Electronic Supplementary Material (ESI) for Dalton Transactions

Supporting Information

Polydentate-ligand-supported Self-assembly of Heterometallic T-shaped Co_4RE (RE = Gd, Tb, Y) Clusters: Synthesis, Structure, and Magnetism

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Table S1 Selected bond lengths (Å) and angles (°) for compounds **1-3**

1		**2**		**3**	
Co1-O22	1.878(3)	Co1-O22	1.891(3)	Co1-O22	1.887(4)
Co1-O24	1.915(3)	Co1-O24	1.912(3)	Co1-O24	1.912(4)
Co1-O27	1.891(3)	Co1-O27	1.888(3)	Co1-O27	1.891(4)
Co1-O29	1.903(3)	Co1-O29	1.921(3)	Co1-O29	1.916(4)
Co1-N5	1.886(4)	Co1-N5	1.894(3)	Co1-N5	1.889(5)
Co1-N6	1.900(4)	Co1-N6	1.889(3)	Co1-N6	1.897(4)
Co2-O2	1.883(3)	Co2-O2	1.893(3)	Co2-O2	1.892(4)
Co2-O4	1.916(3)	Co2-O4	1.904(3)	Co2-O4	1.907(4)
Co2-O7	1.885(3)	Co2-O7	1.876(3)	Co2-O7	1.880(4)
Co2-O10	1.909(3)	Co2-O10	1.918(3)	Co2-O10	1.919(3)
Co2-N3	1.894(4)	Co2-N3	1.890(3)	Co2-N3	1.892(4)
Co2-N4	1.885(4)	Co2-N4	1.905(3)	Co2-N4	1.902(4)
Co3-O9	2.088(3)	Co3-O9	2.095(3)	Co3-O9	2.089(4)
Co3-O14	2.110(3)	Co3-O14	2.114(3)	Co3-O14	2.111(4)
Co3-O15	2.055(3)	Co3-O15	2.059(3)	Co3-O15	2.051(4)
Co3-O19	2.131(3)	Co3-O19	2.137(3)	Co3-O19	2.127(4)
Co3-O20	2.054(3)	Co3-O20	2.062(3)	Co3-O20	2.067(4)
Co3-O23	2.097(3)	Co3-O23	2.079(3)	Co3-O23	2.082(4)
Co4-O12	1.894(3)	Co4-O12	1.899(3)	Co4-O12	1.902(4)
Co4-O15	1.882(3)	Co4-O15	1.881(3)	Co4-O15	1.885(4)
Co4-O17	1.904(3)	Co4-O17	1.914(3)	Co4-O17	1.906(4)
Co4-O20	1.894(3)	Co4-O20	1.896(3)	Co4-O20	1.892(4)
Co4-N1	1.904(4)	Co4-N1	1.908(3)	Co4-N1	1.903(4)
Co4-N2	1.899(4)	Co4-N2	1.903(3)	Co4-N2	1.898(4)
Gd1-O4	2.419(3)	Tb1-O4	2.433(3)	Y1-O4	2.415(4)
Gd1-O5	2.467(3)	Tb1-O5	2.455(3)	Y1-O5	2.421(4)
Gd1-O9	2.239(3)	Tb1-O9	2.236(3)	Y1-O9	2.206(4)
Gd1-O10	2.470(3)	Tb1-O10	2.416(3)	Y1-O10	2.388(4)
Gd1-O23	2.247(3)	Tb1-O23	2.232(3)	Y1-O23	2.207(4)
Gd1-O24	2.437(3)	Tb1-O24	2.462(3)	Y1-O24	2.435(4)
Gd1-O29	2.438(3)	Tb1-O29	2.402(3)	Y1-O29	2.380(3)
Gd1-O30	2.454(3)	Tb1-O30	2.477(3)	Y1-O30	2.455(4)
Co1-O24-Gd1	105.71(13)	Co1-O24-Tb1	103.84(11)	Co1-O24-Y1	103.89(15)
Co1-O29-Gd1	106.07(13)	Co1-O29-Tb1	105.76(11)	Co1-O29-Y1	105.81(15)
Co2-O4-Gd1	105.49(13)	Co2-O4-Tb1	105.80(12)	Co2-O4-Y1	105.49(16)
Co2-O10-Gd1	103.83(13)	Co2-O10-Tb1	106.02(12)	Co2-O10-Y1	106.09(16)
Co3-O9-Gd 1	99.53(13)	Co3-O9-Tb1	99.32(11)	Co3-O9-Y1	99.73(15)
Co3-O23-Gd1	98.99(13)	Co3-O23-Tb1	99.90(11)	Co3-O23-Y1	99.91(15)
Co3-O15-Co4	97.04(14)	Co3-O15-Co4	97.11(12)	Co3-O15-Co4	97.21(16)
Co3-O20-Co4	96.71(14)	Co3-O20-Co4	96.58(12)	Co3-O20-Co4	96.49(16)
Co1 ⋯ Gd1	3.4833(7)	Co1 ⋯ Tb1	3.4595(6)	Co1 ⋯ Y1	3.4381(9)
Co2 ⋯ Gd1	3.4641(6)	Co2 ⋯ Tb1	3.4744(6)	Co2 ⋯ Y1	3.4533(9)
Co3 ⋯ Gd1	3.3048(7)	Co3 ⋯ Tb1	3.3017(6)	Co3 ⋯ Y1	3.2846(9)
Co3 ⋯ Co4	2.9520(9)	Co3 ⋯ Co4	2.9562(8)	Co3 ⋯ Co4	2.9553(10)

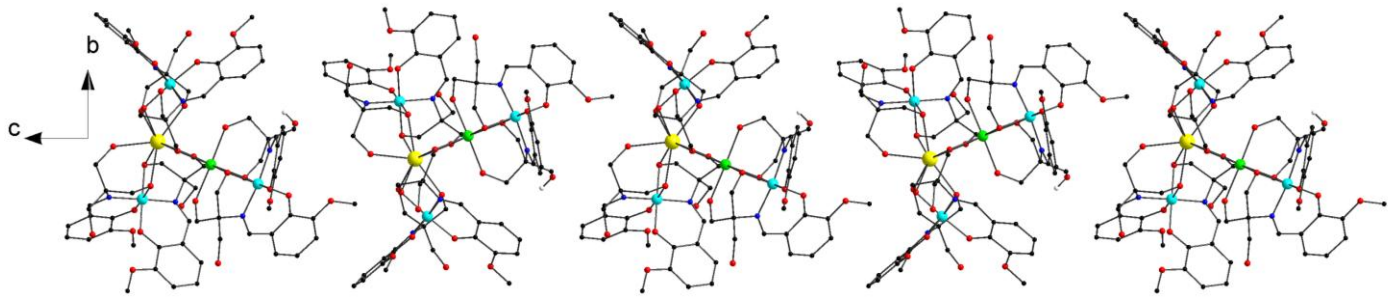

Fig. S1 The crystal packing of **2** showing the 1-D chain along a-axis.

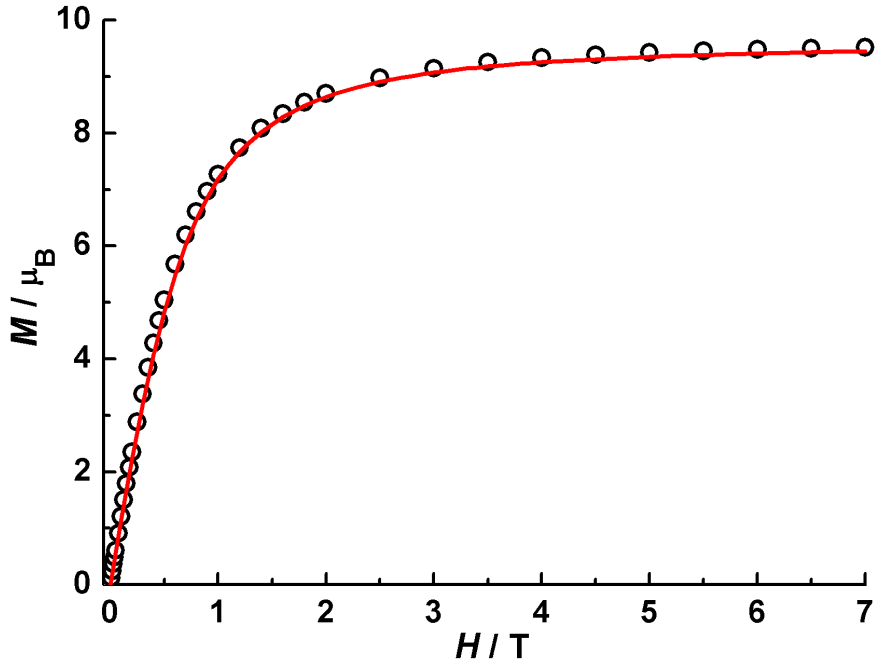

Fig. S2 *M* vs *H* plot of **1** collected at 2 K. Data were simulated using MAGPACK (solid line), see the main text for parameters.

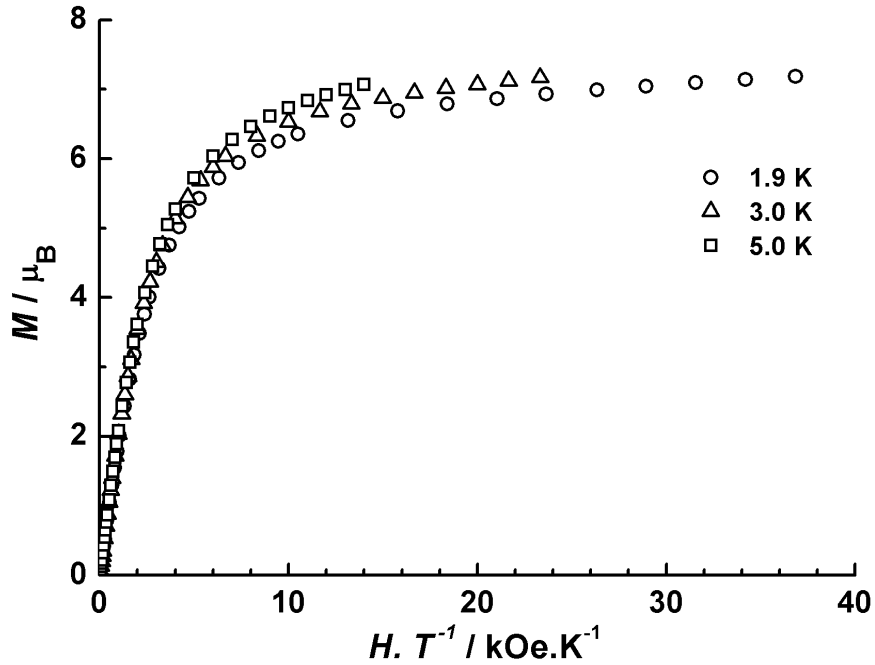

Fig. S3 Plot of *M* versus *H*/*T* for **2** at different temperatures below 5 K.

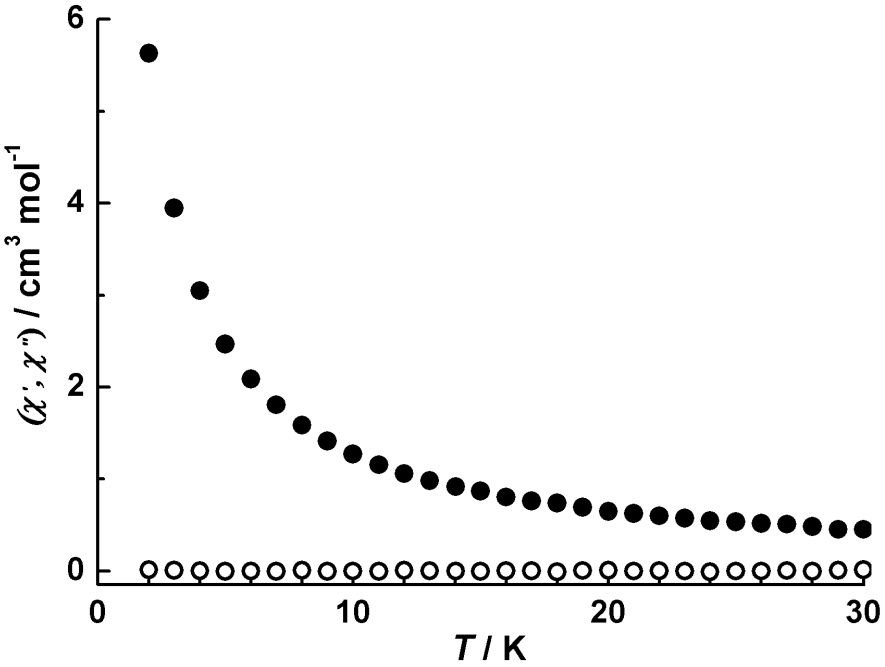

Fig. S4 Temperature dependences of in-phase (χ') (top) and out-of-phase (χ'') (bottom) ac susceptibilities of **2** at 997 Hz in 600 Oe applied dc field and 3 Oe ac field.