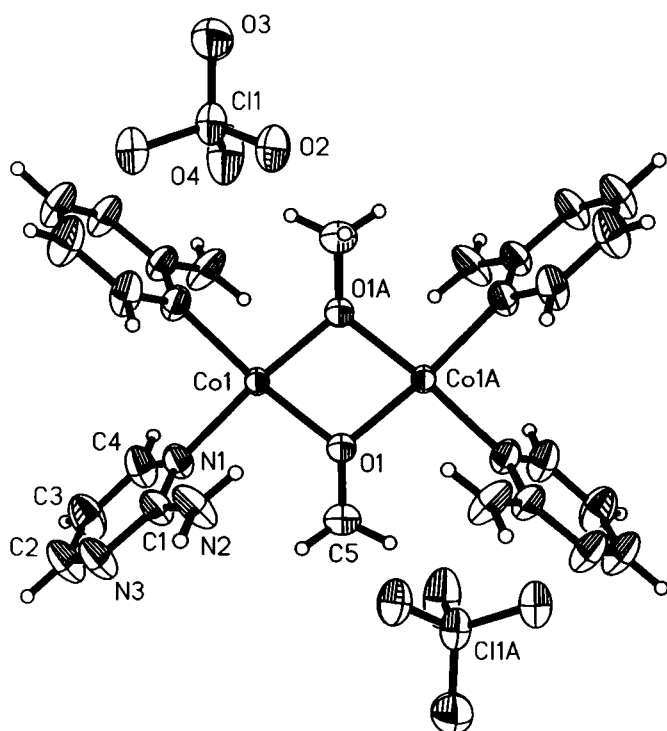


Crystal structure of tetra(2-aminopyrimidine)dimethanolato-dicobalt(II) diperchlorate, $[\text{Co}_2(\text{CH}_3\text{O})_2(\text{C}_4\text{H}_5\text{N}_3)_4][\text{ClO}_4]_2$

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Abstract

$\text{C}_{18}\text{H}_{26}\text{Cl}_2\text{Co}_2\text{N}_{12}\text{O}_{10}$, monoclinic, $C12/m1$ (no. 12), $a = 16.466(5)$ Å, $b = 14.969(5)$ Å, $c = 12.003(4)$ Å, $\beta = 132.40(1)^\circ$, $V = 2184.8$ Å³, $Z = 2$, $R_{\text{gt}}(F) = 0.053$, $wR_{\text{ref}}(F^2) = 0.188$, $T = 293$ K.

Source of material

Cobalt(II) perchlorate and 2-aminopyrimidine in a molar ratio of 1:2 were dissolved in methanol, and the resulting solution was kept standing still in air overnight. The crystals precipitated were filtered and washed with methanol for three times, and were dried in vacuo using CaCl_2 (yield 56 %). The presence of salicylaldehyde would increase the yield of the product (from 56 % to 80–95 %).

Discussion

Co(II,III) complexes with organic ligands-containing nitrogen donor atoms have been a hot topics in the field of coordination chemistry for many years. Recently, there were many cobalt(II, III) complexes being structurally determined by single X-ray analysis [1–4]. We have been interested in preparing some mono-, di- or trinuclear metal complexes and assaying their biological

relevant activities and succeeded in preparing the trinuclear cobalt complexes [5]. But using the same method we failed to isolate the similar trinuclear cobalt complexes when the 2-aminopyridine was replaced by 2-aminopyrimidine and obtained the title compound.

The title complex is a dinuclear cobalt(II) complex, and the crystal structure consists of the coordination dication and two uncoordinated perchlorate anions. In the cation, each of the cobalt(II) atoms is four-coordinated by two nitrogen atoms from two monodentate 2-aminopyrimidine molecules and by two oxygen atoms from two deprotonated methanol molecules. The latter acted as a bidentate ligand, two of which bridged the two cobalt subunits to form one dication. The separation of the two metals in each dimer is 2.951(6) Å. The mean deviation of the plane constituted from the four coordination atoms around each metal was 0.115(5) Å, and the metal was in the plane. The dihedral angles between the metal plane and the two adjacent pyrimidine rings were both $112.8(2)^\circ$, and the two neighboring aromatic rings were almost perpendicular each other. Two oxygen atoms in each perchlorate group and all the amine groups and the uncoordinated nitrogen atoms in the pyrimidine molecules contributed to the formation of hydrogen bonds, which link the complexes to form a three-dimensional network structure.

Table 1. Data collection and handling.

Crystal:	red prism, size $0.28 \times 0.28 \times 0.40$ mm
Wavelength:	Mo $K\alpha$ radiation (0.71073 Å)
μ :	9.30 cm^{-1}
Diffractometer, scan mode:	Bruker SMART CCD, φ/ω
$2\theta_{\text{max}}$:	53.08°
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$:	4544, 2359
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 1864
$N(\text{param})_{\text{refined}}$:	109
Program:	SHELXTL [6]

Table 2. Atomic coordinates and displacement parameters (in Å²).

Atom	Site	Occ.	x	y	z	U_{iso}
H(3A)	8j		0.2488	0.1793	0.4354	0.08
H(3B)	8j		0.1893	0.1194	0.2929	0.08
H(2A)	8j		0.0170	0.3786	0.3349	0.08
H(3C)	8j		−0.1484	0.3463	0.0893	0.08
H(4A)	8j		−0.1466	0.2330	−0.0432	0.08
H(5A)	8j	0.5	0.0152	−0.0557	0.2612	0.08
H(5B)	8j	0.5	0.0303	0.0483	0.2796	0.08
H(5C)	8j	0.5	−0.0838	0.0074	0.1409	0.08

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Table 3. Atomic coordinates and displacement parameters (in Å²).

Atom	Site	x	y	z	U ₁₁	U ₂₂	U ₃₃	U ₁₂	U ₁₃	U ₂₃
Co(1)	4g	0	0.09856(4)	0	0.0543(5)	0.0309(4)	0.0359(4)	0	0.0271(3)	0
O(1)	4i	0.0254(3)	0	0.1238(4)	0.060(2)	0.045(2)	0.048(2)	0	0.036(2)	0
O(2)	8j	0.2792(3)	0.4222(2)	0.8604(4)	0.080(2)	0.053(2)	0.101(2)	0.008(2)	0.060(2)	0.007(2)
O(3)	4i	0.1871(5)	½	0.6380(7)	0.118(4)	0.089(4)	0.081(3)	0	0.060(3)	0
O(4)	4i	0.1211(5)	½	0.7646(9)	0.091(4)	0.070(3)	0.197(6)	0	0.110(4)	0
N(1)	8j	0.0090(3)	0.1942(2)	0.1266(4)	0.069(2)	0.047(2)	0.053(2)	0.007(2)	0.035(2)	−0.004(1)
N(2)	8j	0.1883(3)	0.1658(3)	0.3397(4)	0.072(2)	0.087(3)	0.062(2)	0.020(2)	0.028(2)	−0.027(2)
N(3)	8j	0.1047(3)	0.2836(3)	0.3472(4)	0.075(2)	0.071(3)	0.069(2)	0.012(2)	0.038(2)	−0.022(2)
C(1)	8j	0.0996(3)	0.2146(3)	0.2688(5)	0.065(2)	0.055(2)	0.055(2)	0.004(2)	0.035(2)	−0.013(2)
C(2)	8j	0.0152(4)	0.3306(4)	0.2802(6)	0.083(3)	0.075(3)	0.084(3)	0.013(3)	0.047(3)	−0.027(3)
C(3)	8j	−0.0826(5)	0.3128(4)	0.1353(7)	0.079(3)	0.075(3)	0.094(4)	0.019(3)	0.044(3)	−0.013(3)
C(4)	8j	−0.0815(4)	0.2447(3)	0.0599(6)	0.071(3)	0.056(3)	0.072(3)	0.010(2)	0.035(2)	−0.009(2)
C(5)	4i	−0.0055(7)	0	0.2083(8)	0.105(5)	0.080(5)	0.072(4)	0	0.068(4)	0
Cl(1)	4i	0.2145(1)	½	0.7805(2)	0.0606(8)	0.0461(7)	0.088(1)	0	0.0509(8)	0

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