Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

{1,2-Bis[(2-oxidobenzylidene)hydrazono]-1,2-diphenylethane}(methanol)cobalt(II)

Yan Bai,[a] Dong-Bin Dang[a]* and Chun-Ying Duan[b]

[a]Institute of Molecular and Crystal Engineering, School of Chemistry and Chemical Engineering, Henan University, Kaifeng 475001, People's Republic of China, and [b]State Key Laboratory of Coordination Chemistry, Coordination Chemistry Institute, Nanjing University, Nanjing 210093, People's Republic of China

Correspondence e-mail: ddbby@163.com

Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.006 Å
R factor = 0.055
wR factor = 0.149
Data-to-parameter ratio = 12.8

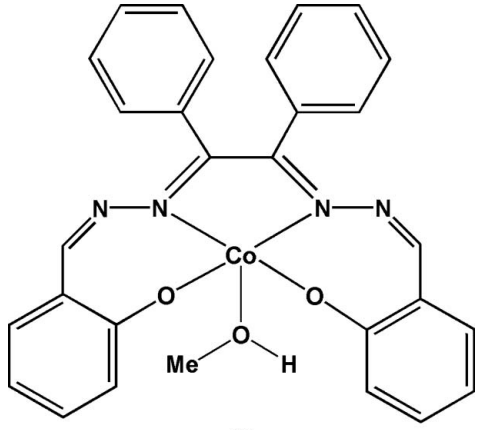
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 21 August 2006
Accepted 7 September 2006

The title complex, $[Co(C_{28}H_{20}N_4O_2)(CH_3OH)]$, can be described as a single-stranded helix with the Co^{II} atom having a distorted trigonal–bipyramidal configuration. Edge-to-face π–π stacking interactions, C—H···π interactions between the aromatic rings and O—H···O hydrogen bonds lead to a three-dimensional network in the crystal structure.

Comment

Within the field of modern supramolecular chemistry, the design of the organic ligand remains a key element for achieving a given metallo-supramolecular architecture (Lehn, 1995; Mulyana *et al.*, 2005). Polydentate diazine ligands containing N—N bridge fragments can produce a variety of structural types, such as helices, polygons and polyhedra, on the basis of the free rotation of the metal coordination planes around the N—N single bond (Grove *et al.*, 2004; Zhao *et al.*, 2004). The study of complexes of these ligands with appropriate metal ions is one of our current interests because of their unusual structures and special physical properties (Bai, Dang *et al.*, 2005; Chowdhury *et al.*, 2003; Gao *et al.*, 2003). As part of our studies of metallo-supramolecular complexes derived from polydentate diazine ligands, we became interested in designing bis-bidentate Schiff base diazine ligands with two symmetrically related coordination capabilities derived from benzil dihydrazone (Bai, Duan *et al.*, 2005; Sun *et al.*, 2006). In our previous work, a single-stranded helicate copper(II) complex generated from benzil bis[(2-oxidobenzylidene)hydrazone] (H_2L) was reported (Bai *et al.*, 2006). Here we report a new complex, (I), of cobalt(II) which was constructed using the same ligand.



(I)

The title cobalt(II) complex, (I), exhibits a single-stranded helical construction (Fig. 1) just like that found in the related

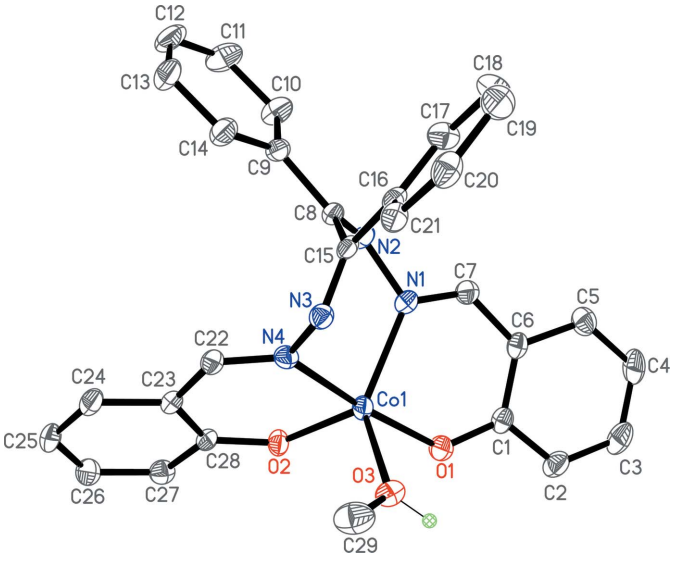


Figure 1
The molecular structure, showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms (except that of the methanol hydroxyl group) have been omitted for clarity.

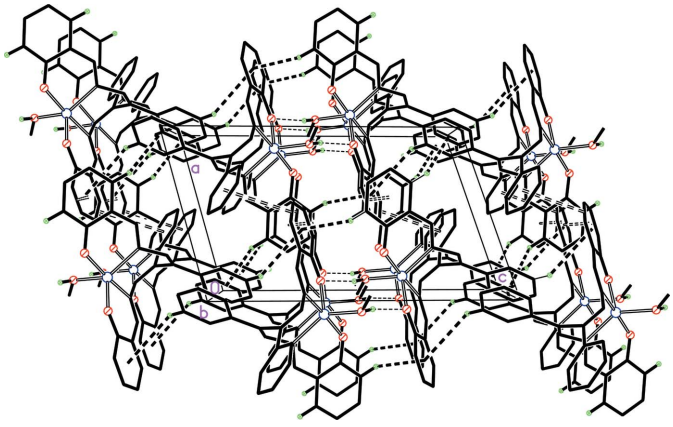


Figure 2
Intermolecular edge-to-face π–π stacking (dashed open lines), C—H$\cdots\pi$ stacking (dashed solid lines) and O—H$\cdots$O hydrogen-bond interactions (dashed lines) in the title complex, viewed along the *b* axis. H atoms other than those of hydroxyl have been omitted for clarity.

copper(II) complex (Bai *et al.*, 2006). The ligand loses two protons and coordinates to the cobalt center as a bisbidentate ligand, forming a mononuclear neutral complex. The cobalt center is coordinated in a distorted trigonal–bipyramidal configuration by two imine N atoms, two alkoxide O atoms and one methanol O atom. The Co—O and Co—N distances are in normal ranges (Table 1). The ligand adopts a twist helical conformation with N2—C8—C15—N3, C7—N1—N2—C8 and C15—N3—N4—C22 torsion angles of 71.1 (4), 130.0 (3) and 105.1 (3)°, respectively. The dihedral angle between the C9–C14 and C16–C21 phenyl rings is 89.9 (1)°. These results are similar to the values in related compounds (Bai, Duan *et al.*, 2005; Bai *et al.*, 2006; Chowdhury *et al.*, 2003).

In the crystal structure, molecules interact with each other forming a three-dimensional network through edge-to-face π–π stacking, C—H$\cdots\pi$ stacking and intermolecular hydrogen-bond interactions (Fig. 2). In the π–π interactions, the shortest atom–atom separations are 3.445 (7) and 3.588 (6) Å for C6$\cdots$C26^{i} and C16$\cdots$C25^{i} [symmetry code: (i) 1 + *x*, *y*, *z*], respectively. The dihedral angles between the interacting pair are 50.6 (1)° for C1–C6 and C23^{i}–C28^{i} and 61.1 (1)° for C16–C21 and C23^{i}–C28^{i}. Intermolecular hydrogen bonds and C—H$\cdots\pi$ interactions are also important factors in the stabilization of the crystal stucture (Table 2).

Experimental

All chemicals were of reagent grade quality, obtained from commercial sources and used without further purification. Benzil bis(salicylidenehydrazone) (H_2L) was readily prepared by the reaction of benzil dihydrazone with salicylaldehyde according to the literature methods (Bai *et al.*, 2006). The ligand H_2L (0.2 mmol, 0.088 g) and $Co(ClO_4)_2{\cdot}6H_2O$ (0.2 mmol, 0.074 g) were mixed in methanol (40 ml). The solution was left for 10 d at room temperature to afford red crystals (yield 83%). Analysis calculated for $C_{29}H_{24}CoN_4O_3$: C 65.0, H 4.5, N 10.5%; found: C 65.3, H 4.2, N 10.3%.

Crystal data

$[Co(C_{28}H_{20}N_4O_2)(CH_4O)]$
M_r = 535.45
Triclinic, $P\overline{1}$
a = 9.298 (2) Å
b = 10.455 (2) Å
c = 14.523 (3) Å
α = 95.668 (4)°
β = 103.721 (4)°
γ = 112.567 (4)°
V = 1237.8 (5) Å^3
Z = 2
D_x = 1.437 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.73 mm^{-1}
T = 293 (2) K
Block, red
0.22 × 0.20 × 0.18 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: none
6207 measured reflections
4310 independent reflections
3617 reflections with $I > 2\sigma(I)$
R_{int} = 0.083
θ_{max} = 25.1°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.055
$wR(F^2)$ = 0.149
S = 1.01
4310 reflections
337 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0888P)^2 + 0.024P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.71 e Å^{-3}
$\Delta\rho_{min}$ = −0.35 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Co1—O1	1.951 (2)	Co1—N4	2.074 (3)
Co1—O2	1.954 (2)	Co1—N1	2.091 (3)
Co1—O3	2.073 (2)		
O1—Co1—O2	100.42 (10)	O3—Co1—N4	89.79 (10)
O1—Co1—O3	86.66 (10)	O1—Co1—N1	89.15 (10)
O2—Co1—O3	107.04 (10)	O2—Co1—N1	121.73 (10)
O1—Co1—N4	171.45 (10)	O3—Co1—N1	130.97 (10)
O2—Co1—N4	88.05 (10)	N4—Co1—N1	87.31 (10)

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O3—H3A···O2^{i}	0.82	1.92	2.699 (3)	159
C29—H29C···O1^{i}	0.96	2.60	3.313 (6)	131
C2—H2A···$Cg1^{i}$	0.93	2.74 (1)	3.404 (8)	127 (1)
C5—H5A···$Cg1^{ii}$	0.93	3.13 (1)	3.90 (2)	139 (1)
C5—H5A···$Cg2^{iii}$	0.93	2.98 (1)	3.804 (8)	145 (1)

Symmetry codes: (i) $-x, -y+1, -z+1$; (ii) $-x, -y+1, -z+2$; (iii) $-x+1, -y+1, -z+2$. $Cg1$ and $Cg2$ are the centroids of the C23–C28 and C9–C14 benzene rings, respectively.

The H atoms bonded to C and O atoms were constrained to ride on their parent atoms, with distances of 0.82 Å for OH, 0.96 Å for CH_3 and 0.93 Å for other C—H; $U_{iso}(H) = 1.2U_{eq}(O)$ for OH, $1.5U_{eq}(C)$ for CH_3 and $1.2U_{eq}(C)$ for other C—H.

Data collection: *SMART* (Bruker, 2000); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 2000); program(s) used to solve structure: *SHELXTL* (Bruker, 2000); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

We are grateful for financial support from the Natural Science Foundation of Henan Province and the Foundation of the Education Department of Henan Province.

References

Bai, Y., Dang, D. B. & Duan, C. Y. (2006). *Acta Cryst.* E**62**, m1805–m1807.
Bai, Y., Dang, D. B., Duan, C. Y., Song, Y. & Meng, Q. J. (2005). *Inorg. Chem.* **44**, 5972–5974.
Bai, Y., Duan, C. Y., Cai, P., Dang, D. B. & Meng, Q. J. (2005). *Dalton Trans.* 2678–2680.
Bruker (2000). *SMART* (Version 5.625), *SAINT* (Version 6.02) and *SHELXTL* (Version 6.10). Bruker AXS Inc., Madison, Wisconsin, USA.
Chowdhury, S., Iveson, P. B., Drew, M. G. B., Tocher, D. A. & Datta, D. (2003). *New J. Chem.* **27**, 193–196.
Gao, E. Q., Bai, S. Q., Wang, Z. M. & Yan, C. H. (2003). *J. Am. Chem. Soc.* **125**, 4984–4985.
Grove, H., Kelly, T. L., Thompson, L. K., Zhao, L., Xu, Z. Q., Abedin, T. S. M., Miller, D. O., Goeta, A. E., Wilson, C. & Howard, J. A. K. (2004). *Inorg. Chem.* **43**, 4278–4288.
Lehn, J. M. (1995). *Supramolecular Chemistry: Concept and Perspectives.* edited by Lehn, pp. 139–160. Weinheim: VCH.
Mulyana, Y., Kepert, C. J., Lindoy, L. F., Parkin, A. & Turner, P. (2005). *Dalton Trans.* pp. 1598–1601.
Sun, Q. Z., Bai, Y., He, G. J., Duan, C. Y., Lin, Z. H. & Meng, Q. J. (2006). *Chem. Commun.* pp. 2777–2779.
Zhao, L., Niel, V., Thompdon, L. K., Xu, Z. Q., Milway, V. A., Harvey, R. G., Miller, D. O., Wilson, C., Leech, M., Howard, J. A. K. & Heath, S. L. (2004). *Dalton Trans.* pp. 1446–1455.