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Key indicators

Single-crystal X-ray study
 $T = 296$ K
Mean $\sigma(\text{C}-\text{C}) = 0.003$ Å
 R factor = 0.034
 wR factor = 0.061
Data-to-parameter ratio = 13.1For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.**(E)-5-[(3-Chlorophenyl)diazenyl]-2-hydroxy-3-methoxybenzaldehyde**

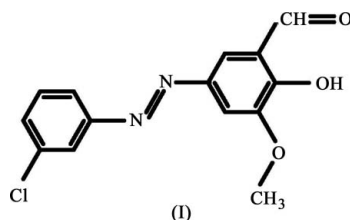
The title compound, $\text{C}_{14}\text{H}_{11}\text{ClN}_2\text{O}_3$, contains an azo group ($-\text{N}=\text{N}-$), and the configuration around the $-\text{N}=\text{N}-$ double bond is *trans*. There are intramolecular $\text{O}-\text{H}\cdots\text{O}$ and intermolecular $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds, and the crystal packing is stabilized by $\text{C}-\text{H}\cdots\pi$ and $\pi-\pi$ stacking interactions, forming a two-dimensional network.

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Comment

Azobenzene and its derivatives have attracted much attention for their high potential in industrial applications, such as liquid crystals, light-driven switches and image-storage devices (Liu *et al.*, 1990; Ikeda & Tsutsumi, 1995). In addition, azo compounds represent the dominant class of synthetic colorant employed in the textile, printing, agrochemical and pharmaceutical industries. As a result of the presence of the stable chromophoric azo group ($-\text{N}=\text{N}-$), linking different aromatic systems with electron-donating and/or electron-attracting groups, dyes can be designed to resist chemical or photochemical degradation processes (Evans *et al.*, 1980; Griffiths & Allen, 1980; Leaver *et al.*, 1980; Sharma *et al.*, 2002; Neta & Levanon, 1977; Flamingi & Monti, 1985).



The title compound, (I), contains two benzene groups linked through a diazene bridge. The dihedral angle between the mean planes of the C1–C6 benzene ring and the C1–N1=N2–C7 azo group is 10.51 (13)°, and that between the planes of the azo group and the C7–C12 benzene ring is 3.33 (13)°. The angle between the two benzene rings is 8.37 (11)°.

The O1–C14 bond length [1.429 (2) Å] is approximately equal to that usually associated with a C–O bond in a methoxy group attached to an azobenzene [1.419 (6) and 1.434 (4) Å; Crano *et al.*, 1994]. All the C–C bond lengths in the benzene rings have typical values; the average C–C bond lengths of these two rings are 1.376 and 1.388 Å. The C10–O2 bond length is 1.350 (2) Å, consistent with literature values (Jottier *et al.*, 1991; Stomberg *et al.*, 1998).

Analysis of the crystal packing (shown in Fig. 2) reveals that the molecules are linked by intramolecular $\text{O}-\text{H}\cdots\text{O}$ and weak intermolecular $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds (Table 2), forming a chain running parallel to the b axis. The crystal

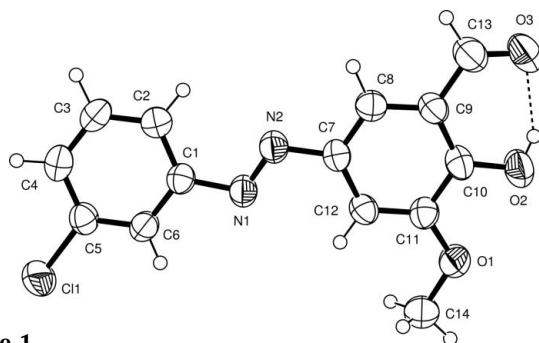


Figure 1
An ORTEP-3 drawing (Farrugia, 1997) of (I), showing the atom-numbering scheme and with 50% probability displacement ellipsoids. The dashed line indicates a hydrogen bond.

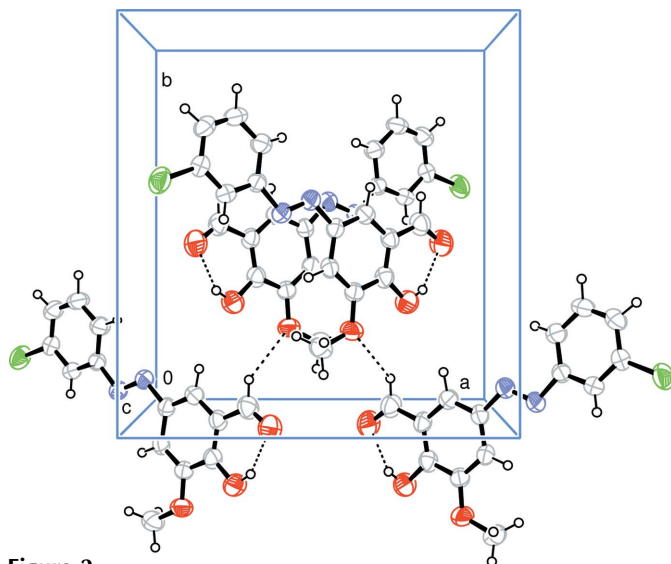


Figure 2
A packing view of (I). Hydrogen bonds are shown as dashed lines.

packing is further stabilized by π - π stacking interactions between the C1–C6 and C7–C12 benzene rings of molecules related by an inversion centre [the centroid–centroid distance is 3.8351 (13) Å], and by a C–H $\cdots\pi$ interaction [C14 \cdots Cgⁱⁱ = 3.743 (3) Å, H14B \cdots Cgⁱⁱ = 3.32 Å and C14–H14B \cdots Cgⁱⁱ = 109°; Cg is the centroid of the C1–C6 ring; symmetry code: (ii) $\frac{3}{2} - x, -\frac{1}{2} + y, z$].

Experimental

The title compound was prepared as described by Odabaşoğlu *et al.* (2003), using *o*-vanillin and 3-chloroaniline as starting materials (m.p. 427–429 K, yield 83%). Well shaped crystals were obtained by slow evaporation of an acetic acid solution.

Crystal data

C₁₄H₁₁ClN₂O₃
M_r = 290.70
Orthorhombic, *Pbcn*
a = 12.3199 (15) Å
b = 13.0849 (17) Å
c = 16.6349 (16) Å
V = 2681.6 (5) Å³
Z = 8
D_x = 1.440 Mg m⁻³

Mo K α radiation
Cell parameters from 4559 reflections
 θ = 2.3–26.2°
 μ = 0.29 mm⁻¹
T = 296 (2) K
Prism, red
0.42 × 0.25 × 0.16 mm

Data collection

Stoe IPDS-2 diffractometer
 ω scans
Absorption correction: integration
(*X-RED32*; Stoe & Cie, 2002)
T_{min} = 0.916, T_{max} = 0.971
10851 measured reflections
2364 independent reflections

1325 reflections with $I > 2\sigma(I)$
R_{int} = 0.055
 θ_{max} = 25.0°
h = -14 → 13
k = -15 → 15
l = -18 → 19

Refinement

Refinement on F²
R[F² > 2 σ (F²)] = 0.034
wR(F²) = 0.061
S = 0.93
2364 reflections
181 parameters

H-atom parameters constrained
w = 1/[$\sigma^2(F_o^2) + (0.0183P)^2$]
where P = (F_o² + 2F_c²)/3
(Δ/σ)_{max} < 0.001
 $\Delta\rho_{max}$ = 0.11 e Å⁻³
 $\Delta\rho_{min}$ = -0.16 e Å⁻³

Table 1

Selected geometric parameters (Å, °).

C1–C5	1.731 (2)	O3–C13	1.221 (2)
O1–C11	1.356 (2)	N1–N2	1.252 (2)
O1–C14	1.429 (2)	N1–C1	1.431 (2)
O2–C10	1.350 (2)	N2–C7	1.420 (2)
C4–C5–C11	119.30 (17)	O2–C10–C11	117.12 (18)
C6–C5–C11	119.61 (16)	O1–C11–C12	125.87 (19)
O2–C10–C9	122.14 (19)	O3–C13–C9	124.5 (2)
N2–N1–C1–C2	11.0 (3)	N1–N2–C7–C8	176.46 (18)

Table 2

Hydrogen-bond geometry (Å, °).

D–H \cdots A	D–H	H \cdots A	D \cdots A	D–H \cdots A
O2–H1 \cdots O3	0.82	1.91	2.629 (2)	146
C13–H13 \cdots O1 ⁱ	0.93	2.83	3.531 (3)	133

Symmetry code: (i) $-x + \frac{1}{2}, y + \frac{1}{2}, z$.

All H atoms were refined using a riding model, with C–H distances of 0.93 [$U_{iso}(H) = 1.2U_{eq}(C)$] or 0.96 Å [$U_{iso}(H) = 1.5U_{eq}(C)$] for methyl groups, and with an O–H distance of 0.82 Å [$U_{iso}(H) = 1.5U_{eq}(O)$].

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED32* (Stoe & Cie, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *PLATON* (Spek, 2003); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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