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2,2′-[(Propane-1,3-diyldioxy)bis(nitrilomethylidyne)]diphenol

Jin-Gui Duan,[a] Chen-Ming Dong,[b]* Jun-Yan Shi,[a] Lei Wu[a] and Wen-Kui Dong[a]

[a]School of Chemical and Biological Engineering, Lanzhou Jiaotong University, Lanzhou 730070, People's Republic of China, and [b]The Second Affiliated Hospital, Lanzhou University, Lanzhou 730070, People's Republic of China

Correspondence e-mail: dongwk@mail.lzjtu.cn

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Key indicators

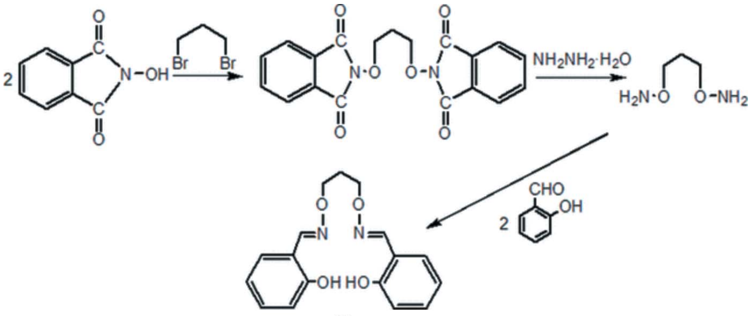
Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.005 Å
R factor = 0.038
wR factor = 0.108
Data-to-parameter ratio = 7.8

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

The title chelating bis-oxime compound, $C_{17}H_{18}N_2O_4$, has been synthesized by the reaction of 1,3-bis(aminooxy)propane with salicylaldehyde in ethanol. An O—H···N intramolecular hydrogen bond is observed between a hydroxyl group and an oxime N atom.

Comment

The study of Schiff bases is important as they can accommodate one, two or more metal centers to form complexes with interesting properties (Ikawa *et al.*, 1993; Erxleben, 2001) with applications, for example, in the preparation of dyes (Sheikhshoaie & Fabian, 2006) and as liquid crystals (Bagheri *et al.*, 2001; Ogiri *et al.*, 1999) and corrosion inhibitors (Hosseini *et al.*, 2007). Furthermore, they are involved in the mechanism of many biochemical processes (Schaur, 2003). Recently, we have reported organic compounds and metal–organic coordination complexes constructed by the formation of Schiff bases (Dong *et al.*, 2006; Akine *et al.*, 2005). As an extension of our work in this area we synthesized the title compound, (I), and determined its crystal structure.



(I)

The structure of (I) is shown in Fig. 1. The molecule adopts an extended conformation in which the two salicylaldoxime units are well separated from each other. The oxime groups and phenolic groups have *anti* conformations, and there is a strong O—H···N intramolecular hydrogen bond involving the hydroxyl O2 and N1 atoms. Three C atoms, one N atom, one O atom and one H atom generate a six-membered ring through this hydrogen bond, which stabilizes the three-dimensional network.

Although most Schiff base derivatives are stable in solution and in the solid state, C═N bonds often suffer exchange reaction as well as hydrolysis. Rate constants of oxime formation are smaller than those of imine formation and the equilibrium constants are larger by several orders (Akine *et al.*, 2005). Hence, the title compound should be stable enough to resist the metathesis of the C═N bonds (Akine *et al.*, 2001).

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Experimental

The title compound was synthesized according to a method reported previously (Akine *et al.*, 2005, 2006). To an ethanol solution (20 ml) of salicylaldehyde (251.7 mg, 2.02 mmol) was added an ethanol solution (8 ml) of 1,3-bis(aminooxy)propane (106.2 mg, 1.00 mmol). The mixture was stirred at 328K for 4 h. After cooling to room temperature, the precipitate was filtered, and washed successively with ethanol and ethanol–hexane (1:4). The product was dried under vacuum and purified by recrystallization from ethanol to yield 235.8 mg of colorless microcrystals (yield 75.0%; m.p. 353-354 K). IR: ν C═N, 1608 cm^{-1}, ν Ar—O, 1198 cm^{-1}, and δ ArO—H, 1271 cm^{-1}. Analysis calculated for $C_{17}H_{18}N_2O_4$: C 64.96, H 5.77, N 8.91%; found: C 64.82, H 5.65, N 8.96%. Single crystals suitable for X-ray diffraction studies were obtained after several weeks by slow evaporation of an ethanol solution.

Crystal data

$C_{17}H_{18}N_2O_4$
M_r = 314.33
Orthorhombic, *Pnn*2
a = 6.285 (2) Å
b = 26.910 (3) Å
c = 4.780 (2) Å
V = 808.4 (5) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 298 (2) K
0.60 × 0.17 × 0.16 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2002)
$T_{\min}$ = 0.946, $T_{\max}$ = 0.985
3965 measured reflections
819 independent reflections
654 reflections with $I > 2\sigma(I)$
$R_{\rm int}$ = 0.054

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.108
S = 1.02
819 reflections
105 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{\max}$ = 0.12 e Å^{-3}
$\Delta\rho_{\min}$ = −0.14 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2···N1	0.82	1.90	2.624 (4)	147

All H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H = 0.97 (CH_2) or 0.93 Å (CH), O—H = 0.82 Å and $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(C) or 1.5$U_{\rm eq}$(O). In the absence of significant anomalous scattering effects, Friedel pairs were merged.

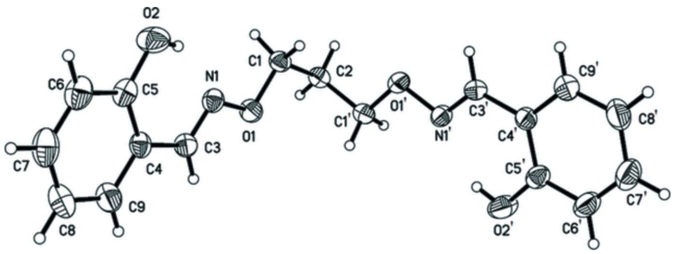

Figure 1
The molecular structure and atom numbering of the title compound. Displacement ellipsoids for non-H atoms are drawn at the 30% probability level.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT*; data reduction: *SAINT* (Bruker, 2003); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Sheldrick, 1997); software used to prepare material for publication: *SHELXTL*.

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