Crystal structure of bis(cyclopropyl-4-bromosalicylaldiminato)cobalt(II), $Co(C_{20}H_{18}BrNO)_2$

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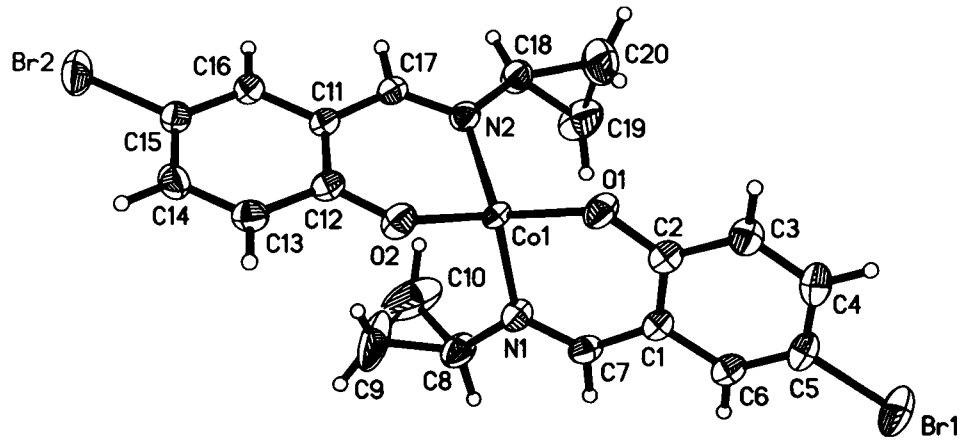
Received June 8, 2006, accepted and available on-line August 5, 2006; CCDC no. 1267/1813



Abstract

$C_{20}H_{18}Br_2CoN_2O_2$, orthorhombic, *Pbca* (no. 61), a = 13.295(2) Å, b = 13.113(2) Å, c = 23.252(3) Å, V = 4053.7 Å^3, Z = 8, $R_{gt}(F)$ = 0.051, $wR_{ref}(F^2)$ = 0.151, T = 298 K.

Source of material

Reagents and solvents used were of commercially available quality. 5-Bromosalicylaldehyde (201.3 mg, 1.0 mmol), cyclopropylamine (57.2 mg, 1.0 mmol) and $Co(CH_3COO)_2 \cdot 6H_2O$ (142.6 mg, 0.5 mmol) were stirred and refluxed in ethanol at about 351 K for 30 min to give a red solution. Red block-shaped crystals, suitable for X-ray structural determination were formed by slow evaporation of the solution in dark for about a week.

Elemental analysis – found: C, 44.89 %; H, 3.45 %; N, 5.13 %; calc. for $C_{20}H_{18}Br_2CoN_2O_2$: C, 44.72 %; H, 3.38 %; N, 5.22 %.

Experimental details

The large ADP anisotropy for the C9 and C10 atoms is due to the disorder of the C8/C9/C10 cyclopropane ring.

Discussion

Cobalt complexes of Schiff bases have been extensively studied. They play an important role in both synthetic and structural research [1-3]. Recent research show that certain cobalt complexes are potent antiviral reagents [4]. Herein we report the synthesis and crystal structure of a cobalt(II) complex derived from the Schiff base 4-bromo-2-(cyclopropyliminomethyl)phenol. The Co^{II} atom in the title complex is four-coordinated by two O and two N atoms from two Schiff base ligands, forming a tetrahedral coordination. All the bond lengths and angles subtended at the Co center are comparable to the corresponding values observed in other Schiff base cobalt complexes [5-7].

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Table 1. Data collection and handling.

Crystal:	red block, size 0.17 × 0.18 × 0.23 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	48.07 cm^{-1}
Diffractometer, scan mode:	Siemens P4, ω
$2\theta_{max}$:	54°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	32106, 4416
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 2873
$N(param)_{refined}$:	244
Program:	SHELXTL [8]

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

Atom	Site	x	y	z	U_{iso}
H(3)	8c	0.2653	0.2022	0.0673	0.065
H(4)	8c	0.3488	0.0879	0.0103	0.073
H(6)	8c	0.3315	−0.1225	0.1325	0.061
H(7)	8c	0.2635	−0.0925	0.2206	0.059
H(8)	8c	0.1969	−0.1098	0.3046	0.081
H(9A)	8c	0.1516	0.0832	0.3576	0.181
H(9B)	8c	0.1702	−0.0239	0.3920	0.181
H(10A)	8c	0.0132	0.0084	0.3079	0.185
H(10B)	8c	0.0318	−0.0988	0.3423	0.185
H(13)	8c	0.2207	0.3138	0.3993	0.061
H(14)	8c	0.1165	0.3697	0.4714	0.066
H(16)	8c	−0.1229	0.3199	0.3718	0.055
H(17)	8c	−0.1128	0.2553	0.2824	0.051
H(18)	8c	−0.1468	0.1746	0.2041	0.069
H(19A)	8c	0.0101	0.0338	0.1711	0.118
H(19B)	8c	−0.1072	0.0267	0.1506	0.118
H(20A)	8c	−0.0936	0.1898	0.1069	0.118
H(20B)	8c	0.0239	0.1969	0.1274	0.118

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)	8c	0.14002(4)	0.16039(4)	0.23959(3)	0.0312(3)	0.0279(3)	0.0409(4)	0.0032(2)	0.0059(3)	–0.0042(2)
Br(1)	8c	0.41091(6)	–0.12480(6)	0.01803(3)	0.1057(6)	0.0730(5)	0.0843(6)	0.0039(4)	0.0392(4)	–0.0271(4)
Br(2)	8c	–0.10138(6)	0.39344(7)	0.48750(3)	0.0908(5)	0.1022(6)	0.0502(4)	0.0092(4)	0.0141(3)	–0.0187(4)
O(1)	8c	0.2092(3)	0.1855(3)	0.1696(2)	0.064(2)	0.039(2)	0.063(2)	0.008(2)	0.020(2)	0.000(2)
O(2)	8c	0.1780(2)	0.2500(3)	0.3011(2)	0.043(2)	0.054(2)	0.063(2)	–0.000(2)	0.002(2)	–0.014(2)
N(1)	8c	0.1860(3)	0.0161(3)	0.2512(2)	0.050(2)	0.041(2)	0.054(3)	0.002(2)	0.012(2)	0.001(2)
N(2)	8c	–0.0071(3)	0.1938(3)	0.2403(2)	0.043(2)	0.043(2)	0.048(2)	0.004(2)	–0.003(2)	–0.008(2)
C(1)	8c	0.2695(3)	0.0127(4)	0.1574(2)	0.040(3)	0.040(3)	0.049(3)	0.000(2)	0.004(2)	–0.005(2)
C(2)	8c	0.2515(3)	0.1142(4)	0.1375(3)	0.041(3)	0.042(3)	0.055(3)	–0.003(2)	0.003(2)	–0.004(2)
C(3)	8c	0.2799(4)	0.1377(4)	0.0817(3)	0.060(3)	0.048(3)	0.055(3)	–0.004(2)	0.009(3)	0.000(3)
C(4)	8c	0.3285(4)	0.0692(5)	0.0471(3)	0.062(4)	0.070(4)	0.050(3)	–0.011(3)	0.015(3)	–0.008(3)
C(5)	8c	0.3476(4)	–0.0284(4)	0.0673(2)	0.056(3)	0.055(3)	0.055(3)	–0.001(3)	0.015(3)	–0.016(3)
C(6)	8c	0.3188(4)	–0.0564(4)	0.1201(2)	0.047(3)	0.045(3)	0.061(4)	0.004(2)	0.003(3)	–0.006(3)
C(7)	8c	0.2404(4)	–0.0273(4)	0.2121(2)	0.045(3)	0.043(3)	0.058(3)	0.009(2)	0.003(2)	0.003(2)
C(8)	8c	0.1641(5)	–0.0430(4)	0.3022(3)	0.084(4)	0.051(3)	0.068(4)	0.021(3)	0.027(3)	0.015(3)
C(9)	8c	0.147(1)	0.0094(7)	0.3572(4)	0.30(2)	0.075(6)	0.073(6)	0.068(8)	0.101(9)	0.024(4)
C(10)	8c	0.0608(8)	–0.0370(9)	0.3264(5)	0.134(9)	0.131(9)	0.20(1)	0.064(7)	0.105(9)	0.091(9)
C(11)	8c	0.0084(3)	0.2807(3)	0.3332(2)	0.039(3)	0.036(2)	0.044(3)	0.004(2)	0.001(2)	–0.002(2)
C(12)	8c	0.1133(4)	0.2801(4)	0.3407(2)	0.044(3)	0.036(3)	0.052(3)	0.003(2)	0.001(2)	–0.001(2)
C(13)	8c	0.1515(4)	0.3141(4)	0.3934(2)	0.048(3)	0.043(3)	0.061(4)	0.000(2)	–0.013(3)	–0.005(2)
C(14)	8c	0.0893(5)	0.3481(4)	0.4367(2)	0.074(4)	0.047(3)	0.044(3)	0.002(3)	–0.014(3)	–0.006(2)
C(15)	8c	–0.0140(4)	0.3500(4)	0.4284(2)	0.056(3)	0.045(3)	0.042(3)	0.006(2)	0.003(2)	0.001(2)
C(16)	8c	–0.0537(4)	0.3175(4)	0.3773(2)	0.049(3)	0.043(3)	0.044(3)	0.005(2)	0.002(2)	–0.001(2)
C(17)	8c	–0.0440(4)	0.2429(3)	0.2836(2)	0.040(3)	0.040(3)	0.047(3)	0.006(2)	0.003(2)	–0.001(2)
C(18)	8c	–0.0754(4)	0.1622(4)	0.1965(3)	0.047(3)	0.068(4)	0.056(4)	0.006(3)	–0.006(3)	–0.018(3)
C(19)	8c	–0.0516(6)	0.0699(6)	0.1623(4)	0.088(5)	0.084(5)	0.121(7)	0.012(4)	–0.030(5)	–0.059(5)
C(20)	8c	–0.0431(7)	0.1709(7)	0.1351(3)	0.110(6)	0.120(7)	0.064(5)	0.007(5)	–0.015(4)	–0.030(5)

Acknowledgment. The authors thank the Education Office of Anhui Province, P. R. China, for research grant (no. 2004kj326).

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