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Crystal structure of tetrakis(μ_3 -2-(*N*-(2-hydroxyethyl)amino)ethoxo)-tetrachloro-tetracobalt(II) methanol solvate, $C_{17}H_{44}Cl_4Co_4N_4O_9$

Table 1: Data collection and handling.

Crystal:	Red block
Size:	0.15 × 0.13 × 0.10 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	24.1 cm ⁻¹
Diffractometer, scan mode:	Bruker APEX2, φ and ω
$2\theta_{\max}$, completeness:	52°, >97%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	40621, 6179, 0.031
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 5670
$N(\text{param})_{\text{refined}}$:	343
Programs:	Bruker [8], SHELX [9, 10]

The crystal structure is shown in the figure. Tables 1 and 2 contain details on crystal structure and measurement conditions and a list of the atoms including atomic coordinates and displacement parameters.

Source of material

All reagents and solvents employed were commercially available and used as received without further purification. A mixture of $CoCl_2 \cdot 6H_2O$ (1 mmol, 0.238 g), diethanolamine(H_2L) (2 mmol, 0.212 g) and sodium methoxide (2 mmol, 0.108 g) were mixed in methanol (10 mL) and heated at 413 K for 2 days in a sealed 15 mL Teflon-lined stainless steel vessel under autogenous pressure. After cooling to room temperature at a rate of 10 K · h⁻¹, red block crystals were isolated, washed with methanol and then dried in air in 37% yield.

Experimental details

H atoms were treated as riding atoms with U_{iso} in the range 1.2–1.5 U_{eq} .

Discussion

With the discovery of the first single-molecule magnet (SMM) [1], $[Mn_{12}O_{12}(O_2CR)_{16}(H_2O)_4]$, research on SMMs has been one of the most active fields in the past decade, and is still developing rapidly. SMMs can provide almost ideal systems for investigating the coexistence of classic and quantum effects, and are hopeful for applications in information storage and

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Abstract

$C_{17}H_{44}Cl_4Co_4N_4O_9$, triclinic, $P\bar{1}$ (no. 2), $a = 10.918(14)$ Å, $b = 11.899(15)$ Å, $c = 13.327(17)$ Å, $\alpha = 91.286(13)^\circ$, $\beta = 91.755(14)^\circ$, $\gamma = 111.673(13)^\circ$, $V = 1607(4)$ Å³, $Z = 2$, $R_{\text{gt}}(F) = 0.0308$, $wR_{\text{ref}}(F^2) = 0.1257$, $T = 293(2)$ K.

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Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²).

Atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso} [*] / <i>U</i> _{eq}
Co1	0.74728(4)	0.72262(4)	0.18724(3)	0.02577(13)
Co2	0.47158(4)	0.67519(4)	0.27845(3)	0.02595(13)
Co3	0.72137(4)	0.86328(4)	0.39842(3)	0.02657(13)
Co4	0.64563(4)	0.94054(4)	0.18769(3)	0.02663(13)
O1	0.4344(3)	0.4832(2)	0.23426(19)	0.0415(6)
H1AA	0.4812	0.4401	0.2633	0.050*
O2	0.5729(2)	0.74993(19)	0.14904(15)	0.0261(4)
O3	0.5544(2)	0.86680(18)	0.32173(15)	0.0260(4)
O4	0.7509(3)	1.1291(2)	0.2526(2)	0.0530(7)
H4C	0.8404	1.1606	0.2708	0.064*
O5	0.6584(2)	0.68699(18)	0.32948(15)	0.0257(4)
O6	0.5918(3)	0.8067(2)	0.53207(17)	0.0404(5)
H6C	0.5157	0.8233	0.5401	0.048*
O7	0.8076(2)	0.7774(2)	0.03144(18)	0.0403(6)
H7C	0.7481	0.7772	−0.0201	0.048*
O8	0.8015(2)	0.90059(19)	0.24975(16)	0.0276(4)
O11	0.0622(4)	0.6036(4)	0.3198(3)	0.0885(12)
H11D	0.1426	0.6297	0.3403	0.106*
N1	0.3032(3)	0.6298(3)	0.1724(2)	0.0361(6)
H1AB	0.2454	0.6611	0.1974	0.043*
N2	0.4922(3)	1.0146(3)	0.1855(2)	0.0371(6)
H1AC	0.4432	0.9888	0.1271	0.044*
N3	0.8317(3)	0.7874(2)	0.4935(2)	0.0337(6)
H1AD	0.9186	0.8352	0.4916	0.040*
N4	0.9589(3)	0.7705(3)	0.1999(2)	0.0357(6)
H1AE	0.9759	0.7179	0.2415	0.043*
C1	0.3325(4)	0.4311(3)	0.1575(3)	0.0494(9)
H1A	0.2876	0.3452	0.1672	0.059*
H1B	0.3705	0.4413	0.0919	0.059*
C2	0.2356(4)	0.4948(4)	0.1640(3)	0.0516(10)
H2A	0.1771	0.4733	0.1045	0.062*
H2B	0.1821	0.4671	0.2219	0.062*
C3	0.3511(3)	0.6896(3)	0.0761(2)	0.0352(7)
H3A	0.3478	0.7700	0.0777	0.042*
H3B	0.2939	0.6432	0.0206	0.042*
C4	0.4929(3)	0.6989(3)	0.0599(2)	0.0307(6)
H4A	0.4940	0.6192	0.0445	0.037*
H4B	0.5278	0.7497	0.0036	0.037*
C5	0.4778(3)	0.9336(3)	0.3591(2)	0.0327(7)
H5A	0.5355	1.0073	0.3942	0.039*
H5B	0.4150	0.8855	0.4059	0.039*
C6	0.4045(3)	0.9645(3)	0.2706(3)	0.0367(7)
H6A	0.3316	0.8921	0.2470	0.044*
H6B	0.3682	1.0233	0.2933	0.044*
C7	0.5551(4)	1.1485(3)	0.1854(3)	0.0501(9)
H7A	0.4889	1.1832	0.1970	0.060*
H7B	0.5899	1.1723	0.1198	0.060*
C8	0.6638(5)	1.1976(4)	0.2633(4)	0.0593(11)
H8A	0.7125	1.2829	0.2539	0.071*
H8B	0.6284	1.1883	0.3298	0.071*
C9	0.7902(4)	0.7903(4)	0.5982(3)	0.0457(9)
H9A	0.8262	0.8729	0.6253	0.055*
H9B	0.8254	0.7421	0.6393	0.055*
C10	0.6408(4)	0.7421(4)	0.6033(3)	0.0441(8)
H10A	0.6044	0.6560	0.5864	0.053*

Table 2 (continued)

Atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso} [*] / <i>U</i> _{eq}
H10B	0.6156	0.7548	0.6705	0.053*
C11	0.8147(3)	0.6645(3)	0.4525(3)	0.0344(7)
H11A	0.8207	0.6153	0.5072	0.041*
H11B	0.8847	0.6713	0.4072	0.041*
C12	0.6818(3)	0.6032(3)	0.3963(2)	0.0300(6)
H12A	0.6815	0.5326	0.3583	0.036*
H12B	0.6123	0.5769	0.4440	0.036*
C13	1.0035(4)	0.7529(4)	0.0983(3)	0.0433(8)
H13A	0.9748	0.6670	0.0817	0.052*
H13B	1.0991	0.7869	0.0986	0.052*
C14	0.9478(4)	0.8134(4)	0.0184(3)	0.0444(8)
H14A	0.9907	0.9007	0.0257	0.053*
H14B	0.9635	0.7884	−0.0483	0.053*
C15	1.0211(3)	0.8951(3)	0.2469(3)	0.0403(8)
H15A	1.1064	0.9357	0.2186	0.048*
H15B	1.0353	0.8893	0.3185	0.048*
C16	0.9355(3)	0.9707(3)	0.2300(3)	0.0342(7)
H16A	0.9673	1.0425	0.2741	0.041*
H16B	0.9413	0.9964	0.1611	0.041*
Cl1	0.33997(8)	0.62193(8)	0.42471(6)	0.0418(2)
Cl2	0.69837(9)	0.51180(7)	0.14353(7)	0.0412(2)
Cl3	0.83190(9)	1.06927(7)	0.46498(7)	0.0427(2)
Cl4	0.71411(8)	0.99727(8)	0.01694(6)	0.0403(2)
C17	−0.0297(6)	0.4788(6)	0.3360(6)	0.098(2)
H17A	−0.1151	0.4671	0.3065	0.148*
H17B	0.0028	0.4220	0.3057	0.148*
H17C	−0.0367	0.4665	0.4069	0.148*

quantum computing in the future [2–4]. To date, several oxo-bridged Mn(III)- or Fe(III)-based SMMs have been reported. As a large anisotropic ion, Co(II) might be another possible candidate ion for SMMs, and its strong Ising-type anisotropic contribution has been demonstrated in some single-chain magnets (SCMs) [5, 6]. However, among the abundant Co(II)-based clusters, only a few behave as SMMs [2, 7]. To extend the research field of Co(II)-based clusters, we report here the synthesis and crystal structure of a new {Co₄O₄} core complex.

The title structure consists of a distorted {Co₄O₄} cubane. The four alkoxide groups of the mono-deprotonated diethanolamine ligands provide four μ₃-O donors. Each amine group and the remaining four O atoms of the diethanolamine ligands are monodentate. The final site of each cobalt(II) centre are filled by a terminal Cl ligand. The coordination environment at each cobalt is distorted octahedral due to the imposed ligand bite angles. Each Co₄ cubane is hydrogen-bonded to four neighbouring cubanes through two N—H···Cl contacts [N—H···Cl distances = 3.428(4) and 3.451(5) Å, respectively].

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