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Key indicators

Single-crystal X-ray study
T = 293 K
Mean $\sigma(\text{C}-\text{C}) = 0.009 \text{ \AA}$
Disorder in main residue
R factor = 0.064
wR factor = 0.207
Data-to-parameter ratio = 23.3

For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

Di- μ_2 -methanolato-bis[tetrakis(pyrimidin-2-amine- κN^1)cobalt(II)] bis(tetrafluoroborate)

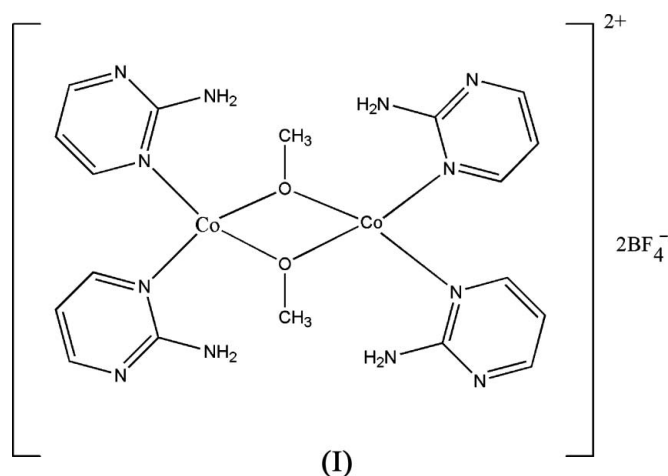
The title compound, $[\text{Co}_2(\text{CH}_3\text{O})_2(\text{C}_4\text{H}_5\text{N}_3)_4](\text{BF}_4)_2$, consists of a discrete dimeric Co^{II} complex. The asymmetric unit consists of one pyrimidin-2-amine ligand, which occupies a general position, and one methanolate group, as well as one Co^{II} cation and one tetrafluoroborate anion, which are located in special positions. The Co^{II} cation lies on a twofold rotation axis, whereas the tetrafluoroborate anion and the methanolate group lie on mirror planes. The N atoms of the pyrimidin-2-amine ligand are involved in intermolecular hydrogen bonding. From this arrangement, large channels are formed, which elongate in the direction of the crystallographic *c* axis.

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Comment

Cobalt complexes are of great interest in coordination chemistry in relation to catalysis and enzymatic reactions, magnetism, and molecular architectures (Billson *et al.*, 2000; Fritsky *et al.*, 2003; Kotera *et al.*, 2003). Until recently, only a few cobalt complexes with pyrimidin-2-amine as ligand have been reported. In all of these compounds, the Co atom is coordinated by the N atom of the pyrimidine ring. Most of these compounds represent discrete mononuclear complexes (Kistenmacher *et al.*, 1978; Masaki *et al.*, 2002; Song *et al.*, 2005) but in some of them the Co atoms are connected into polymers, $[\text{C}_{16}\text{H}_{10}\text{CO}_2\text{N}_{18}]_n$ (Jensen *et al.*, 2000). To date, there is one dinuclear compound, $[\text{C}_8\text{H}_{22}\text{Co}_2\text{N}_6\text{O}_{14}\text{S}_2 \cdot 2\text{H}_2\text{O}]$, in which the two Co atoms are connected by two sulfate anions (Lumme *et al.*, 1996). We report here the structure of another dinuclear Co compound with pyrimidin-2-amine, (I).



The structure of compound (I), is presented in Fig. 1. The Co atom lies on a twofold rotation axis, whereas the tetrafluoroborate anion and the methanolate group lie on mirror

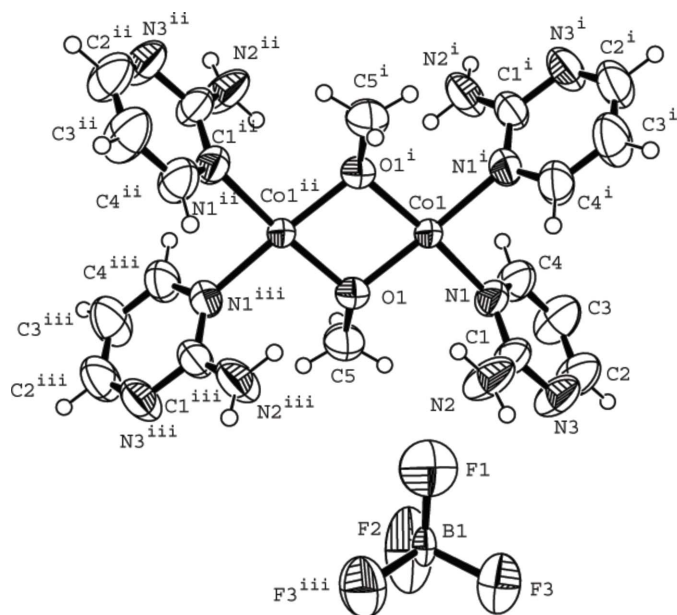


Figure 1
Crystal structure of (I), with displacement ellipsoids drawn at the 30% probability level. Only one disorder component is shown. [Symmetry codes: (i) $-x, y, -z$; (ii) $-x, -y, -z$; (iii) $x, -y, z$.]

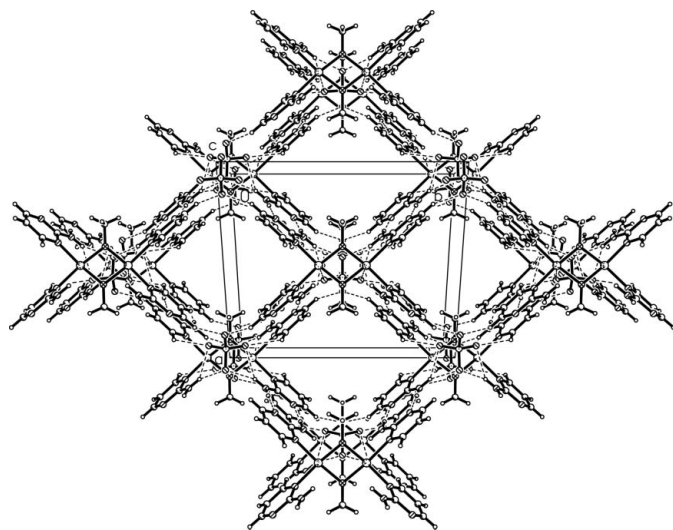


Figure 2
Packing diagram of (I), viewed along the c axis (hydrogen bonding is shown as dashed lines).

planes. The cobalt centres are four-coordinated by two O atoms of the methanolate group and two N atoms of two symmetry-related pyrimidin-2-amine ligands. The Co—O bond lengths of 1.920 (2) Å and the Co—N bond lengths of 2.014 (3) Å are comparable to those of similar Co complexes. The *cis*-angles at the Co^{II} centre range from 79.86 (17) to 95.33 (14)°, which indicates a slightly distorted square geometry of Co atoms. Two Co atoms are connected by two methanolate groups *via* μ -O,O' coordination into dimers, which are located on site $2/m$. The tetrafluoroborate anions are located 3.4471 Å above the plane formed by the two Co

and the two O atoms. The complexes are connected *via* N—H...N and N—H...F hydrogen bonding. From this arrangement, large channels are formed, which elongate in the direction of the c axis (Fig. 2). The channel volume was calculated using PLATON (Spek, 2003) to be 41.8% of the unit-cell volume.

Experimental

All chemicals were of AR grade. $\text{Co}(\text{CH}_3\text{COO})_2 \cdot 4\text{H}_2\text{O}$ (0.2 mmol, 49.8 mg) and pyrimidin-2-amine (0.2 mmol, 37.6 mg) were dissolved in methanol (20 ml). A solution of sodium fluoroborate (0.1 mmol, 10.9 mg) in water (3 ml) was then added. The mixture was stirred for 30 min at 353 K and the remaining solid was filtered off. After slow evaporation of the solvent from the filtrate red block-shaped crystals of (I) grew within 10 d. Analysis found: C 29.23, H 3.62, N 22.85%; calculated for $\text{C}_{18}\text{H}_{26}\text{B}_2\text{Co}_2\text{F}_8\text{N}_{12}\text{O}_2$: C 29.46, H 3.57, N 22.90%.

Crystal data

$[\text{Co}_2(\text{CH}_3\text{O})_2(\text{C}_4\text{H}_5\text{N}_3)_4](\text{BF}_4)_2$
 $M_r = 733.99$
 Monoclinic, $C2/m$
 $a = 16.338$ (6) Å
 $b = 14.704$ (2) Å
 $c = 12.040$ (4) Å
 $\beta = 132.34$ (1)°
 $V = 2138.0$ (11) Å³

$Z = 2$
 $D_x = 1.140$ Mg m⁻³
 Mo $K\alpha$ radiation
 $\mu = 0.84$ mm⁻¹
 $T = 293$ (2) K
 Block, red
 $0.32 \times 0.28 \times 0.20$ mm

Data collection

Bruker APEX area-detector diffractometer
 φ and ω scans
 Absorption correction: multi-scan (SADABS; Bruker, 2001)
 $T_{\min} = 0.775$, $T_{\max} = 0.850$

2626 measured reflections
 2541 independent reflections
 2010 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.032$
 $\theta_{\text{max}} = 27.5^\circ$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.064$
 $wR(F^2) = 0.207$
 $S = 1.11$
 2541 reflections
 109 parameters
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.1252P)^2 + 2.7158P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} = 0.003$
 $\Delta\rho_{\text{max}} = 0.86$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.60$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D\text{---}H\cdots A$	$D\text{---}H$	$H\cdots A$	$D\cdots A$	$D\text{---}H\cdots A$
N2—H2B...N3 ^{iv}	0.90	2.10	3.001 (6)	176
N2—H2A...F3 ^v	0.90	2.15	3.022 (6)	163
N2—H2A...F1 ^{vi}	0.90	2.40	3.091 (6)	134

Symmetry codes: (iv) $-x + \frac{1}{2}, -y + \frac{1}{2}, -z + 1$; (v) $-x, y, -z + 1$; (vi) $-x, -y, -z + 1$.

All C-bound H atoms were placed in idealized positions and were refined using a riding model, with C—H = 0.93 Å and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ for aromatic H atoms, and C—H = 0.96 Å and $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$ for methyl H atoms. The N-bound H atoms were located in a difference map, their bond lengths were set to 0.90 Å and they were refined using a riding model [$U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{N})$]. The methyl H

atoms are disordered due to symmetry; site occupancy factors are 0.5. There are no indications that the channels are filled with solvent molecules.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINTE* (Bruker, 2001); data reduction: *SAINTE*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

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