Crystal structure of nitratodi(1,3-propanediamine)cobalt(II) mononitrate monohydrate, $[Co(C_3H_{10}N_2)_2(NO_3)]NO_3 \cdot H_2O$

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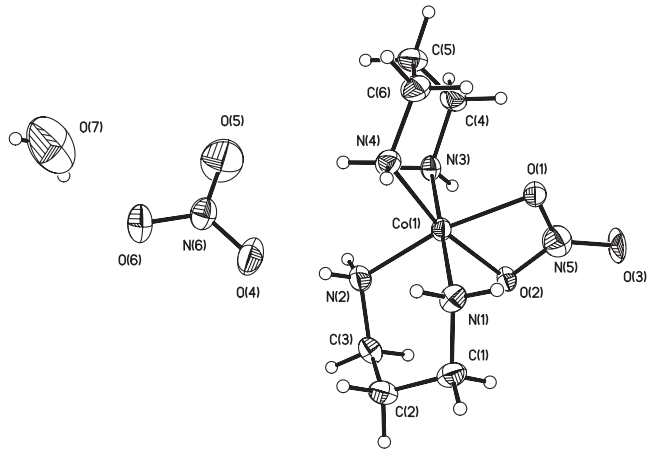

Abstract

$C_6H_{22}CoN_6O_7$, monoclinic, $P12_1/c1$ (No. 14), a = 8.76(1) Å, b = 10.22(1) Å, c = 15.83(2) Å, β = 93.45(2)°, V = 1414.3 Å^3, Z = 4, $R_{gt}(F)$ = 0.053, $wR_{ref}(F^2)$ = 0.131, T = 293 K.

Source of material

0.4256 g $Co(NO_3)_2 \cdot 6H_2O$ (1.460 mmol) and 0.2172 g 1,3-propanediamine (2.93 mmol) were dissolved in 15 ml H_2O. Orange single crystals were obtained after the solution was allowed to stand at room temperature for about three weeks.

Discussion

The structure of the title complex consists of divalent cobalt cation coordinated by two 1,3-propanediamine neutral molecules and one nitrate anion. The cobalt cation is bounded to four N atoms from the two 1,3-propanediamine molecules and two O atoms from a nitrate. The two six-membered rings were constructed by the coordination of 1,3-propanediamine molecules to cobalt cation, while a four-membered ring was formed through the chelated coordination of the nitrate anion to the divalent cobalt cation. The bond distances of Co—N range from 1.945(4) Å to 1.957(4) Å, and the Co—O bond distances are 1.913(3) Å and 1.918(3) Å and compared with the analogous complexes the present Co—O bond distances are short ones [1-3]. The distance of Co1—N5 is 2.326(5) Å, which indicates that there also exists a certain of valence between the cobalt cation and the nitrogen atom. The Co—N bond distances is also shorter than that of the complexes mentioned above. The angles of N–Co–N are in the range from 89.4(1)° to 179.4(1)° and the angles dealing with N–Co–O range from 89.5(1)° to 167.5(1)°, while the angle of O–Co–O is 68.7(1)°. The angles of nitrate anions are 124.9(4)°, 124.2(4)° and 110.9(4)° for coordinated nitrate anion, whereas the angles of the uncoordinated nitrate anions are 120.7(5)°, 121.0(5)° and 118.3(5)°. Obviously, the chelated coordination mode of the nitrate anion makes the O–N–O angle be compressed. The bond distances and the angles indicate that the divalent cobalt cation is located in a distorted octahedral environment. The complex cations pile up along the c axis to form one-dimensional chains and hydrogen bondings which are from the complex cations, uncoordinated nitrate anions and the uncoordinated water molecules make them connect to each other to form the crystal structure.

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Table 1. Data collection and handling.

Crystal:	orange prism, size 0.07 × 0.28 × 0.37 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	12.55 cm^{-1}
Diffractometer, scan mode:	Bruker SMART CCD, φ/ω
$2\theta_{max}$:	52.82°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	6322, 2842
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 1871
$N(param)_{refined}$:	181
Programs:	SHELXS-97 [4] SHELXL-97 [5]

Table 2. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	x	y	z	U_{iso}
H(1A)	4*e*	1.1058	0.8202	0.2491	0.048
H(1B)	4*e*	1.0327	0.6952	0.2308	0.048
H(2A)	4*e*	0.8889	0.6334	0.0789	0.060
H(2B)	4*e*	0.8674	0.7225	0.0077	0.060
H(3A)	4*e*	0.8207	0.9872	0.0196	0.043
H(3B)	4*e*	0.7190	0.8763	0.0264	0.043
H(4A)	4*e*	0.7067	0.7204	0.1608	0.050
H(4B)	4*e*	0.7990	0.7355	0.2395	0.050
H(1C)	4*e*	1.2846	0.6798	0.2113	0.056
H(1D)	4*e*	1.2671	0.7925	0.1442	0.056
H(2C)	4*e*	1.1300	0.5453	0.1246	0.065
H(2D)	4*e*	1.2753	0.5889	0.0789	0.065
H(3C)	4*e*	1.1270	0.7473	0.0038	0.059
H(3D)	4*e*	1.0708	0.6042	–0.0168	0.059
H(4C)	4*e*	0.5959	1.0656	0.0518	0.056
H(4D)	4*e*	0.7133	1.0897	0.1291	0.056
H(5A)	4*e*	0.5041	0.8799	0.1172	0.063
H(5B)	4*e*	0.4865	1.0026	0.1751	0.063
H(6A)	4*e*	0.7022	0.9388	0.2591	0.060
H(6B)	4*e*	0.5760	0.8299	0.2579	0.060
H(1)	4*e*	0.4199	0.2895	–0.0030	0.080
H(2)	4*e*	0.3320	0.2216	0.0608	0.080

Table 3. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	*x*	*y*	*z*	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Co(1)	4*e*	0.92306(6)	0.85165(5)	0.13210(3)	0.0325(3)	0.0256(3)	0.0352(3)	–0.0038(3)	0.0008(2)	–0.0001(2)
N(1)	4*e*	1.0770(4)	0.7644(4)	0.2070(2)	0.039(2)	0.040(2)	0.039(2)	–0.003(2)	–0.000(2)	0.011(2)
N(2)	4*e*	0.9283(4)	0.7040(4)	0.0540(2)	0.043(2)	0.039(2)	0.067(3)	0.001(2)	–0.009(2)	–0.015(2)
N(3)	4*e*	0.7709(4)	0.9384(3)	0.0565(2)	0.041(2)	0.028(2)	0.038(2)	–0.004(2)	0.001(2)	0.002(2)
N(4)	4*e*	0.7578(4)	0.7790(4)	0.1942(2)	0.036(2)	0.038(2)	0.051(2)	–0.002(2)	0.005(2)	0.005(2)
N(5)	4*e*	1.0615(5)	1.0457(5)	0.1439(3)	0.066(3)	0.059(3)	0.057(3)	0.001(3)	–0.003(2)	0.000(2)
N(6)	4*e*	0.6752(5)	0.4486(5)	0.1383(2)	0.051(3)	0.047(3)	0.047(2)	–0.009(2)	–0.003(2)	0.007(2)
O(1)	4*e*	0.9545(3)	1.0113(3)	0.1944(2)	0.040(2)	0.038(2)	0.034(2)	–0.008(1)	0.011(1)	–0.005(1)
O(2)	4*e*	1.0806(3)	0.9552(3)	0.0868(2)	0.043(2)	0.029(2)	0.031(1)	–0.006(1)	0.006(1)	–0.005(1)
O(3)	4*e*	1.1308(4)	1.1507(3)	0.1485(2)	0.076(3)	0.033(2)	0.082(2)	–0.035(2)	0.025(2)	–0.018(2)
O(4)	4*e*	0.8047(5)	0.4832(4)	0.1592(3)	0.057(3)	0.058(2)	0.113(3)	–0.021(2)	–0.012(2)	–0.004(2)
O(5)	4*e*	0.5801(6)	0.5334(5)	0.1176(3)	0.089(4)	0.098(4)	0.150(4)	0.015(3)	–0.035(3)	0.034(3)
O(6)	4*e*	0.6397(5)	0.3352(4)	0.1410(3)	0.081(3)	0.045(3)	0.126(4)	–0.023(2)	0.021(3)	–0.007(2)
O(7)	4*e*	0.3664(8)	0.2804(6)	0.0431(4)	0.176(5)	0.140(5)	0.211(5)	0.021(4)	–0.111(5)	–0.074(5)
C(1)	4*e*	1.2156(5)	0.7183(5)	0.1680(3)	0.033(3)	0.052(3)	0.055(3)	0.003(2)	0.000(2)	0.006(2)
C(2)	4*e*	1.1801(6)	0.6197(5)	0.1001(3)	0.044(3)	0.044(3)	0.075(3)	0.011(2)	0.009(3)	–0.002(3)
C(3)	4*e*	1.0802(6)	0.6703(5)	0.0272(3)	0.054(3)	0.038(3)	0.056(3)	0.002(2)	0.006(2)	–0.012(2)
C(4)	4*e*	0.6597(5)	1.0226(5)	0.0957(3)	0.044(3)	0.041(3)	0.053(3)	0.012(2)	–0.002(2)	0.000(2)
C(5)	4*e*	0.5604(5)	0.9443(5)	0.1517(3)	0.042(3)	0.051(3)	0.064(3)	0.011(3)	0.010(2)	–0.002(3)
C(6)	4*e*	0.6479(5)	0.8745(5)	0.2236(3)	0.044(3)	0.055(3)	0.053(3)	–0.003(2)	0.015(2)	0.002(2)

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