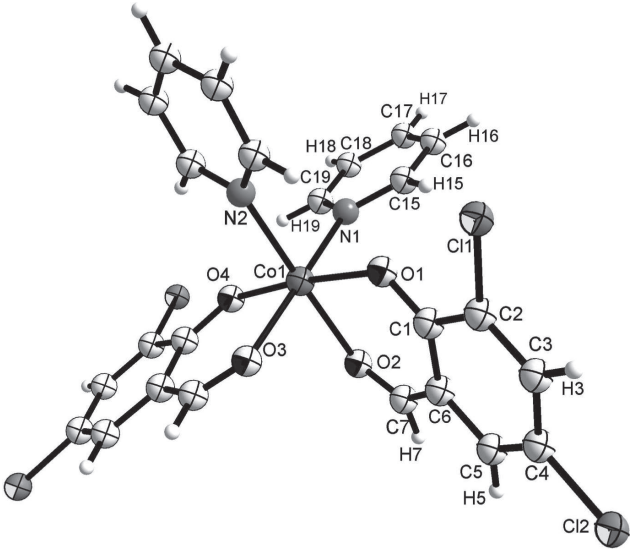
Open Access

Qiong Su and Yan-Bin Wang*

Crystal structure of bis(pyridine)-bis(2-formyl-4,6-dichlorophenolato)cobalt(II), $C_{24}H_{16}Cl_4CoN_2O_4$



DOI 10.1515/ncrs-2016-0386
Received January 3, 2017; accepted June 16, 2017; available online July 14, 2017

Abstract

$C_{24}H_{16}Cl_4CoN_2O_4$, triclinic, $P\bar{1}$, (no. 2) $a = 8.6148(13)$ Å, $b = 12.2201(16)$ Å, $c = 13.4807(16)$ Å, $\alpha = 115.198(12)°$, $\beta = 101.596(11)°$, $\gamma = 96.518(12)°$, $V = 1225.8(3)$ Å^3, $Z = 2$, $R_{gt}(F) = 0.0524$, $wR_{ref}(F^2) = 0.1109$, $T = 173(1)$ K.

CCDC no.: 1523793

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

***Corresponding author: Yan-Bin Wang,** College of Chemical Engineering, Northwest University for Nationalities, Lanzhou 730030, P. R. China; and Key Laboratory for Utifity of Environment-friendly Composite, Materials and Biomass in Universities of Gansu Province, Lanzhou 730030, P. R. China, e-mail: ybwang@126.com
Qiong Su: College of Chemical Engineering, Northwest University for Nationalities, Lanzhou 730030, P. R. China; and Key Laboratory for Utifity of Environment-friendly Composite, Materials and Biomass in Universities of Gansu Province, Lanzhou 730030, P. R. China

Table 1: Data collection and handling.

Crystal:	Violet block
Size:	0.25 × 0.23 × 0.21 mm
Wavelength:	Mo $K\alpha$ radiation (0.71073 Å)
μ:	11.7 cm^{-1}
Diffractometer, scan mode:	SuperNova Dual, ω scans
$2\theta_{max}$, completeness:	52°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	8572, 4822, 0.044
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 3276
$N(param)_{refined}$:	316
Programs:	SHELX [1], CrysAlis^{PRO} [2]

Source of materials

A solution of cobalt(II) acetate tetrahydrate (0.01 mmol) in acetone (2 mL) was added dropwise to a solution of 2-formyl-4,6-dichlorophenol (0.01 mmol) in chloroform (2 mL) at room temperature. The color of the mixing solution turned to brown immediately, then 1 mL pyridine was added and stirred for 1 h at room temperature. The mixture was filtered off, and the filtrate was allowed to stand at room temperature for one week to form violet block crystals suitable for X-ray crystallographic analysis (yield 78.0%, **m.p.** 477–478 K). **Elemental analysis**-Anal. calcd. for $C_{24}H_{16}Cl_4CoN_2O_4$: C, 48.27%; H, 2.70%; N, 4.69%; Co, 9.87%; Found: C, 48.31%; H, 2.68%; N, 4.72%; Co, 9.89%.

Experimental details

Hydrogen atoms were placed in their geometrically idealized positions and constrained to ride on their parent atoms.

Comment

Salicylaldehyde derivatives play an important role in the modern coordination chemistry [3–7]. In general, they can act as bridging bidentate ligands *via* the phenolic oxygen and formyl group oxygen atoms to build coordination networks [8] as well as interlink the one-dimensional or two-dimensional molecules into frameworks *via* the hydrogen bonds [9, 10] or π-π stacking interactions [11–13].

The title compound consists of a mononuclear cobalt(II) complex. The Co centre is hexa-coordinated with a distorted octahedral geometry. Bond lengths and angles are in the expected ranges.

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

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
Co1	0.32944(7)	0.47584(4)	0.24647(4)	0.02622(16)
Cl4	0.19575(14)	0.13685(9)	−0.13505(8)	0.0397(3)
Cl1	0.39082(16)	0.79832(9)	0.62842(8)	0.0492(3)
Cl2	0.86342(15)	1.09512(9)	0.59419(10)	0.0528(3)
Cl3	0.78793(17)	0.03394(10)	−0.06078(10)	0.0600(4)
O4	0.3144(3)	0.3253(2)	0.10052(19)	0.0306(7)
O1	0.3618(3)	0.6353(2)	0.38993(18)	0.0265(6)
O2	0.4366(3)	0.5898(2)	0.18370(19)	0.0306(7)
O3	0.5678(3)	0.4619(2)	0.3077(2)	0.0346(7)
N2	0.2276(4)	0.3698(3)	0.3190(2)	0.0301(8)
N1	0.0886(4)	0.4832(3)	0.1736(2)	0.0277(8)
C15	0.0240(5)	0.5759(4)	0.2328(3)	0.0373(11)
H15	0.0841	0.6336	0.3064	0.045*
C6	0.5571(5)	0.7703(3)	0.3643(3)	0.0240(9)
C7	0.5249(5)	0.6946(3)	0.2438(3)	0.0301(9)
H7	0.5771	0.7288	0.2061	0.036*
C5	0.6773(5)	0.8816(3)	0.4152(3)	0.0324(10)
H5	0.7343	0.9016	0.3712	0.039*
C14	0.4209(5)	0.2647(3)	0.0697(3)	0.0254(9)
C9	0.5801(5)	0.2850(3)	0.1405(3)	0.0266(9)
C8	0.6380(5)	0.3844(3)	0.2559(3)	0.0330(10)
H8	0.7425	0.3901	0.2959	0.040*
C19	−0.0022(5)	0.3995(3)	0.0678(3)	0.0291(9)
H19	0.0392	0.3330	0.0255	0.035*
C2	0.5037(5)	0.8271(3)	0.5460(3)	0.0283(9)
C1	0.4686(5)	0.7362(3)	0.4293(3)	0.0240(9)
C13	0.3870(5)	0.1653(3)	−0.0440(3)	0.0306(10)
C11	0.6469(6)	0.1195(3)	−0.0104(3)	0.0357(10)
C4	0.7097(5)	0.9594(3)	0.5281(3)	0.0313(10)
C3	0.6222(5)	0.9339(3)	0.5943(3)	0.0327(10)
H3	0.6438	0.9891	0.6713	0.039*
C12	0.4947(6)	0.0964(3)	−0.0827(3)	0.0357(11)
H12	0.4664	0.0337	−0.1575	0.043*
C18	−0.1538(5)	0.4091(3)	0.0201(3)	0.0327(10)
H18	−0.2128	0.3503	−0.0535	0.039*
C16	−0.1261(6)	0.5899(4)	0.1904(4)	0.0452(12)
H16	−0.1665	0.6558	0.2347	0.054*
C24	0.1448(6)	0.2527(3)	0.2521(3)	0.0418(11)
H24	0.1445	0.2168	0.1758	0.050*
C10	0.6901(5)	0.2114(3)	0.0999(3)	0.0352(10)
H10	0.7920	0.2254	0.1482	0.042*
C22	0.0597(6)	0.2312(4)	0.3980(4)	0.0465(13)
H22	0.0013	0.1860	0.4246	0.056*
C23	0.0604(6)	0.1820(4)	0.2882(4)	0.0508(13)
H23	0.0043	0.1009	0.2373	0.061*
C17	−0.2173(5)	0.5059(4)	0.0817(3)	0.0421(11)
H17	−0.3192	0.5145	0.0509	0.051*
C20	0.2281(7)	0.4136(4)	0.4261(3)	0.0648(17)
H20	0.2876	0.4939	0.4765	0.078*
C21	0.1461(8)	0.3485(4)	0.4691(4)	0.077(2)
H21	0.1502	0.3848	0.5460	0.093*

References

1. Sheldrick, G. M.: A short history of SHELX. Acta Crystallogr. **A64** (2008) 112–122.
2. Oxford Diffraction Ltd., CrysAlis^{PRO}, Abingdon, Oxfordshire, England (2006).
3. Dong, W. K.; Zhang, X. Y.; Sun, Y. X.; Dong, X. Y.; Li, G.; Wang, J.: A 2D supramolecular copper(II) complex with an asymmetric Salamo-type ligand: synthesis, crystal structure, and fluorescent property. Synth. React. Inorg. Met.-Org. Nano-Met. Chem. **45** (2015) 956–962.
4. Song, X. Q.; Xiao, Z. R.; Zhao, M. M.; Qian, W. H.: Two coordination polymers with the ligand salicylamide: synthesis, crystal structure and luminescent properties. Z. Anorg. Allg. Chem. **640** (2014) 1769–1775.
5. Sun, Y. X.; Zhang, S. T.; Ren, Z. L.; Dong, X. Y.; Wang, L.: Synthesis, characterization and crystal structure of a new supramolecular Cd(II) complex with halogen substituted Salen-type bisoxime. Synth. React. Inorg. Met.-Org. Nano-Met. Chem. **43** (2013) 995–1000.
6. Dong, W. K.; Ma, J. C.; Dong, Y. J.; Zhu, L. C.; Zhang, Y.: Di- and tetranuclear heterometallic 3d-4f cobalt(II)-lanthanide(III) complexes derived from a hexadentate bisoxime: syntheses, structures and magnetic properties. Polyhedron **115** (2016) 228–235.
7. Dong, W. K.; Ma, J. C.; Zhu, L. C.; Sun, Y. X.; Akogun, S. F.; Zhang, Y.: A series of heteromultinuclear zinc(II)-lanthanide(III) complexes based on 3-MeOsalamo: syntheses, structural characterizations, and luminescent properties. Cryst. Growth Des. **16** (2016) 6903–6914.
8. Li, B. Y.; Tong, J. F.; Dong, W. K.; Yao, J.; Wu, J. C.: Bis(*N*,*N*-dimethylformamide)bis(2,4,6-trinitrophenolato) copper(II). Acta Crystallogr. **E65** (2009) m1.
9. Wang, P.; Zhao, L.: An infinite 2D supramolecular cobalt(II) complex based on an asymmetric Salamo-type ligand: synthesis, crystal structure, and spectral properties. Synth. React. Inorg. Met.-Org. Nano-Met. Chem. **46** (2016) 1095–1101.
10. Dong, W. K.; Zhu, L. C.; Dong, Y. J.; Ma, J. C.; Zhang, Y.: Mono, di and heptanuclear metal(II) complexes based on symmetric and asymmetric tetradentate Salamo-type ligands: syntheses, structures and spectroscopic properties. Polyhedron **117** (2016) 148–154.
11. Dong, W. K.; Zhang, L. S.; Sun, Y. X.; Zhao, M. M.; Li, G.; Dong, X. Y.: Synthesis, crystal structure and spectroscopic properties of a supramolecular zinc(II) complex with N_2O_2 coordination sphere. Spectrochim. Acta **A121** (2014) 324–329.
12. Dong, W. K.; Sun, Y. X.; Zhao, C. Y.; Dong, X. Y.; Xu, L.: Synthesis, structure and properties of supramolecular Mn(II), Co(II), Ni(II) and Zn(II) complexes containing Salen-type bisoxime ligands. Polyhedron **29** (2010) 2087–2097.
13. Dong, W. K.; Zhang, J. T.; Dong, Y. J.; Zhang, Y.; Wang, Z. K.: Construction of mononuclear copper(II) and trinuclear cobalt(II) complexes based on asymmetric Salamo-type ligands. Z. Anorg. Allg. Chem. **642** (2016) 189–196.