

Supporting Information

Synthesis, Characterization and Modeling of Magnetic Properties of a Hexanuclear Aminoalcohol-Supported $\{\text{Co}_2^{\text{II}}\text{Co}_2^{\text{III}}\text{Dy}_2^{\text{III}}\}$ Pivalate Cluster

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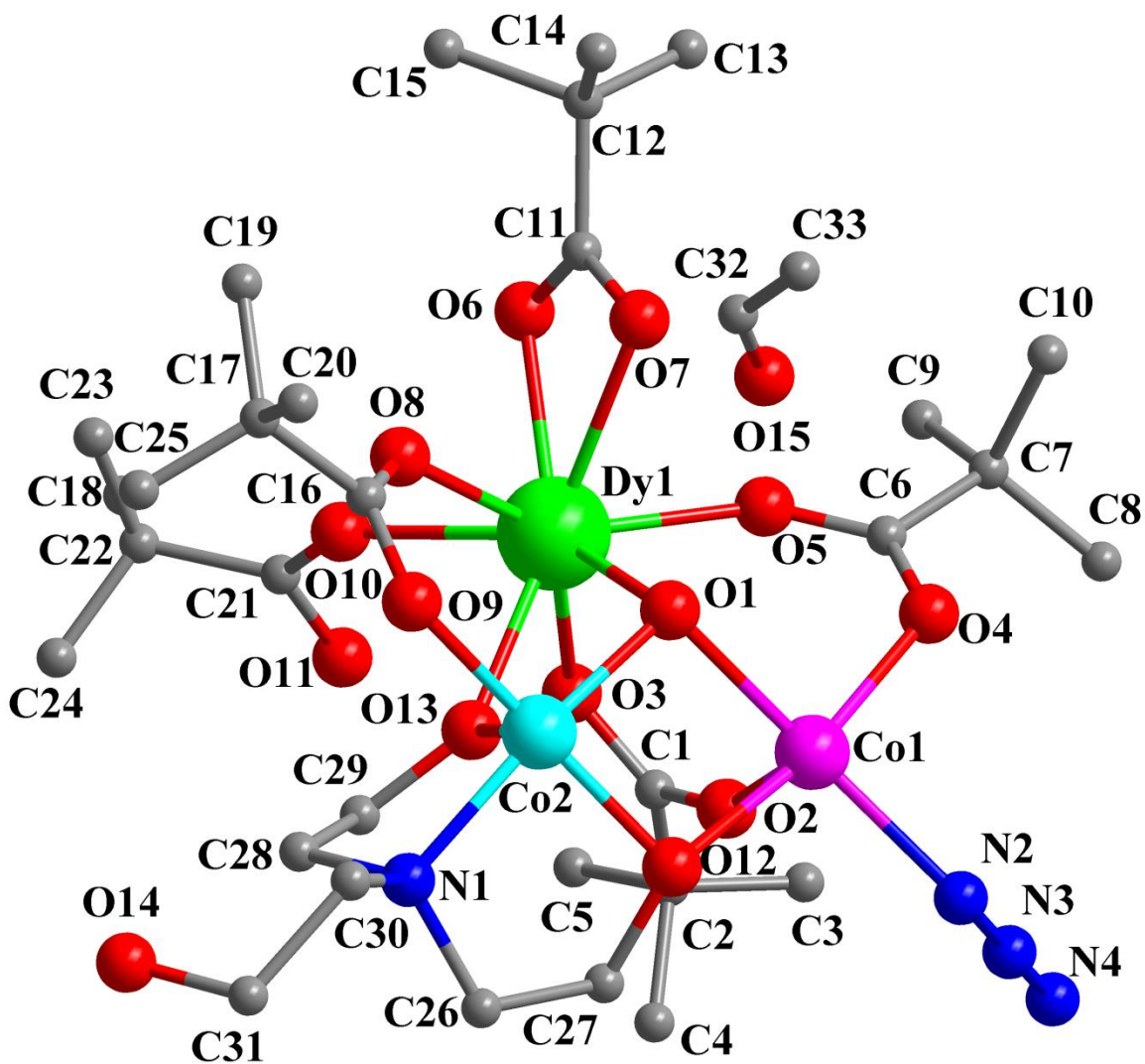


Figure S1. Asymmetric unit in $[\text{Co}_4\text{Dy}_2(\text{OH})_2(\text{O}_2\text{CCMe}_3)_8(\text{HO}_2\text{CCMe}_3)_2(\text{teaH})_2(\text{N}_3)_2] \cdot 2(\text{EtOH})$ (1) with atom numbering scheme. Hydrogen atoms are omitted for clarity.

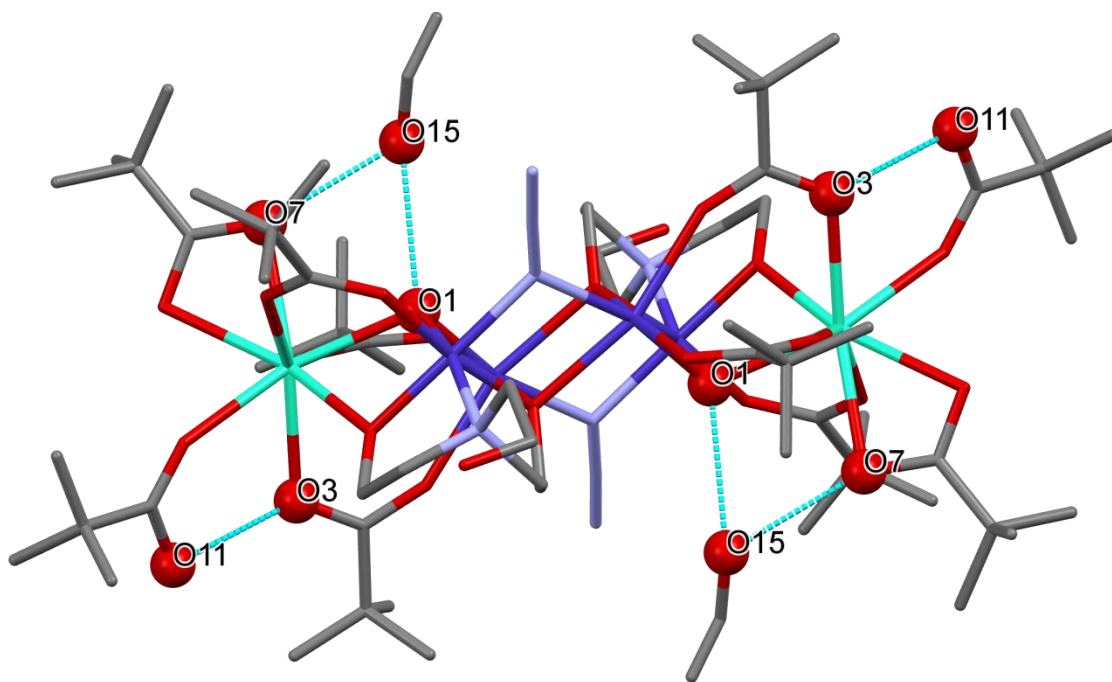


Figure S2. The O–H...O hydrogen bonds formed in **1** between solvate EtOH molecules (O15) and OH⁻ (O1) and chelating pivalate (O7) groups, and between the monodentate (O11) and bridging (O3) pivalates.

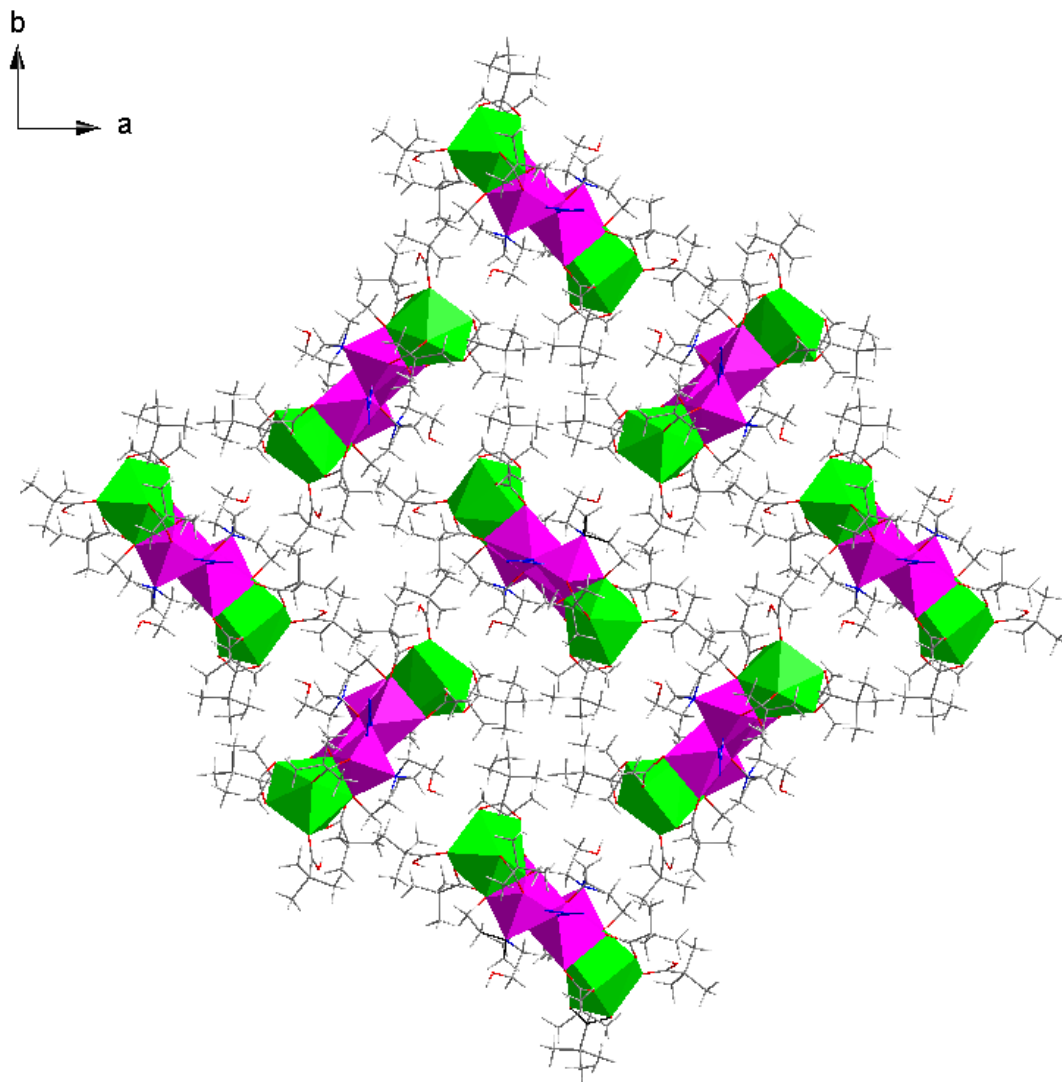


Figure S3. The crystal packing diagram for **1**. The Co and Dy atoms are highlighted as pink and green polyhedra, respectively.

Table S1. Selected Angles (°) for **1**

O1–Dy1–O3	110.61(14)	O1–Co1–O4	95.15(17)
O1–Dy1–O5	83.87(15)	O1–Co1–O12	75.60(15)
O1–Dy1–O6	131.29(15)	O1–Co1–N2	163.88(19)
O1–Dy1–O7	78.08(14)	O1–Co1–O12 _a	92.84(15)
O1–Dy1–O8	82.98(14)	O2–Co1–O4	87.83(18)
O1–Dy1–O10	145.47(15)	O2–Co1–O12	93.15(17)
O1–Dy1–O13	65.28(14)	O2–Co1–N2	93.7(2)
O3–Dy1–O5	74.12(17)	O2–Co1–O12 _a	162.85(16)
O3–Dy1–O6	109.76(16)	O4–Co1–O12	170.72(17)
O3–Dy1–O7	146.11(17)	O4–Co1–N2	92.50(19)
O3–Dy1–O8	140.64(17)	O4–Co1–O12 _a	101.51(16)
O3–Dy1–O10	72.74(16)	O12–Co1–N2	96.63(18)
O3–Dy1–O13	76.11(15)	O12–Co1–O12 _a	79.96(16)
O5–Dy1–O6	82.04(16)	O12 _a –Co1–N2	71.71(18)
O5–Dy1–O7	74.44(18)	O1–Co2–O9	98.87(17)
O5–Dy1–O8	145.22(18)	O1–Co2–O12	84.43(17)
O5–Dy1–O10	128.08(17)	O1–Co2–O13	81.92(17)
O5–Dy1–O13	125.13(16)	O1–Co2–N1	164.56(19)
O6–Dy1–O7	53.23(16)	O1–Co2–N2 _a	92.34(19)
O6–Dy1–O8	82.80(16)	O9–Co2–O12	170.86(18)
O6–Dy1–O10	73.12(16)	O9–Co2–O13	93.54(18)
O6–Dy1–O13	152.05(15)	O9–Co2–N1	90.71(19)
O7–Dy1–O8	71.40(18)	O9–Co2–N2 _a	89.46(19)
O7–Dy1–O10	119.18(17)	O12–Co2–O13	95.37(17)
O7–Dy1–O13	133.89(15)	O12–Co2–N1	87.96(19)
O10–Dy1–O13	83.30(15)	O12–Co2–N2 _a	81.86(19)
O8–Dy1–O10	76.02(17)	O13–Co2–N1	85.45(19)
O8–Dy1–O13	77.02(15)	O13–Co2–N2 _a	173.9(2)
O1–Co1–O2	100.70(17)	N1–Co2–N2 _a	99.9(2)

Symmetry transformations used to generate equivalent atoms: a = 1-x,-y,-z

Table S2. Spherical Coordinates of the Ligand Atoms Composing Coordination Sphere of the Dy^{III} Ion of the {Co₄Dy₂} Cluster in the Crystallographic Frame of Reference

<i>Atoms</i>	1 (O)	2 (O)	3 (O)	4 (O)	5 (O)	6 (O)	7 (O)	8 (O)
<i>R / Å</i>	2.289	2.343	2.328	2.395	2.422	2.394	2.273	2.477
<i>θ / °</i>	116.3	85.4	156.2	62.8	122.8	89.7	12.0	86.1
<i>φ / °</i>	306.4	246.6	185.7	2.6	46.0	115.3	166.6	168.6

Spherical coordinates of the local surrounding of the both Dy^{III} ions are related through the inversion operation.

Table S3. Crystal Field Parameters as Functions of the Phenomenological Parameter G of the Exchange Charge Model

a_{20}	a_{21}	b_{21}
$(7.3 \cdot G - 16.9 \cdot Z)\alpha$	$(-16.3 \cdot G - 281.3 \cdot Z)\alpha$	$(23.4 \cdot G + 281.4 \cdot Z)\alpha$
a_{22}	b_{22}	a_{40}
$(-3.8 \cdot G + 117.4 \cdot Z)\alpha$	$(-14.9 \cdot G - 328.8 \cdot Z)\alpha$	$(10.6 \cdot G + 48.4 \cdot Z)\beta$
a_{41}	b_{41}	a_{42}
$(17.7 \cdot G + 95.2 \cdot Z)\beta$	$(3.6 \cdot G + 23.7 \cdot Z)\beta$	$(32.4 \cdot G + 146.8 \cdot Z)\beta$
b_{42}	a_{43}	b_{43}
$(7.7 \cdot G + 53.7 \cdot Z)\beta$	$(210.4 \cdot G + 1025.6 \cdot Z)\beta$	$(17.7 \cdot G + 59.7 \cdot Z)\beta$
a_{44}	a_{44}	a_{60}
$(-8.4 \cdot G - 22.3 \cdot Z)\beta$	$(-1.7 \cdot G - 19.0 \cdot Z)\beta$	$(1.7 \cdot G + 3.2 \cdot Z)\gamma$
a_{61}	b_{61}	a_{62}
$(-7.7 \cdot G - 14.9 \cdot Z)\gamma$	$(7.2 \cdot G + 13.8 \cdot Z)\gamma$	$= (7.8 \cdot G + 15.0 \cdot Z)\gamma$
b_{62}	a_{63}	b_{63}
$(-0.5 \cdot G - 1.2 \cdot Z)\gamma$	$(-7.8 \cdot G - 14.7 \cdot Z)\gamma$	$(-4.5 \cdot G - 8.6 \cdot Z)\gamma$
a_{64}	b_{64}	a_{65}
$(-8.1 \cdot G - 15.5 \cdot Z)\gamma$	$(10.1 \cdot G + 19.2 \cdot Z)\gamma$	$(49.8 \cdot G + 94.0 \cdot Z)\gamma$
b_{65}	a_{66}	b_{66}
$(-6.7 \cdot G - 12.5 \cdot Z)\gamma$	$(45.2 \cdot G + 85.3 \cdot Z)\gamma$	$(-3.2 \cdot G - 6.4 \cdot Z)\gamma$