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6-Methoxy-5-(phenyldiazenyl)salicylaldehyde

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.002 Å
R factor = 0.042
wR factor = 0.100
Data-to-parameter ratio = 14.2

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

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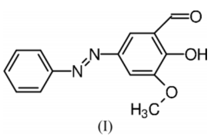
The structure of the title compound, $C_{14}H_{12}N_2O_3$, determined at room temperature, shows that the molecule is approximately planar in the solid state, as found for other diazene (azobenzene) derivatives. The compound exhibits *trans* geometry with respect to the azo double bond.

Comment

Diazenes have been the most widely used class of dyes, owing to their versatile applications in various fields, such as dyeing textile fibres, colouring different materials and plastics, biological–medical studies, and lasers, liquid-crystalline displays, electro-optical devices and ink-jet printers in high-technology areas (Catino & Farris, 1985; Gregory, 1991). The crystal and molecular structures of the title compound, (I), have been investigated in order to determine the conformation and also to confirm the stereochemistry.



(I)

A view of the molecule of (I) is shown in Fig. 1, and selected bond distances and angles are given in Table 1. The structure of (I) is very similar to those of azo compounds studied previously (Maginn, 1993; Işik *et al.*, 1997, 1998; Zhang *et al.*, 1998; Odabaşoğlu *et al.*, 2003). The two aromatic rings are in a *trans* configuration with respect to the azo double-bond.

The C—O(hydroxyl) [1.342 (2) Å], —N=N— [1.255 (2) Å, indicative of a double bond] and C—N [1.432 (2) Å, indicative of a single bond] bond lengths are consistent with values observed in related compounds (Işik *et al.*, 1997, 1998; Odabaşoğlu *et al.*, 2003). The C14—O3 bond [1.417 (2) Å] is approximately equal to that usually associated with a methyl C—O bond in a methoxy group attached to an aromatic ring (1.424 Å; Allen *et al.*, 1987).

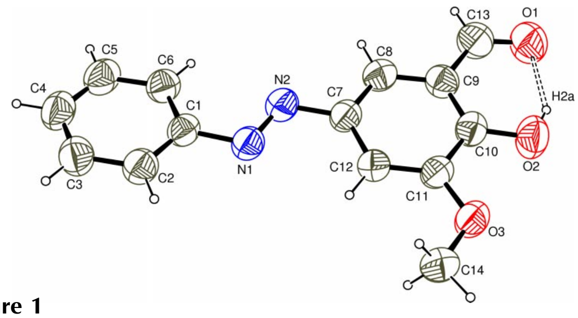


Figure 1
A view of the molecule of (I), showing the atom-labelling scheme and with displacement ellipsoids drawn at the 50% probability level.

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In (I), the dihedral angle θ_1, between the mean planes of the phenyl ring (C1–C6) and the C1—N1═N2—C7 azo bridge, is 8.9 (1)°. The angle θ_2 between the C1—N1═N2—C7 azo group and the substituted phenyl ring (C7–C12) is 1.0 (1)°. The angle θ_3 between the planes of the rings is 8.02 (8)°; thus the molecule is approximately planar.

The molecule of (I) contains a strong intramolecular O···O hydrogen bond [2.627 (2) Å; see Table 2 for details].

Experimental

The title compound, (I), was prepared using the literature method of Odabaşoğlu *et al.* (2003), with *o*-vanilline and aniline as starting materials (yield 95%; m.p. 422–424 K).

Crystal data

$C_{14}H_{12}N_2O_3$
$M_r = 256.26$
Orthorhombic, *Pbcn*
$a = 10.6039\ (11)$ Å
$b = 12.9904\ (14)$ Å
$c = 18.1168\ (14)$ Å
$V = 2495.6\ (4)$ Å^3
$Z = 8$
$D_x = 1.364$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 7873 reflections
$\theta = 1.9$–26.5°
$\mu = 0.10$ mm^{-1}
$T = 293\ (2)$ K
Prism, brown
0.40 × 0.37 × 0.31 mm

Data collection

Stoe IPDS2 diffractometer
ω scans
Absorption correction: by integration (*X-RED*32; Stoe & Cie, 2002)
$T_{\min} = 0.962$, $T_{\max} = 0.977$
16 964 measured reflections
2457 independent reflections
1503 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.137$
$\theta_{\max} = 26.0°$
$h = -13 \rightarrow 12$
$k = -16 \rightarrow 16$
$l = -22 \rightarrow 21$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.042$
$wR(F^2) = 0.100$
$S = 0.84$
2457 reflections
173 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0654P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.25$ e Å^{-3}
$\Delta\rho_{\min} = -0.17$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

C1—N1	1.4315 (18)	C13—O1	1.224 (2)
C7—N2	1.4176 (18)	C14—O3	1.4166 (19)
C10—O2	1.3425 (17)	N1—N2	1.2553 (17)
C11—O3	1.3578 (16)		
C6—C1—N1	123.64 (14)	O3—C11—C12	126.27 (14)
C2—C1—N1	116.68 (13)	O3—C11—C10	114.21 (12)
C8—C7—N2	115.15 (12)	O1—C13—C9	124.87 (16)
C12—C7—N2	124.64 (13)	N2—N1—C1	112.99 (12)
O2—C10—C9	122.46 (14)	N1—N2—C7	115.72 (12)
O2—C10—C11	117.62 (12)	C11—O3—C14	116.83 (11)

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2*A*···O1	0.82	1.91	2.627 (2)	146

H atoms were added at calculated positions and refined using a riding model, with isotropic displacement parameters equal to 1.2 (or 1.5 for methyl and hydroxyl H atoms) times the equivalent isotropic displacement parameter of the atom to which they are attached.

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED*32 (Stoe & Cie, 2002); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1990); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*-3 *for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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