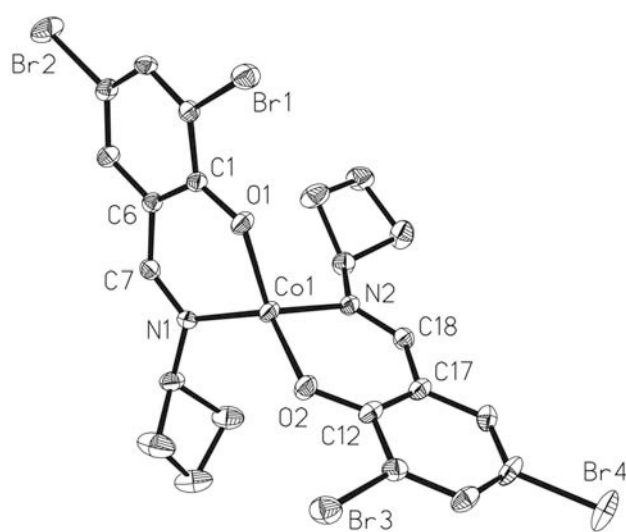


Crystal structure of bis(3,5-dibromo-*N*-cyclobutylsalicylaldiminato)-cobalt(II), Co(C₁₁H₁₀Br₂NO)₂

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Abstract

C₂₂H₂₀Br₄CoN₂O₂, triclinic, *P* $\bar{1}$ (no. 2), *a* = 8.088(1) Å, *b* = 12.299(2) Å, *c* = 12.796(2) Å, α = 93.166(8)°, β = 108.219(7)°, γ = 95.718(8)°, *V* = 1198.0 Å³, *Z* = 2, *R*_{gt}(*F*) = 0.037, *wR*_{ref}(*F*²) = 0.088, *T* = 296 K.

Source of material

3,5-Dibromosalicylaldehyde (56 mg, 0.2 mmol) and cyclobutylamine (14 mg, 0.2 mmol) were dissolved in an aqueous acetonitrile solution (5 mL). The mixture was stirred for 5 min to give an orange solution, which was added to a methanol solution (1 mL) of Co(NO₃)₂ · 6H₂O (28 mg, 0.1 mmol). The mixture was stirred for another 5 min at room temperature to give a red solution and then filtered. The filtrate was kept in air for 5 d, forming red block-shaped crystals. The crystals were isolated, washed three times with distilled water and dried in a vacuum desiccator containing anhydrous CaCl₂ (yield 75 %). All reagents and solvents were used as obtained without further purification.

Experimental details

All H atoms were positioned geometrically with *d*(C—H) = 0.93–0.98 Å, and refined as riding with *U*_{iso}(H) = 1.2 *U*_{eq}(C).

Discussion

Transition metal complexes of Schiff-base ligands have been extensively investigated in the past decades due to their novel structures and potential applications in many fields [1–6].

The title crystal structure contains the mononuclear cobalt(II) complexes. In the molecule, cobalt(II) atom is in a distorted tetrahedral manner four-coordinated by two N atom and two O atoms from two independent Schiff base ligands. The average bond lengths of Co1—O and Co1—N are 1.907(3) and 1.992(3) Å, respectively. The angles subtended at the Co(II) ion of the distorted tetrahedral geometry (CoN₂O₂) are in the range 95.1(4)°–123.5(4)°. The dihedral angle between the six-membered rings Co1/O1/C1/C6/C7/N1 and Co1/O2/C12/C17/C18/N2 is 89.0(2)°. Some weak interactions play an important role in the crystal structure of the title complex.

Table 1. Data collection and handling.

Crystal:	red block, size 0.22 × 0.30 × 0.40 mm
Wavelength:	Mo <i>K</i> _α radiation (0.71073 Å)
μ :	74.09 cm ^{−1}
Diffractometer, scan mode:	Bruker SMART Apex CCD, φ/ω
2 θ _{max} :	52°
<i>N</i> (<i>hkl</i>) _{measured} , <i>N</i> (<i>hkl</i>) _{unique} :	6681, 4621
Criterion for <i>I</i> _{obs} , <i>N</i> (<i>hkl</i>) _{gt} :	<i>I</i> _{obs} > 2 σ (<i>I</i> _{obs}), 3365
<i>N</i> (<i>param</i>) _{refined} :	280
Program:	SHELXTL [7]

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

Atom	Site	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso}
H(3)	2i	−0.1261	0.2316	0.0259	0.037
H(5)	2i	−0.3448	0.5028	−0.0692	0.039
H(7)	2i	−0.2450	0.6708	0.0284	0.035
H(8)	2i	−0.2089	0.8364	0.0882	0.047
H(9A)	2i	0.1542	0.8979	0.2129	0.086
H(9B)	2i	0.0500	0.9384	0.0963	0.086
H(10A)	2i	0.0420	1.0394	0.2885	0.075
H(10B)	2i	−0.1150	1.0415	0.1757	0.075
H(11A)	2i	−0.2619	0.9043	0.2437	0.065
H(11B)	2i	−0.0818	0.8722	0.3243	0.065
H(14)	2i	0.6558	0.9188	0.7082	0.047
H(16)	2i	0.1951	0.7835	0.7215	0.041
H(18)	2i	−0.0280	0.7035	0.5693	0.040
H(19)	2i	−0.2957	0.6745	0.3522	0.044
H(20A)	2i	−0.1885	0.4625	0.3316	0.062
H(20B)	2i	−0.3298	0.5186	0.2399	0.062
H(21A)	2i	−0.5287	0.5068	0.3405	0.060
H(21B)	2i	−0.4214	0.4123	0.3996	0.060
H(22A)	2i	−0.3674	0.6198	0.5009	0.061
H(22B)	2i	−0.2175	0.5402	0.5319	0.061

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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)	2i	0.08127(8)	0.67109(5)	0.30778(5)	0.0315(3)	0.0302(3)	0.0247(3)	−0.0010(2)	0.0059(2)	−0.0039(2)
Br(1)	2i	0.16619(6)	0.29610(4)	0.22260(4)	0.0452(3)	0.0356(3)	0.0435(3)	0.0101(2)	0.0033(2)	0.0027(2)
Br(2)	2i	−0.41160(7)	0.27486(5)	−0.16330(5)	0.0501(3)	0.0509(3)	0.0520(3)	−0.0045(2)	−0.0120(3)	−0.0192(3)
Br(3)	2i	0.64737(6)	0.88365(4)	0.48103(5)	0.0368(3)	0.0466(3)	0.0563(3)	−0.0031(2)	0.0190(2)	0.0012(2)
Br(4)	2i	0.50630(8)	0.89925(6)	0.88565(4)	0.0542(4)	0.1080(5)	0.0303(3)	0.0108(3)	−0.0034(3)	−0.0202(3)
N(1)	2i	−0.0796(4)	0.7163(3)	0.1683(3)	0.034(2)	0.022(2)	0.029(2)	0.000(2)	0.009(2)	0.003(2)
N(2)	2i	−0.0376(4)	0.6682(3)	0.4222(3)	0.031(2)	0.031(2)	0.026(2)	−0.004(2)	0.007(2)	−0.001(2)
O(1)	2i	0.0931(4)	0.5284(2)	0.2460(2)	0.036(2)	0.034(2)	0.027(2)	0.004(1)	0.003(1)	−0.005(1)
O(2)	2i	0.2877(4)	0.7608(3)	0.3984(2)	0.035(2)	0.045(2)	0.030(2)	−0.009(1)	0.011(1)	−0.005(1)
C(1)	2i	−0.0180(5)	0.4782(3)	0.1560(3)	0.025(2)	0.027(2)	0.027(2)	−0.003(2)	0.008(2)	−0.000(2)
C(2)	2i	−0.0148(5)	0.3665(3)	0.1284(3)	0.030(2)	0.029(2)	0.029(2)	0.001(2)	0.012(2)	0.002(2)
C(3)	2i	−0.1316(5)	0.3061(3)	0.0386(4)	0.035(3)	0.023(2)	0.035(3)	−0.005(2)	0.014(2)	−0.001(2)
C(4)	2i	−0.2591(5)	0.3578(4)	−0.0338(4)	0.026(2)	0.036(3)	0.031(3)	−0.007(2)	0.005(2)	−0.005(2)
C(5)	2i	−0.2637(6)	0.4683(4)	−0.0173(4)	0.028(2)	0.034(3)	0.032(3)	0.003(2)	0.006(2)	−0.001(2)
C(6)	2i	−0.1466(5)	0.5300(3)	0.0776(3)	0.025(2)	0.028(2)	0.028(2)	−0.002(2)	0.009(2)	−0.001(2)
C(7)	2i	−0.1635(5)	0.6451(3)	0.0876(4)	0.029(2)	0.029(2)	0.029(2)	0.002(2)	0.008(2)	0.005(2)
C(8)	2i	−0.1132(6)	0.8311(4)	0.1565(4)	0.043(3)	0.026(3)	0.040(3)	0.004(2)	0.002(2)	0.000(2)
C(9)	2i	0.0426(9)	0.9166(4)	0.1666(6)	0.079(5)	0.039(3)	0.113(6)	0.005(3)	0.056(4)	0.006(3)
C(10)	2i	−0.0407(7)	0.9958(4)	0.2247(6)	0.047(3)	0.039(3)	0.097(5)	0.001(3)	0.019(3)	−0.011(3)
C(11)	2i	−0.1400(7)	0.8967(4)	0.2527(5)	0.052(3)	0.035(3)	0.076(4)	0.009(2)	0.023(3)	0.000(3)
C(12)	2i	0.3256(6)	0.7890(3)	0.5038(4)	0.030(2)	0.029(2)	0.031(3)	0.005(2)	0.003(2)	−0.006(2)
C(13)	2i	0.4935(5)	0.8485(3)	0.5615(4)	0.028(2)	0.030(2)	0.038(3)	0.004(2)	0.007(2)	0.002(2)
C(14)	2i	0.5452(6)	0.8807(4)	0.6728(4)	0.028(3)	0.039(3)	0.039(3)	0.008(2)	−0.003(2)	−0.008(2)
C(15)	2i	0.4308(6)	0.8556(4)	0.7316(4)	0.033(3)	0.052(3)	0.029(3)	0.010(2)	−0.004(2)	−0.014(2)
C(16)	2i	0.2698(6)	0.8000(4)	0.6806(4)	0.038(3)	0.042(3)	0.026(2)	0.010(2)	0.011(2)	0.004(2)
C(17)	2i	0.2137(6)	0.7667(4)	0.5673(4)	0.031(2)	0.032(3)	0.030(3)	0.004(2)	0.003(2)	−0.005(2)
C(18)	2i	0.0376(6)	0.7101(4)	0.5213(4)	0.036(3)	0.037(3)	0.031(3)	−0.003(2)	0.016(2)	0.003(2)
C(19)	2i	−0.2222(6)	0.6203(4)	0.3894(4)	0.030(3)	0.041(3)	0.037(3)	−0.002(2)	0.009(2)	0.002(2)
C(20)	2i	−0.2783(7)	0.5115(4)	0.3182(5)	0.042(3)	0.052(3)	0.057(4)	−0.013(2)	0.019(3)	−0.016(3)
C(21)	2i	−0.4135(7)	0.4868(4)	0.3785(5)	0.041(3)	0.048(3)	0.062(4)	−0.009(2)	0.021(3)	0.000(3)
C(22)	2i	−0.3007(7)	0.5713(5)	0.4725(4)	0.039(3)	0.071(4)	0.043(3)	−0.005(3)	0.019(2)	0.000(3)

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