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Crystal structure of diaqua-bis(2-bromo-4-chloro-6-formylphenolato- $\kappa^2 O, O'$)cobalt(II), $C_{16}H_{16}Cl_2CrN_3O_7$

<https://doi.org/10.1515/ncrs-2017-0240>

Received June 7, 2018; accepted August 9, 2018; available online September 1, 2018

Abstract

$C_{16}H_{10}Br_2Cl_2CoO_6$, monoclinic, $P2_1/c$ (no. 14), $a = 7.578(2)$ Å, $b = 27.729(11)$ Å, $c = 8.634(2)$ Å, $\beta = 101.36(3)^\circ$, $V = 1778.8(10)$ Å³, $Z = 4$, $R_{gt}(F) = 0.0668$, $wR_{ref}(F^2) = 0.1452$, $T = 293(2)$ K.

CCDC no.: 1846664

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 materials

3-Bromo-5-chlorosalicylaldehyde (1 mmol, 2.35 mg) was dissolved in 2:1 ethanol/methanol mixture (30 mL) to obtain a colorless solution. Then, $Co(Ac)_2 \cdot 4H_2O$ (0.249 g, 1 mmol) was slowly added to the above solution and kept stirring at room temperature for 2 h to afford a clear reddish brown solution. After this, the filtrate was sealed in a beaker and kept undisturbed at room temperature. The brown block crystals of title compound were formed after one week.

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Table 1: Crystal collection and handling.

Crystal:	Block, brown
Size:	$0.10 \times 0.12 \times 0.26$ mm
Wavelength:	Mo $K\alpha$ radiation ($\lambda = 0.71073$ Å)
μ :	5.786 mm^{-1}
Diffractometer, scan mode:	Xcalibur, Φ and ω -scans
$\theta_{\max}$, completeness:	25° , $>99\%$
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	9450, 3115, 0.1022
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2\sigma(I_{\text{obs}})$, 1764
$N(\text{param})_{\text{refined}}$:	228
Programs:	CrysAlis ^{PRO} [1], OLEX2 [2], SHELX [3]

Experimental details

Hydrogen atoms were placed in calculated positions and included in the refinement in the riding model approximation, with $U_{\text{iso}}(\text{H})$ set to $1.2U_{\text{eq}}(\text{C})$. The H atoms attached to water were found in the electron density map and fixed with the U_{iso} values of the hydrogen atoms of water molecules set to $1.5U_{\text{eq}}(\text{O})$.

Comment

Cobalt complexes have received much attention owing to their potential applications in many fields such as artificial photosynthesis, magnetic material, biotechnology [4–8]. To date, considerable progress has been made by developing various ligands to construct new cobalt complexes including pyridine, carboxylates, Schiff base etc. [9–12]. However, related research involving halogenated salicylic aldehyde ligands is rare. Hence, we selected 3-bromo-5-chlorosalicylaldehyde and cobalt acetate as starting material, and isolated a new cobalt-base complex $[Cr(C_{16}H_{16}Cl_2N_2O_2)(H_2O)_2] \cdot NO_3$. To the best of our knowledge, the title compound also represents the first coordination compound constructed from 3-bromo-5-chlorosalicylaldehyde.

The crystal structure of title compound consists of one mononuclear cobalt(II) complex. The center Co(II) atom lies on the inversion center of the whole complex (*cf.* the figure). The equatorial sites are chelated by four oxygen atoms from two 3-bromo-5-chlorosalicylaldehyde ligands. The average bond length of Co–O is 2.06 Å. The bond distance between

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

Atom	x	y	z	<i>U</i> _{iso} */ <i>U</i> _{eq}
Co1	0.21392(11)	0.52086(4)	0.84194(11)	0.0298(3)
Br1	0.38231(11)	0.56600(4)	1.41362(10)	0.0521(3)
Br2	0.24357(12)	0.36696(4)	1.15597(10)	0.0533(3)
Cl1	0.5372(3)	0.74846(10)	1.2240(3)	0.0693(8)
Cl2	−0.0539(3)	0.27386(11)	0.6037(4)	0.0894(10)
O1	0.2546(6)	0.5537(2)	1.0591(6)	0.0381(15)
O2	0.2391(6)	0.4513(2)	0.9276(5)	0.0360(14)
O3	0.1809(6)	0.4916(2)	0.6191(6)	0.0385(15)
O4	0.1787(6)	0.5900(2)	0.7457(5)	0.0367(15)
O5	−0.0679(5)	0.5182(2)	0.8167(5)	0.0375(15)
H5A	−0.0998	0.4893	0.8295	0.056
H5B	−0.0993	0.5361	0.8864	0.056
O6	0.4861(5)	0.5267(2)	0.8310(5)	0.0406(15)
H6A	0.5158	0.5036	0.7755	0.061
H6B	0.5035	0.5536	0.7876	0.061
C1	0.3083(8)	0.5975(3)	1.0914(9)	0.033(2)
C2	0.3818(9)	0.6112(3)	1.2521(9)	0.037(2)
C3	0.4481(9)	0.6571(4)	1.2879(10)	0.047(3)
H3	0.4956	0.6650	1.3925	0.056
C4	0.4457(10)	0.6921(3)	1.1706(9)	0.041(2)
C5	0.3713(9)	0.6813(3)	1.0218(9)	0.041(2)
H5	0.3604	0.7051	0.9448	0.049
C6	0.3092(9)	0.6347(3)	0.9791(8)	0.033(2)
C7	0.2345(9)	0.6272(3)	0.8127(9)	0.040(2)
H7	0.2285	0.6544	0.7490	0.048
C8	0.1811(8)	0.4122(3)	0.8546(9)	0.032(2)
C9	0.1262(9)	0.4097(3)	0.6866(9)	0.038(2)
C10	0.0586(10)	0.3652(3)	0.6152(10)	0.049(3)
H10	0.0232	0.3642	0.5058	0.059
C11	0.0434(11)	0.3252(3)	0.6967(11)	0.053(3)
C12	0.0962(10)	0.3259(3)	0.8591(10)	0.051(3)
H12	0.0851	0.2985	0.9184	0.061
C13	0.1659(9)	0.3680(3)	0.9322(8)	0.034(2)
C14	0.1379(9)	0.4497(3)	0.5846(9)	0.037(2)
H14	0.1089	0.4430	0.4770	0.045

the Co(II) atom and the phenolic O atom is longer than that between the Co(II) atom and the aldehyde O atom.

In the apical the Co^{II} center is coordinated with two oxygen atoms from two water ligands. The bond lengths of Co—O(1) is 2.46 Å and Co—O(3) is 2.20 Å, respectively. In the stacking arrangement, adjacent complexes are pairwise linked to each other *via* O—H···O hydrogen bonds between apical water molecule (O3) and adjacent phenoxy oxygen (O2) atoms to form a dimer.

Acknowledgements: This work was supported by the National Science Foundation of China (Nos. 31760257, 21761017), the agricultural plastic film and products research and development of Plateau area (No. DH1606), the Joint

Research Projects of Yunnan province of Local of institutions (partial) of higher education (2017FH001–002) and the Kunming University Chemistry and Chemical engineering students' science and technology innovation project HXHG1808.

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