Asian Journal of Chemistry Vol. 20, No. 6 (2008), 4963-4965

NOTE

Synthesis and Crystal Structure of $phen_2Co\text{-}2N_3$

JIAN-HONG BI*†, RONG-JIN DING, ZI-XIAN HUANG‡,
YAN CHEN and NAI-LIANG HU
Department of Chemistry, Hefei Teachers College, 327, Jinzhai Street
Hefei, Anhui 230061, P.R. China
E-mail: hxx010101@126.com

A novel cobalt complex $phen_2Co\text{-}2N_3$, where phen is 1,10-phenanthroline, was synthesized and characterized by IR spectra, elemental analysis and single-crystal X-ray. The crystal is triclinic, space group P-1 with unit cell parameters: a = 8.090 Å, b = 12.7351 (5) Å, c = 14.2705 (3) Å, α = 82.912 (15)º, β = 73.595(16)º, γ = 72.122(13)º, V = 1341.22 (6) $Å^3$, Z = 2, Mr = 543.93, Dc = 1.347 Mg/cm^3, μ = 0.681 mm^{-1}, F(000) = 559, T = 293(2)K, R = 0.0782, wR = 0.2482 for 10293 reflections with $I > 2\sigma(I)$. The crystal structure analysis shows that the Co(II) is a six-coordinated in a slightly distorted octahedron environment.

Key Words: Cobalt(II), 1,10-Phenanthroline, Crystal structure, Sodium azide.

Recently, the chemistry of transition metal coordination compounds of multidentate nitrogen organic ligand has become increasingly important[1-3]. It has been reported useful catalysts for many reactions, resulting in higher selectivity, mild conditions and easier operation[4-8]. The study of inorganic-organic hybrid materials may contribute to the development of modern chemistry. In this communication, the synthesis and the structure of a novel 3D-complex $phen_2Co\text{-}2N_3$ (phen = 1,10-phenanthroline) has been reported.

IR spectrum was recorded on an Nexus-870 spectromer. Elemental analyses on an Elementar Vario EL-III elemental analyzer.

Synthesis: A mixture of $CoSO_4$ (1 mmol), 1,10-phenanthroline (2 mmol), sodium azide (2 mmol) and H_2O (20 mL) was sealed in a 25 mL cone bottle under normal atmospheric temperature and normal pressure for 7 d. The product was brown pillar-shaped crystal. IR spectrum (KBr, ν_{max}, cm^{-1}): (N-H) 3340, (N=N=N) 2050, (C=N) 1620, 1580, (phen) 845, 725. Elemental analysis (%) calcd. for $phen_2Co\text{-}N_3$: C, 52.99; H, 3.72; N, 25.82. Found: (%) C, 53.03; H, 3.70; N, 25.79.

†School of Chemistry and Chemical Engineering, Anhui University, Hefei 230039, P.R. China.
‡Fujian Institute of Research on the Structure of Matter, Chinese Academy of Science, Fuzhou, 350002, P.R. China.

Crystal structure determination: A brown crystal (0.40 mm × 0.35 mm × 0.10 mm) was selected for crystallographic data collection at 293(2) K and structure determinated with graphite-monochromatic MoK_α radiation ($\lambda = 0.71073$ Å). A total of 10293 reflections were collected in the range of $2.20^\circ \leq \theta \leq 27.48^\circ$, of which 6056 reflections were unique with $R_{int} = 0.0170$ and R = 0.0782, wR = 0.2482; where $w = 1/[\sigma^2(F_0^2) + (0.1805P)^2 + 0.4947P]$ and $P = (F_0^2 + 2F_C^2)/3$. The maximum and minimum peaks on the final difference Fourier map are corresponding to 1.198 and -0.326 e/Å^3 (CCDC No. 646141), respectively.

The atomic coordinates and thermal parameters are listed in Table-1, and the selected bond lengths and bond angles in Table-2. Fig. 1 shows the molecular structure of $phen_2Co\text{-}2N_3$. Fig. 2 shows the packing diagram of the title compound. From the Fig. 1, the cobalt(II) ion is coordinated with six nitrogen atoms, and six Co-N bonds are varied. So it is obviously that Co atom is in a slightly distorted octahedral geometry. Fig. 2 depicts the packing diagram in the unit cell, shows that the moleculars are linked to the neighbours by π-π stacking interactions. And through the π-π stacking interactions, the molecules formed a three-dimensional frameworks. In addition, there are molecular channels in the supermolecule frameworks which suggest a potential application foreground of this compound in the fields of molecular sieve, selective sorbent and selective catalyzer, *etc*.

TABLE-1
ATOMIC COORDINATES (× 10^4) AND THERMAL PARAMETERS (× 10^3 Å^2)

Atom	X	Y	Z	U(eq)
Co	-21(1)	2991(1)	1337(1)	40(1)
N(1)	-1258(4)	4025(3)	457(2)	46(1)
N(4)	-431(7)	1741(4)	871(4)	77(2)
N(11)	1379(5)	1943(3)	2136(3)	48(1)
N(12)	2255(4)	2718(3)	350(2)	42(1)
N(21)	229(4)	4260(3)	1881(2)	43(1)
N(22)	-2288(4)	3265(3)	2323(2)	45(1)

TABLE-2
SELECTED BOND DISTANCES (Å) AND ANGLES (°)

Bond	Length	Angle	(°)	Angle	(°)
Co-N(22)	1.933(3)	N(22)-Co-N(12)	179.84(13)	N(1)-Co-N(21)	88.22(13)
Co-N(1)	1.951(3)	N(22)-Co-N(11)	95.91(14)	N(4)-Co-N(21)	175.81(14)
Co-N(21)	1.963(3)	N(22)-Co-N(4)	91.73(15)	N(11)-Co-N(21)	92.22(14)
Co-N(4)	1.948(4)	N(22)-Co-N(1)	88.39(14)	N(12)-Co-N(21)	95.76(13)
Co-N(11)	1.947(3)	N(12)-Co-N(1)	91.67(13)	N(22)-Co-N(21)	84.10(14)
Co-N(12)	1.938(3)	N(11)-Co-N(1)	175.75(13)	N(4)-Co-N(21)	92.00(15)

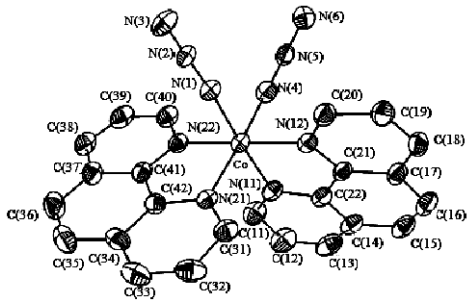

Fig. 1. Molecular structure of the $phen_2Co\text{-}2N_3$

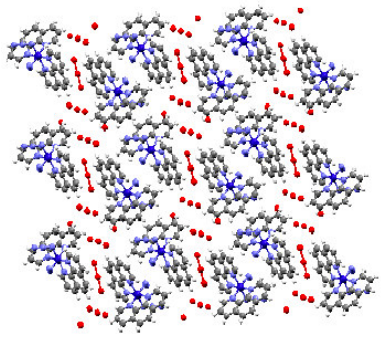

Fig. 2. Packing diagram of the $phen_2Co\text{-}2N_3$

Conclusion

We have reported a novel cobalt complex $phen_2Co\text{-}2N_3$, which was confirmed structually by IR spectra, elemental analysis and single-crystal X-ray diffraction analysis.

ACKNOWLEDGEMENTS

This work is financially supported by Nature Science Foundation of Anhui Universities.

REFERENCES

1. B. Moulton and M. Zaworotko, *J. Chem. Rev.*, **107**, 1629 (2001).
2. G.F. Swiegers and T. Malefetse, *J. Chem. Rev.*, **100**, 3483 (2000).
3. J.H. Bi, J.M. Song, Z.X. Huang, Y.H. Wang and L.T. Kong, *Asian J. Chem.*, **18**, 2365 (2006).
4. D. Villemin, *J. Chem. Soc. Chem. Commum.*, **19**, 1092 (1986).
5. J.H. Bi, F.H. Yao, Z.X. Huang, H.L. Wang and N.L. Hu, *Asian J. Chem.*, **19**, 5360 (2007).
6. L.J. Henderson, J.R. Fronezek and W.R. Cherry, *J. Am. Chem. Soc.*, **106**, 5876 (1984).
7. O. Kahn, *J. Angew. Chem. Int. Ed. Engl.*, **24**, 834 (1985).
8. J.H. Bi, L.Q. Chen, Z.Q. F.X. Xie, X.D. Zhao and S.S. Ni, *Asian J. Chem.*, **14**, 1621 (2002).

(*Received*: 27 December 2007; *Accepted*: 15 March 2008) AJC-6487