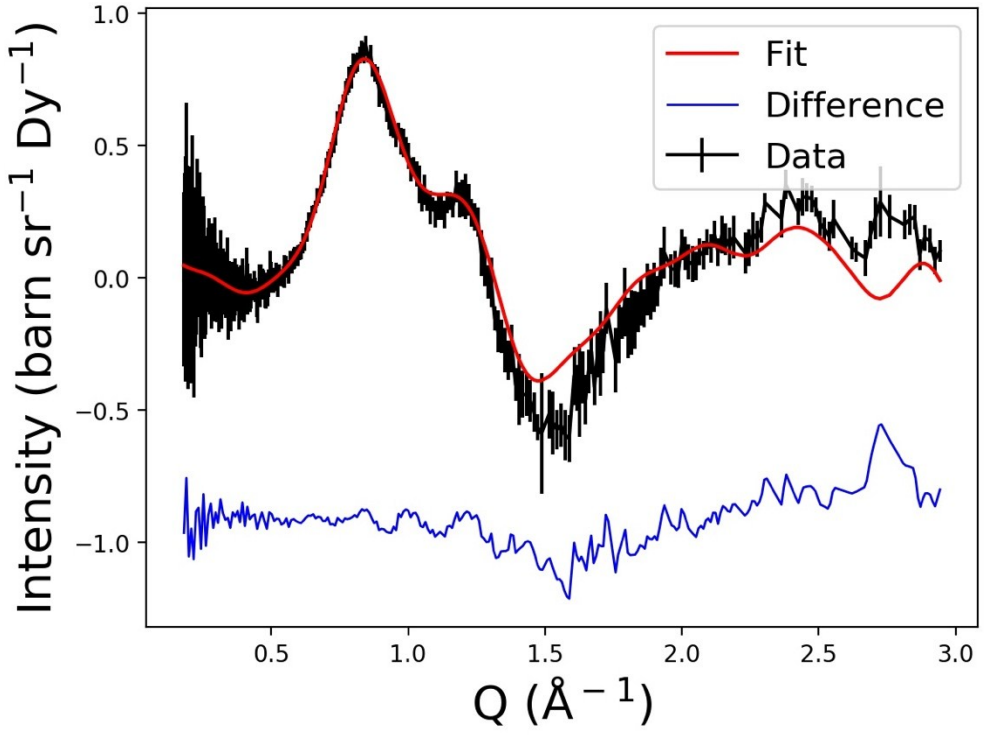

Figure S6*: Reverse Monte Carlo fit at 1.5 K for $DyODCO_3$ using the four site Ising model, determined from $TbODCO_3$.*

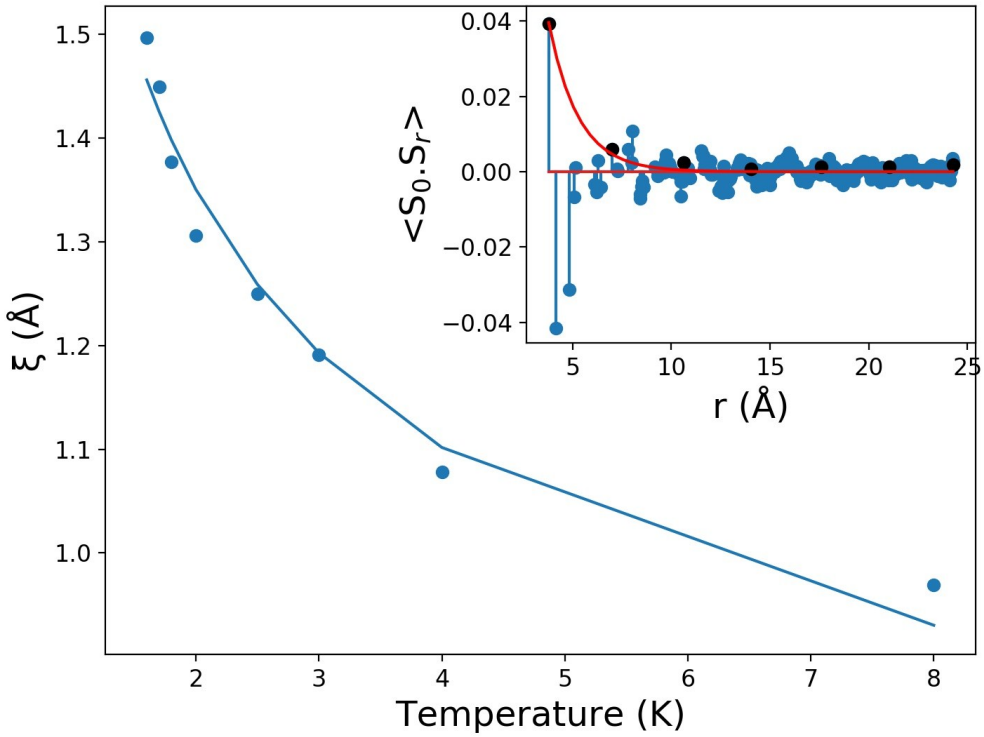

Figure S7: *Fit to the chain correlation length of $DyODCO_3$ using a Heisenberg model. The fit to the base temperature at 1.5 K in the insert.*

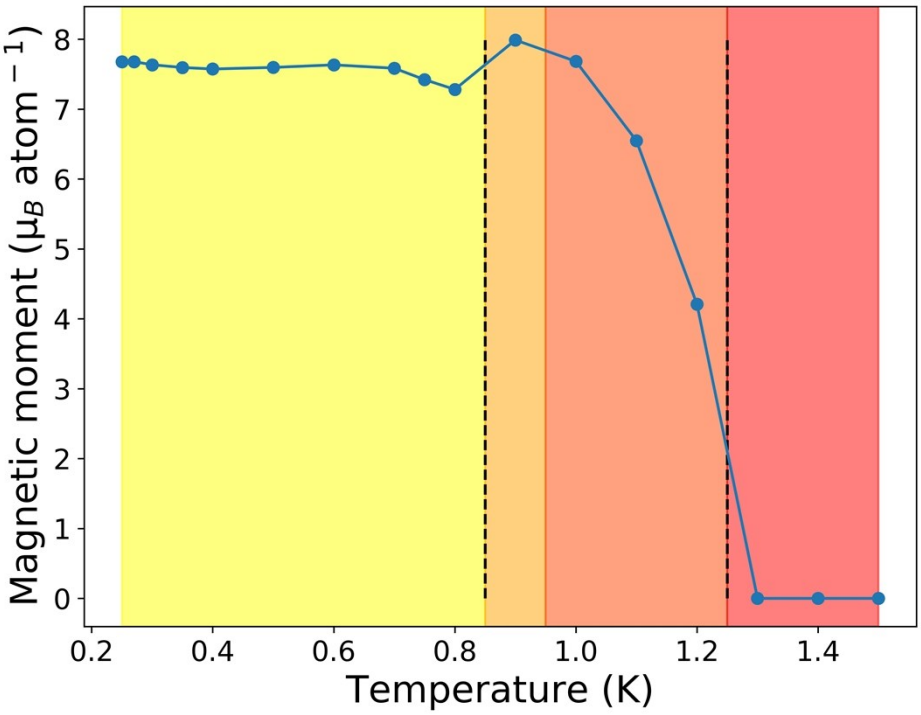

Figure S8: *$HoODCO_3$ phase diagram. Phase fraction have not been refined and so magnetic moments are the average of all magnetic sites. Yellow, orange and red correspond to the **k**=0, incommensurate and paramagnetic phases, respectively. The data point at 0.9 K is the sum of two coexisting phases and highlighted in dark.*

Table S1: Summary of the fractional coordinates, isotropic displacement and occupation of the atoms in the nuclear unit cell of $HoODCO_3$ at 0.25 K, determined from Rietveld refinement.

Atom	x	y	z	Isotropic Displacement	Occupation
Ho	-0.0002(19)	0.1155(5)	0.1649(4)	1.29(13)	1.00000
C	0.515(2)	0.4494(7)	0.1646(6)	0.20(13)	1.00000
D	-0.1158(13)	-0.2618(13)	0.0378(8)	2.8(3)	0.97(2)
O1	-0.273(2)	0.4270(16)	0.1251(10)	2.1(2)	1.00000
O2	0.539(2)	0.0575(9)	0.2014(6)	0.22(14)	1.00000
O3	0.024(2)	-0.1982(8)	0.1155(8)	0.50(14)	1.00000
O4	0.272(2)	0.3914(12)	0.0906(10)	0.24(20)	1.00000

Table S2: Summary of the bond distances of $HoODCO_3$ at 0.25 K, determined from Rietveld refinement.

Atom 1	Atom 2	Distance (Å)
Ho	O1	2.554(12)
Ho	O1	2.563(11)
Ho	O2	2.270(13)
Ho	O3	2.224(7)
Ho	O3	2.262(7)
Ho	O4	2.405(10)
Ho	O4	2.415(10)
C	O1	1.082(13)
C	O2	1.381(8)
C	O4	1.383(13)
D	D	2.489(9)
D	D	2.489(9)
D	O	2.408(14)
D	O3	1.037(11)
D	O3	2.177(11)
O1	Ho	2.554(12)
O1	Ho	2.563(11)
O1	C	1.082(13)
O1	D	2.408(14)
O1	O2	2.143(12)
O1	O4	2.218(14)
O2	Ho	2.270(13)
O2	C	1.381(8)
O2	O1	2.143(12)
O2	O4	2.287(11)
O3	Ho	2.224(7)
O3	Ho	2.262(7)
O3	D	1.037(11)
O3	D	2.177(11)
O4	Ho	2.405(10)
O4	Ho	2.415(10)
O4	C	1.383(13)
O4	O1	2.218(14)
O4	O2	2.287(11)