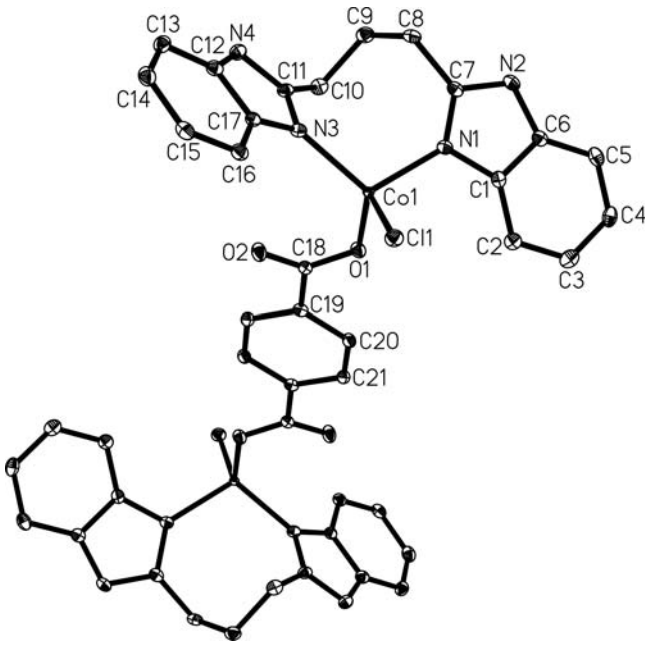
Crystal structure of dichlorobis[1,3-bis(benzimidazolyl)propane]-(terephthalato)dicobalt(II), $Co_2Cl_2(C_{17}H_{16}N_4)_2(C_8H_4O_4)$

Yan Wang*

Baoji University of Arts and Science, Department of Chemistry and Chemical Engineering, Baoji 721013, Shaanxi, P. R. China

Received January 14, 2011, accepted and available on-line February 9, 2011; CCDC no. 1267/3365



Abstract

$C_{42}H_{36}Cl_2Co_2N_8O_4$, monoclinic, $P2_1/n$ (no. 14), a = 9.891(2) Å, b = 8.687(2) Å, c = 22.411(5) Å, β = 100.228(3)°, V = 1895.1 Å^3, Z = 2, $R_{gt}(F)$ = 0.039, $wR_{ref}(F^2)$ = 0.093, T = 123 K.

Source of material

A mixture of $CoCl_2 \cdot 6H_2O$ (71.4 mg, 0.3 mmol), 2′,2′-(1,2-propyl)bis(1*H*-benzimidazole) (82.8 mg, 0.3 mmol), terephthalic acid (55.8 mg, 0.3 mmol), NaOH (24.0 mg, 0.6 mmol), and H_2O (14 mL) was sealed in a 25 mL Teflon-lined stainless steel container, which was heated at 423 K for 72 h and then cooled down to room temperature at a rate of 5 K/h. Hereafter, some blue needle-like crystals suitable for analysis were produced with yield of 50 %.

Experimental details

All hydrogen atoms bound to carbon atoms were placed in geometrically idealized positions and allowed to ride on their parent atoms with d(C—H) = 0.95 Å (aromatic), 0.99 Å (methylene) and U_{iso}(H) = 1.2 or 1.5 U_{eq}(C). Hydrogen atoms bound to nitrogen atoms were found in the difference Fourier maps and refined freely.

* e-mail: wangyan7144279@163.com

Discussion

Bisbenzimidazoles are known to be strong chelating agents coordinating through both nitrogen atoms [1]. The complexes of bis(2-benzimidazoles) with cadmium [2], nickel [3] and copper [4,5] have been reported because of their wide-ranging antivirus activity, coordination chemistry in the context of mimicking of biological systems, and importance in selective ion-exchange resins. Several novel cobalt complexes have been reported recently [6,7].

In the title crystal structure, Co(II) is four-coordinated by two nitrogen atoms from the 1,3-bis(benzimidazolyl)propane, one oxygen atom from the terephthalate and a chloride in a distorted tetrahedral arrangement. The bond lengths and angles are in normal range. The terephthalate anions serve as bidentate bridging ligands yielding a dimeric complex molecule. These dimers are interlinked by C–H···Cl hydrogen bonds, forming a two-dimensional layered structure with nearly rectangular apertures along [001].

Table 1. Data collection and handling.

Crystal:	blue needle, size 0.08 × 0.09 × 0.27 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	10.73 cm^{-1}
Diffractometer, scan mode:	AFC10/Saturn724+, φ/ω
$2\theta_{max}$:	54.98°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	14599, 4321
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 3485
$N(param)_{refined}$:	270
Programs:	SHELXS-97, SHELXL-97 [8]

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

Atom	Site	x	y	z	U_{iso}
H(2)	4*e*	0.5745	0.6329	0.5165	0.026
H(3)	4*e*	0.6323	0.7268	0.4263	0.030
H(4)	4*e*	0.7056	0.9794	0.4189	0.028
H(5)	4*e*	0.7198	1.1503	0.5001	0.028
H(8A)	4*e*	0.6526	1.0790	0.7264	0.025
H(8B)	4*e*	0.6282	0.9008	0.7386	0.025
H(9A)	4*e*	0.4091	1.1074	0.6922	0.028
H(9B)	4*e*	0.4492	1.0645	0.7625	0.028
H(10A)	4*e*	0.2596	0.9139	0.7202	0.026
H(10B)	4*e*	0.3370	0.8541	0.6676	0.026
H(13)	4*e*	0.4470	0.5831	0.9210	0.027
H(14)	4*e*	0.5443	0.3358	0.9297	0.030
H(15)	4*e*	0.6135	0.2155	0.8474	0.028
H(16)	4*e*	0.5934	0.3397	0.7534	0.025
H(20)	4*e*	0.2118	0.5692	0.4755	0.022
H(21)	4*e*	0.0200	0.5464	0.3993	0.021
H(2N)	4*e*	0.668(4)	1.168(4)	0.623(2)	0.06(1)
H(4N)	4*e*	0.355(4)	0.823(5)	0.829(2)	0.07(1)

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*	0.50887(3)	0.61362(3)	0.64594(1)	0.0110(2)	0.0087(2)	0.0089(1)	–0.0010(1)	0.0012(1)	–0.0009(1)
Cl(1)	4*e*	0.66898(7)	0.42959(7)	0.63983(3)	0.0256(3)	0.0181(3)	0.0240(3)	0.0028(2)	0.0054(3)	–0.0009(2)
O(1)	4*e*	0.3426(2)	0.5992(2)	0.58250(8)	0.0186(9)	0.0229(9)	0.0176(8)	–0.0051(7)	–0.0009(7)	0.0027(7)
O(2)	4*e*	0.2388(2)	0.4644(2)	0.64551(8)	0.026(1)	0.035(1)	0.0180(9)	–0.0118(9)	–0.0009(8)	0.0065(8)
N(1)	4*e*	0.5837(2)	0.8172(2)	0.62069(9)	0.018(1)	0.015(1)	0.018(1)	0.0000(8)	0.0019(8)	–0.0009(8)
N(2)	4*e*	0.6517(2)	1.0586(2)	0.6122(1)	0.020(1)	0.015(1)	0.024(1)	–0.0017(9)	0.0004(9)	0.0013(9)
N(3)	4*e*	0.4722(2)	0.6325(2)	0.73083(9)	0.018(1)	0.017(1)	0.017(1)	–0.0006(8)	0.0005(8)	–0.0021(8)
N(4)	4*e*	0.3974(2)	0.7414(3)	0.8088(1)	0.020(1)	0.022(1)	0.019(1)	0.0027(9)	0.0037(8)	–0.0013(9)
C(1)	4*e*	0.6125(2)	0.8387(3)	0.5621(1)	0.016(1)	0.016(1)	0.022(1)	0.0022(9)	0.005(1)	0.0027(9)
C(2)	4*e*	0.6033(3)	0.7364(3)	0.5134(1)	0.023(1)	0.020(1)	0.023(1)	0.003(1)	0.004(1)	0.001(1)
C(3)	4*e*	0.6381(3)	0.7929(3)	0.4605(1)	0.025(1)	0.026(1)	0.024(1)	0.009(1)	0.004(1)	0.001(1)
C(4)	4*e*	0.6816(3)	0.9453(3)	0.4560(1)	0.019(1)	0.030(1)	0.024(1)	0.006(1)	0.007(1)	0.008(1)
C(5)	4*e*	0.6908(3)	1.0469(3)	0.5034(1)	0.017(1)	0.022(1)	0.030(1)	–0.001(1)	0.003(1)	0.005(1)
C(6)	4*e*	0.6552(2)	0.9904(3)	0.5569(1)	0.014(1)	0.018(1)	0.023(1)	0.001(1)	0.002(1)	–0.001(1)
C(7)	4*e*	0.6081(2)	0.9527(3)	0.6488(1)	0.013(1)	0.017(1)	0.023(1)	0.0004(9)	0.0001(9)	–0.000(1)
C(8)	4*e*	0.5937(3)	0.9893(3)	0.7124(1)	0.024(1)	0.016(1)	0.022(1)	–0.002(1)	0.001(1)	–0.004(1)
C(9)	4*e*	0.4469(3)	1.0250(3)	0.7209(1)	0.029(1)	0.018(1)	0.024(1)	0.002(1)	0.004(1)	–0.002(1)
C(10)	4*e*	0.3503(3)	0.8849(3)	0.7108(1)	0.019(1)	0.024(1)	0.021(1)	0.004(1)	0.001(1)	–0.000(1)
C(11)	4*e*	0.4066(2)	0.7511(3)	0.7497(1)	0.016(1)	0.021(1)	0.017(1)	–0.001(1)	0.0009(9)	–0.005(1)
C(12)	4*e*	0.4595(2)	0.6031(3)	0.8306(1)	0.016(1)	0.020(1)	0.022(1)	–0.001(1)	0.002(1)	–0.002(1)
C(13)	4*e*	0.4748(3)	0.5337(3)	0.8874(1)	0.020(1)	0.030(2)	0.018(1)	–0.003(1)	0.003(1)	–0.002(1)
C(14)	4*e*	0.5329(3)	0.3882(3)	0.8919(1)	0.022(1)	0.030(2)	0.022(1)	–0.006(1)	–0.000(1)	0.004(1)
C(15)	4*e*	0.5753(3)	0.3160(3)	0.8425(1)	0.022(1)	0.020(1)	0.026(1)	–0.004(1)	–0.000(1)	0.002(1)
C(16)	4*e*	0.5628(2)	0.3881(3)	0.7866(1)	0.018(1)	0.020(1)	0.024(1)	–0.002(1)	0.004(1)	–0.002(1)
C(17)	4*e*	0.5037(2)	0.5343(3)	0.7810(1)	0.015(1)	0.020(1)	0.017(1)	–0.004(1)	0.0009(9)	–0.0016(9)
C(18)	4*e*	0.2394(2)	0.5264(3)	0.5956(1)	0.018(1)	0.016(1)	0.018(1)	–0.003(1)	0.003(1)	–0.0010(9)
C(19)	4*e*	0.1150(2)	0.5144(3)	0.5459(1)	0.017(1)	0.014(1)	0.019(1)	–0.0002(9)	0.001(1)	–0.0016(9)
C(20)	4*e*	0.1257(2)	0.5412(3)	0.4856(1)	0.017(1)	0.018(1)	0.019(1)	–0.002(1)	0.003(1)	0.0009(9)
C(21)	4*e*	0.0118(2)	0.5273(3)	0.4402(1)	0.020(1)	0.017(1)	0.016(1)	–0.001(1)	0.004(1)	0.0007(9)

Acknowledgments. This work was supported by Science and Technology Foundation of the Shaanxi Key Laboratory (grant no. 2010JS069), Scientific Research Project (grant nos. 09JK334, 2010JK409) from Shaanxi Province Office of Education and Key Research Project (grant no. ZK10131) from Baoji University of Arts and Sciences.

References

1. Sun, T.; Ke, L.; Yulin, L.: Aqua[1,3-bis(benzimidazol-2-yl)-2-oxapropane]-diethanolmanganese(II) dipicrate ethanol disovate. Acta Crystallogr. **E66** (2010) m1058-1059.
2. Zhao, W. X.; Wen, P. H.; Feng, G. D.; Wang, Y.; Jiang, L.; Jiang, H. B.: Crystal structure of bis(homophthalato)-bis[2,2′-(1,2-ethanediyl)-bis(1*H*-benzimidazole)]dicadmium(II), $Cd_2(C_9H_6O_4)_2(C_{16}H_{14}N_4)_2$. Z. Kristallogr. NCS. **225** (2010) 785-786.
3. Isele, K.; Broughton, V.; Matthews, C. J.; Williams, A. F.; Bernardinelli, G.; Franz, P.; Decurtins, S.: 1,2-Bis(2-benzimidazolyl)-1,2-ethanediol, a chiral, tridentate, facially coordinating ligand. J. Chem. Soc., Dalton Trans. **20** (2002) 3899-3905.
4. van Albada, G. A.; Mutikainen, I.; Turpeinen, U.; Reedijk, J.: Distortion isomerism of Cu(II) chloride adducts with bis(2-benzimidazolyl)ethane. Synthesis, characterization, X-ray structures and spectroscopy of four different isomers. J. Chem. Cryst. **37** (2007) 489-496.
5. van Albada, G. A.; Mutikainen, I.; Turpeinen, U.; Reedijk, J.: Crystal structure, magnetism and spectroscopy of a dinuclear Cu(II) compound with a chiral ligand; $Cu_2(SL)(\mu\text{-}Cl)(Cl)_2(CH_3OH)$ (HSL = *S*-1,2-bis-(benzimidazol-2-yl)-1-hydroxyethane). Polyhedron **25** (2006) 81-86.
6. An, H. Y.; Wang, E. B.; Xiao, D. R.; Li, Y. G.; Su, Z. M.; Xu, L.: Chiral 3D Architectures with Helical Channels Constructed from Polyoxometalate Clusters and Copper-Amino Acid Complexes. Angew. Chem., Int. Ed. **45** (2006) 904-908.
7. Tian, G.; Zhu, G.; Yang, X.; Fang, Q.; Xue, M.; Sun, J.; Wei, Y.; Qiu, S.: A chiral layered Co(II) coordination polymer with helical chains from a chiral materials. Chem. Commun. **11** (2005) 1396-1398.
8. Sheldrick, G. M.: A short history of SHELX. Acta Crystallogr. **A64** (2008) 112-122.