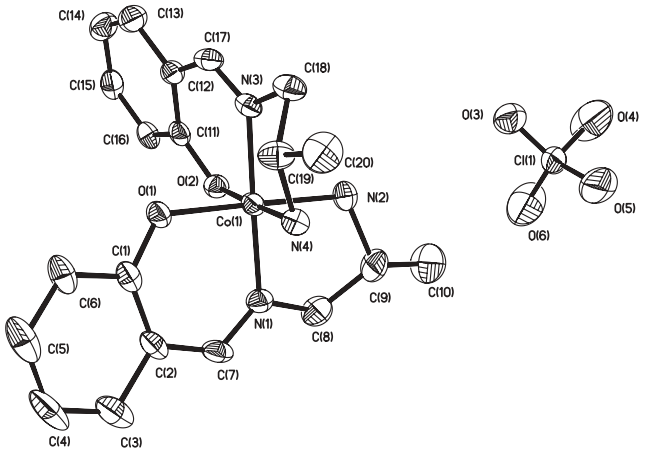
# Crystal structure of bis[*N*-(2-aminopropyl)-salicylaldiminato)]cobalt(III) perchlorate, $C_{20}H_{26}ClCoN_4O_6$

H.-L. Zhu*,[I], W.-J. Liu[I], Y.-F. Wang[I] and D.-Q. Wang[II]

[I] Wuhan Institute of Science and Technology, Department of Environmental and Chemical Engineering, Wuhan, 430073 P. R. China
[II] Liaocheng University, Department of Chemistry, Liaocheng, 252059 P. R.China

Received March 17, 2003, accepted and available on-line June 10, 2003; CCDC-No. 1267/1058




**Abstract**

$C_{20}H_{26}ClCoN_4O_6$, monoclinic, $P12_1/c1$ (No. 14), $a = 9.703(4)$ Å, $b = 24.323(9)$ Å, $c = 10.289(4)$ Å, $\beta = 111.561(6)°$, $V = 2258.4$ Å$^3$, $Z = 4$, $R_{gt}(F) = 0.049$, $wR_{ref}(F^2) = 0.110$, $T = 298$ K.

**Source of material**

Reagents and solvents used were of commercially available quality. The Schiff's base ligand (L) was prepared by the (1 + 1) condensation of salicylaldehyde with 1,2-diaminopropane in methanol at room temperature. Further isolation was not carried out and the ligand solution was subsequently used for the preparation of the metal complexes. To a methanol solution (5 ml) of $CoCl_2 \cdot 6H_2O$ (238 mg, 1 mmol) was added a methanol solution (5 ml) of L (2 mmol) with stirring for 30 min. $NaClO_4$ (100 mg) in methanol (2 ml) was added to the above solution. Upon slow diffusion of diethyl ether into the resulting dark purple solution for four days, large dark purple prismatic crystals of the title complex were deposited and collected by filtration, respectively washed with methanol and diethyl ether and dried in a vacuum desiccator over silica gel (yield 83%). Elemental analysis: found – C, 47.02%; H, 5.18%; N, 10.80%; calc. for $C_{20}H_{26}ClCoN_4O_6$ – C, 46.84%; H, 5.11%; N, 10.92%.

**Experimental details**

Only the hydrogen atoms that could be located from the difference Furier maps were refined. Those hydrogen atoms which could not be located from the difference Fourier maps were geometrically fixed. The displacement $U_{ij}$ parameters for some oxygen atoms (O4, O5, O6) are relatively large. These atoms are presumably disordered.

* Correspondence author (e-mail: hlzhu@wist.edu.cn)

**Discussion**

The discovery that certain cobalt(III) Schiff's base complexes are potent antiviral agents prompted a rapid development on investigation of Co(III) complexes with Schiff's bases of various structures. Reported here is the crystal structure of a cobalt(III) complex with a Schiff's base. The title complex exists as a discrete molecule in the solid state, which consists of one complex cation and one perchlorate anion. In the cation, the Co(III) atom is six-coordinated to form a slightly distorted octahedron with four nitrogen and two phenoxo oxygen atoms from two Schiff's base ligands. As expected, the average Co(III)—N distance (from imine, 1.899(3) Å) is much shorter than the mean Co(III)—N distance (from amine, 1.956(3) Å) in the coordination polyhedron. But all the Co(III)—N and the Co(III)—O bond lengths (with the average 1.891(2) Å) are in the normal ranges comparing to similar bond lengths. There exists a hydrogen bond between the N(2) atom in each cation with O(5) atom in each perchlorate anion.

**Table 1.** Data collection and handling.

| | |
|---|---|
| Crystal: | purple prism, size 0.17 × 0.33 × 0.35 mm |
| Wavelength: | Mo $K_\alpha$ radiation (0.71073 Å) |
| $\mu$: | 9.22 cm$^{-1}$ |
| Diffractometer, scan mode: | Bruker SMART CCD, $\varphi/\omega$ |
| $2\theta_{max}$: | 52.92° |
| $N(hkl)_{measured}$, $N(hkl)_{unique}$: | 12991, 4572 |
| Criterion for $I_{obs}$, $N(hkl)_{gt}$: | $I_{obs} > 2\ \sigma(I_{obs})$, 2328 |
| $N(param)_{refined}$: | 341 |
| Programs: | SHELXTL [1], SHELXTL-plus [2] |

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

| Atom | Site | *x* | *y* | *z* | $U_{iso}$ |
|---|---|---|---|---|---|
| H(1) | 4*e* | –0.1330 | 0.4087 | 1.0089 | 0.122 |
| H(2) | 4*e* | –0.3364 | 0.3521 | 0.9681 | 0.145 |
| H(3) | 4*e* | –0.3715 | 0.2779 | 0.8215 | 0.137 |
| H(4) | 4*e* | –0.2142 | 0.2586 | 0.7133 | 0.099 |
| H(5) | 4*e* | 0.0892 | 0.4311 | 0.9752 | 0.083 |
| H(10A) | 4*e* | 0.4711 | 0.4887 | 0.6845 | 0.198 |
| H(10B) | 4*e* | 0.5446 | 0.4626 | 0.8334 | 0.198 |
| H(10C) | 4*e* | 0.4565 | 0.5179 | 0.8147 | 0.198 |
| H(11) | 4*e* | 0.3044 | 0.1539 | 0.6260 | 0.093 |
| H(12) | 4*e* | 0.4621 | 0.1136 | 0.8246 | 0.102 |
| H(13) | 4*e* | 0.5562 | 0.1639 | 1.0292 | 0.089 |
| H(14) | 4*e* | 0.4916 | 0.2539 | 1.0342 | 0.077 |
| H(15) | 4*e* | 0.1798 | 0.2304 | 0.4985 | 0.074 |
| H(6) | 4*e* | 0.390(4) | 0.423(2) | 0.957(4) | 0.08(1) |
| H(7) | 4*e* | 0.290(3) | 0.484(1) | 0.933(3) | 0.052(9) |
| H(8) | 4*e* | 0.220(4) | 0.473(1) | 0.687(3) | 0.07(1) |

**Table 2.** Continued.

| Atom | Site | *x* | *y* | *z* | $U_{iso}$ |
|---|---|---|---|---|---|
| H(9) | 4*e* | 0.389(4) | 0.384(1) | 0.715(3) | 0.04(1) |
| H(10) | 4*e* | 0.302(4) | 0.404(2) | 0.582(4) | 0.08(1) |
| H(16) | 4*e* | 0.114(4) | 0.349(2) | 0.387(4) | 0.09(1) |
| H(17) | 4*e* | 0.031(4) | 0.294(2) | 0.359(4) | 0.07(1) |
| H(18) | 4*e* | –0.156(4) | 0.328(2) | 0.449(4) | 0.08(1) |

**Table 2.** Continued.

| Atom | Site | *x* | *y* | *z* | $U_{iso}$ |
|---|---|---|---|---|---|
| H(19) | 4*e* | –0.060(4) | 0.404(2) | 0.593(4) | 0.07(1) |
| H(20) | 4*e* | 0.025(3) | 0.419(1) | 0.529(3) | 0.04(1) |
| H(21) | 4*e* | –0.108(5) | 0.410(2) | 0.299(4) | 0.10(2) |
| H(22) | 4*e* | –0.222(6) | 0.352(2) | 0.241(5) | 0.13(2) |
| H(23) | 4*e* | –0.256(6) | 0.407(3) | 0.316(5) | 0.16(2) |

**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* | 0.16303(5) | 0.35087(2) | 0.70452(5) | 0.0518(3) | 0.0565(3) | 0.0513(3) | –0.0057(2) | 0.0269(2) | –0.0054(2) |
| Cl(1) | 4*e* | 0.8186(2) | 0.50765(6) | 0.6644(2) | 0.125(1) | 0.0755(9) | 0.107(1) | 0.0236(8) | 0.0667(9) | 0.0208(8) |
| N(1) | 4*e* | 0.1673(3) | 0.4022(1) | 0.8456(3) | 0.067(2) | 0.058(2) | 0.060(2) | –0.004(2) | 0.026(2) | –0.012(2) |
| N(2) | 4*e* | 0.3149(4) | 0.3982(2) | 0.6791(4) | 0.057(3) | 0.071(3) | 0.072(3) | –0.009(2) | 0.027(2) | 0.006(2) |
| N(3) | 4*e* | 0.1545(3) | 0.3016(1) | 0.5591(3) | 0.051(2) | 0.071(2) | 0.043(2) | –0.005(2) | 0.021(2) | –0.009(2) |
| N(4) | 4*e* | 0.0022(4) | 0.3892(2) | 0.5602(4) | 0.074(3) | 0.063(3) | 0.068(2) | 0.000(2) | 0.037(2) | –0.003(2) |
| O(1) | 4*e* | 0.0206(3) | 0.3056(1) | 0.7355(2) | 0.059(2) | 0.068(2) | 0.067(2) | –0.013(1) | 0.036(1) | –0.007(1) |
| O(2) | 4*e* | 0.3205(2) | 0.3125(1) | 0.8413(2) | 0.057(2) | 0.059(2) | 0.052(1) | –0.002(1) | 0.020(1) | –0.006(1) |
| O(3) | 4*e* | 0.7592(4) | 0.4553(2) | 0.6227(4) | 0.126(3) | 0.098(3) | 0.148(3) | 0.007(2) | 0.070(2) | –0.005(2) |
| O(4) | 4*e* | 0.9396(6) | 0.5105(2) | 0.6180(8) | 0.192(5) | 0.132(4) | 0.440(9) | –0.026(3) | 0.220(6) | –0.028(5) |
| O(5) | 4*e* | 0.7289(7) | 0.5492(2) | 0.5904(5) | 0.359(7) | 0.133(4) | 0.165(4) | 0.136(5) | 0.119(5) | 0.069(3) |
| O(6) | 4*e* | 0.855(1) | 0.5152(2) | 0.7977(5) | 0.57(1) | 0.143(4) | 0.076(3) | –0.039(6) | 0.069(5) | –0.019(3) |
| C(1) | 4*e* | –0.0691(4) | 0.3212(2) | 0.7953(4) | 0.052(2) | 0.077(3) | 0.063(2) | 0.010(2) | 0.029(2) | 0.022(2) |
| C(2) | 4*e* | –0.0479(4) | 0.3668(2) | 0.8821(4) | 0.064(3) | 0.089(3) | 0.057(2) | 0.019(2) | 0.036(2) | 0.020(2) |
| C(3) | 4*e* | –0.1484(6) | 0.3787(2) | 0.9494(5) | 0.103(4) | 0.139(5) | 0.083(3) | 0.032(4) | 0.058(3) | 0.016(3) |
| C(4) | 4*e* | –0.2690(7) | 0.3449(3) | 0.9252(6) | 0.091(4) | 0.194(7) | 0.114(5) | 0.039(5) | 0.079(4) | 0.046(5) |
| C(5) | 4*e* | –0.2896(6) | 0.3004(3) | 0.8370(6) | 0.072(4) | 0.172(6) | 0.115(5) | 0.009(4) | 0.054(4) | 0.047(4) |
| C(6) | 4*e* | –0.1957(4) | 0.2887(2) | 0.7731(5) | 0.051(3) | 0.115(4) | 0.090(3) | –0.002(2) | 0.035(3) | 0.024(3) |
| C(7) | 4*e* | 0.0756(5) | 0.4040(2) | 0.9080(4) | 0.091(3) | 0.077(3) | 0.048(2) | 0.022(3) | 0.034(2) | –0.002(2) |
| C(8) | 4*e* | 0.2920(6) | 0.4402(2) | 0.8787(5) | 0.090(4) | 0.077(3) | 0.086(3) | –0.023(3) | 0.024(3) | –0.024(3) |
| C(9) | 4*e* | 0.3215(6) | 0.4514(2) | 0.7511(6) | 0.090(4) | 0.069(3) | 0.104(4) | –0.033(3) | 0.034(3) | –0.013(3) |
| C(10) | 4*e* | 0.4610(6) | 0.4830(2) | 0.7729(6) | 0.107(4) | 0.130(5) | 0.157(5) | –0.040(4) | 0.046(4) | –0.016(4) |
| C(11) | 4*e* | 0.3522(4) | 0.2605(2) | 0.8317(4) | 0.046(2) | 0.066(3) | 0.064(3) | –0.010(2) | 0.033(2) | –0.001(2) |
| C(12) | 4*e* | 0.2972(4) | 0.2297(2) | 0.7070(4) | 0.053(2) | 0.059(3) | 0.072(3) | –0.005(2) | 0.035(2) | –0.007(2) |
| C(13) | 4*e* | 0.3410(5) | 0.1743(2) | 0.7081(5) | 0.078(3) | 0.071(3) | 0.089(3) | –0.006(3) | 0.035(3) | –0.013(3) |
| C(14) | 4*e* | 0.4352(5) | 0.1502(2) | 0.8259(6) | 0.084(3) | 0.062(3) | 0.116(4) | 0.005(3) | 0.045(3) | –0.002(3) |
| C(15) | 4*e* | 0.4912(4) | 0.1804(2) | 0.9483(5) | 0.067(3) | 0.074(3) | 0.091(3) | 0.006(2) | 0.039(3) | 0.023(3) |
| C(16) | 4*e* | 0.4518(4) | 0.2342(2) | 0.9512(4) | 0.051(2) | 0.081(3) | 0.068(3) | –0.006(2) | 0.031(2) | 0.006(2) |
| C(17) | 4*e* | 0.2051(4) | 0.2528(2) | 0.5770(4) | 0.056(2) | 0.071(3) | 0.063(3) | –0.007(2) | 0.029(2) | –0.023(2) |
| C(18) | 4*e* | 0.0626(5) | 0.3222(2) | 0.4212(4) | 0.077(3) | 0.087(4) | 0.055(3) | –0.002(3) | 0.027(2) | –0.016(3) |
| C(19) | 4*e* | –0.0690(5) | 0.3508(2) | 0.4407(4) | 0.069(3) | 0.084(3) | 0.057(2) | 0.008(3) | 0.012(2) | –0.013(2) |
| C(20) | 4*e* | –0.1724(8) | 0.3784(3) | 0.3128(6) | 0.100(4) | 0.108(5) | 0.078(4) | –0.001(4) | 0.009(3) | 0.002(3) |

*Acknowledgment.* The authors thank the Education Office of Hubei Province for the research grant 2002B29002.

## References

1. Sheldrick, G. M.: Siemens SHELXTL (Version 5.0). Siemens Industrial Automation, Inc., Analytical Instrumentation, USA 1995.
2. Sheldrick, G. M.: SHELXTL-plus. Release 4.1. Siemens Analytial X-ray Instruments Inc., Madison Wisconsin, USA 1991.