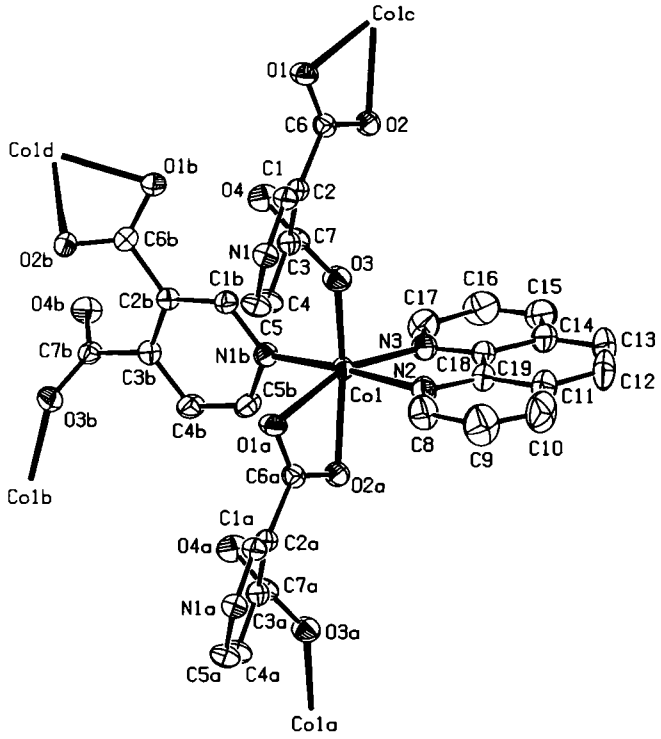
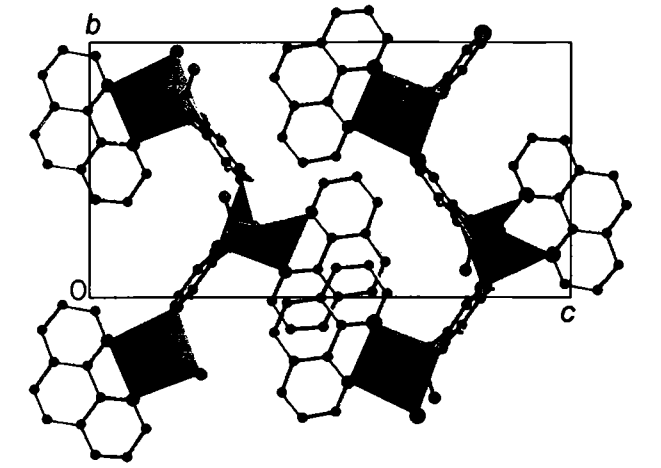
Crystal structure of poly[(1,10-phenanthroline-*N*,*N*′)(μ_3-pyridyl-3,4-dicarboxylato-*N*,*O*,*O*′,*O*″)cobalt(II)], $Co(C_{12}H_8N_2)[NC_5H_3(COO)_2]$

D. Weng[I], Y.-W. Yao*[,II], Q. Cai[I] and G.-Y. Tang[II]

[I] Tsinghua University, Department of Materials Science and Engineering, Beijing, Henan, 100084 P. R. China
[II] Tsinghua University, Graduate School at Shenzhen, Advanced Materials Institute, Shenzhen, Guangdong, 518055 P. R. China

Received October 3, 2005, accepted and available on-line December 3, 2005; CCDC no. 1267/1654





Abstract

$C_{19}H_{11}CoN_3O_4$, monoclinic, $P12_1/n1$ (no. 14), $a = 7.680(2)$ Å, $b = 19.870(4)$ Å, $c = 10.650(2)$ Å, $\beta = 95.15(3)°$, $V = 1618.7$ Å^3, $Z = 4$, $R_{gt}(F) = 0.035$, $wR_{ref}(F^2) = 0.093$, $T = 293$ K.

* Correspondence author (e-mail: yw_yao@yahoo.com)

Source of material

The title compound was synthesized by hydrothermal treatment of a well-stirred mixture containing Co_3O_4, pyridine-3,4-dicarboxylic acid, 1,10-phenanthroline and water in the molar ratio of 1.0:4.8:3.4:224.2 under 413 K for 72 h. The resulting crystals were recovered by filtration, washed with distilled water and dried under ambient conditions.

Discussion

The structure of the title compound contains a two-dimensionally extended framework which is made up of six-coordinated cobalt, pdc (H_2pdc = 3,4-pyridinedicarboxylic acid), and phen (phen = 1,10-phenanthroline) ligand. The Co1 atom has a distorted octahedral environment composed of two phen nitrogen, one pdc nitrogen, and three pdc oxygen atoms (figure, top). The distances of Co—N_{phen} differ significantly with d(Co1—N2) = 2.150(2) Å and d(Co1—N3) = 2.106(2) Å, which has been also observed in $[Co(H_2O)(2,2'\text{-bipy})(p\text{-CPOA})]_n$ (p-H_2CPOA = 4-carboxylphenoxyacetic acid) [1]. The distance of Co1—N1 (2.158(2) Å) is similar to that of Co1—N3. That O1 and O2 coordinate to Co1 renders the pdc a role of chelate ligand. The distances of Co1—O1, Co1—O2 and Co1—O3 are 2.183(2) Å, 2.197(2) Å and 2.011(2) Å, respectively, indicating the relatively strong interaction between Co1 and O3. The Co—O (average 2.138(2) Å) and Co—N distances (average 2.130(2) Å) are comparable to those reported previously [1,2]. The pdc and phen serve as bridging and capping ligands, respectively. One pdc as a quadridentate ligand bridges three Co atoms together, vice versa, giving rise to a 2D framework with the aromatic planes of phen being exposed. The exposed phen ligands from adjacent frameworks overlap to a certain extent (figure, bottom), forming an interdigitated structure of the aromatic planes. The interdigitated structure and the interplanar distance of about 3.84 Å on average reveal the face-to-face π-π interactions between the two nearest overlapped phen ligands. The framework fragments stack together via π-π interactions in ABAB sequence along the b axis, resulting in the three-dimensional structure (figure, bottom).

Table 1. Data collection and handling.

Crystal:	pink needle, size 0.05 × 0.05 × 0.10 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	10.93 cm^{-1}
Diffractometer, scan mode:	Rigaku R-AXIS RAPID IP, ω/φ
$2\theta_{max}$:	54.86°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	12746, 3390
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 3055
$N(param)_{refined}$:	244
Programs:	SHELXS-97 [3], SHELXL-97 [4], DIAMOND [5]

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

Atom	Site	x	y	z	U_{iso}
H(1)	4e	0.0455	0.7126	0.4956	0.028
H(2)	4e	0.5960	0.7278	0.3660	0.035
H(3)	4e	0.5388	0.6635	0.5361	0.035
H(4)	4e	0.7918	0.8340	0.5220	0.051
H(5)	4e	0.7957	0.8985	0.7039	0.073
H(6)	4e	0.7569	1.0132	0.6884	0.074
H(7)	4e	0.7038	1.1163	0.5471	0.077
H(8)	4e	0.6729	1.1610	0.3519	0.071
H(9)	4e	0.6715	1.1447	0.1128	0.060
H(10)	4e	0.6922	1.0724	−0.0540	0.061
H(11)	4e	0.7391	0.9586	−0.0154	0.049

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)	4e	0.76385(4)	0.85936(2)	0.21972(3)	0.0235(2)	0.0181(2)	0.0230(2)	0.0006(1)	0.0015(1)	−0.0008(1)
O(1)	4e	−0.1222(2)	0.76655(9)	0.3000(2)	0.0200(9)	0.0289(9)	0.037(1)	0.0004(7)	0.0027(8)	0.0049(8)
O(2)	4e	0.0482(2)	0.85207(8)	0.2637(2)	0.0272(9)	0.0231(9)	0.0267(9)	0.0010(7)	0.0004(8)	0.0026(7)
O(3)	4e	0.5055(2)	0.84360(9)	0.2214(2)	0.0247(9)	0.030(1)	0.041(1)	−0.0020(7)	0.0060(8)	0.0042(8)
O(4)	4e	0.3082(3)	0.7817(1)	0.1054(2)	0.030(1)	0.046(1)	0.024(1)	−0.0019(9)	0.0046(8)	−0.0004(8)
N(1)	4e	0.2884(3)	0.6827(1)	0.5353(2)	0.024(1)	0.027(1)	0.023(1)	0.0001(8)	0.0042(9)	0.0026(8)
N(2)	4e	0.7648(3)	0.9076(1)	0.4005(2)	0.034(1)	0.027(1)	0.029(1)	0.0030(9)	0.001(1)	−0.0026(9)
N(3)	4e	0.7417(3)	0.9615(1)	0.1678(2)	0.030(1)	0.023(1)	0.035(1)	−0.0008(9)	0.001(1)	0.0031(9)
C(1)	4e	0.1575(3)	0.7159(1)	0.4693(2)	0.021(1)	0.025(1)	0.025(1)	0.0005(9)	0.002(1)	0.0018(9)
C(2)	4e	0.1815(3)	0.7549(1)	0.3634(2)	0.021(1)	0.022(1)	0.021(1)	0.0001(9)	0.002(1)	−0.0002(9)
C(3)	4e	0.3488(3)	0.7602(1)	0.3232(2)	0.025(1)	0.022(1)	0.022(1)	0.0001(9)	0.004(1)	−0.0002(9)
C(4)	4e	0.4828(3)	0.7255(1)	0.3902(3)	0.021(1)	0.039(2)	0.029(1)	0.003(1)	0.007(1)	0.006(1)
C(5)	4e	0.4474(3)	0.6873(1)	0.4935(3)	0.025(1)	0.035(1)	0.027(1)	0.006(1)	0.001(1)	0.007(1)
C(6)	4e	0.0272(3)	0.7933(1)	0.3044(2)	0.025(1)	0.024(1)	0.020(1)	0.0031(9)	0.003(1)	−0.0011(9)
C(7)	4e	0.3883(3)	0.7985(1)	0.2058(2)	0.018(1)	0.027(1)	0.025(1)	0.0044(9)	0.006(1)	0.0028(9)
C(8)	4e	0.7804(5)	0.8805(2)	0.5147(3)	0.057(2)	0.039(2)	0.031(2)	0.005(1)	0.005(1)	0.001(1)
C(9)	4e	0.7805(6)	0.9191(2)	0.6252(3)	0.086(3)	0.064(2)	0.030(2)	0.009(2)	0.002(2)	−0.006(2)
C(10)	4e	0.7582(6)	0.9872(2)	0.6159(4)	0.083(3)	0.061(2)	0.041(2)	0.007(2)	0.001(2)	−0.024(2)
C(11)	4e	0.7373(5)	1.0176(2)	0.4973(3)	0.053(2)	0.038(2)	0.049(2)	0.005(1)	−0.003(2)	−0.019(1)
C(12)	4e	0.7098(6)	1.0883(2)	0.4777(4)	0.079(3)	0.036(2)	0.075(3)	0.009(2)	−0.009(2)	−0.031(2)
C(13)	4e	0.6924(5)	1.1150(2)	0.3613(4)	0.067(2)	0.023(2)	0.084(3)	0.006(2)	−0.007(2)	−0.014(2)
C(14)	4e	0.7034(4)	1.0740(1)	0.2511(4)	0.039(2)	0.022(1)	0.065(2)	−0.001(1)	−0.009(2)	−0.003(1)
C(15)	4e	0.6893(4)	1.0989(2)	0.1274(4)	0.045(2)	0.023(1)	0.077(3)	−0.004(1)	−0.012(2)	0.013(2)
C(16)	4e	0.7018(5)	1.0562(2)	0.0283(4)	0.056(2)	0.038(2)	0.055(2)	−0.006(2)	−0.009(2)	0.021(2)
C(17)	4e	0.7292(4)	0.9874(2)	0.0525(3)	0.050(2)	0.033(2)	0.039(2)	−0.005(1)	−0.001(1)	0.009(1)
C(18)	4e	0.7289(4)	1.0038(1)	0.2671(3)	0.028(1)	0.021(1)	0.044(2)	−0.001(1)	−0.002(1)	−0.002(1)
C(19)	4e	0.7445(4)	0.9754(1)	0.3910(3)	0.035(2)	0.026(1)	0.038(2)	0.002(1)	−0.002(1)	−0.009(1)

Acknowledgments. This work was supported by the National Key Basic Research Development Program of China (grant no. 2004CB719503), the National High-Tech Research Development Program of China (grant no. 2004AA649400), and the National Natural Science Foundation of China (grant no. 20273037).

References

1. Gao, S.; Huo, L. H.; Gu, C. S.; Zhao, H.; Zhao, J. G.: Synthesis and Crystal Structure of 1D Chain Coordination Polymer $[Co(p\text{-}CPOA)(2,2'\text{-bipy})(H_2O)]_n$ with 4-Carboxyphenoxyacetate Ligand. Chin. J. Inorg. Chem. **21** (2005) 701-704.
2. Qi, Y. J.; Wang, Y. H.; Hu, C. W.; Cao, M. H.; Mao, L.; Wang, E. B.: A New Type of Single-Helix Coordination Polymer with Mixed Ligands $[M_2(phen)_2(e,a\text{-}cis\text{-}1,4\text{-}chdc)_2(H_2O)_2]_n$ (M = Co and Ni; phen = 1,10-phenanthroline; chdc = cyclohexanedicarboxylate). Inorg. Chem. **25** (2003) 8519-8523.
3. Sheldrick, G. M.: SHELXS-97. Program for the Solution of Crystal Structures. University of Göttingen, Germany 1997.
4. Sheldrick, G. M.: SHELXL-97. Program for the Refinement of Crystal Structures. University of Göttingen, Germany 1997.
5. Brandenburg, K.: DIAMOND. Visual Crystal Structure Information System. Version 2.1e. Crystal Impact, Bonn, Germany 2001.