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(*E*)-4-[(4-Hydroxyphenyl)diazenyl]benzaldehyde

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.046
wR factor = 0.129
Data-to-parameter ratio = 14.0

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

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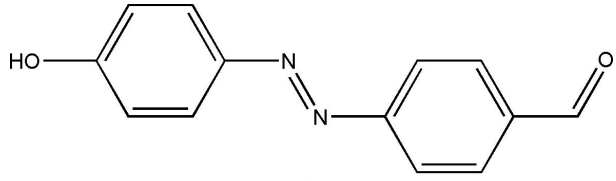
The title compound, $C_{13}H_{10}N_2O_2$, is approximately planar in the solid state and displays a *trans* configuration with respect to the azo double bond. Molecules form infinite chains linked by O—H···O hydrogen bonds along the *a* axis.

Comment

Azo compounds are widely utilized as dyes and indicators in chemistry and as stains in the biological field (Kumar & Neckers, 1989). Moreover, azobenzene and some azobenzene derivatives can undergo *cis–trans* isomerization under photochemical stimulation and may be involved in energy-transfer processes (Murakami *et al.*, 1997). We report here the synthesis and structure of the title compound, (I) (Fig. 1).



(I)

The molecule is approximately planar, with a mean deviation 0.026 (2) Å from the molecular plane. The dihedral angle between the planes of the two aromatic rings is 1.5 (3)°. Moreover, the title compound displays the expected *trans* configuration with respect to the azo double bond. O—H···O hydrogen bonds involving O atoms at either end of the molecule result in the formation of polymeric chains of molecules along the *a* axis (Figs. 2 and 3, and Table 1).

Experimental

Sodium nitrite (5 mmol) in water (10 ml) was added dropwise to 4-aminobenzaldehyde (4 mmol) dispersed in concentrated HCl (2 ml) at 273–278 K and the mixture stirred for 30 m. The resulting solution was added dropwise to Na_2CO_3 (10 mmol) and phenol (5 mmol) in water (40 ml) and stirred for 30 min. The red–orange

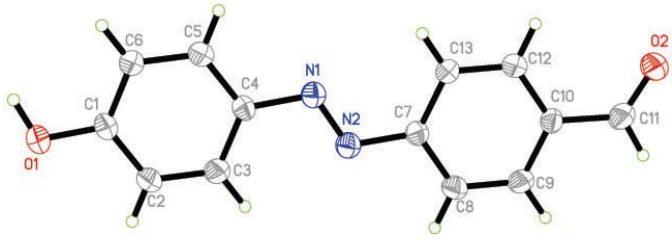


Figure 1
The molecular structure of (I), with atom labels and 30% probability ellipsoids. H atoms are shown as spheres of arbitrary radii.

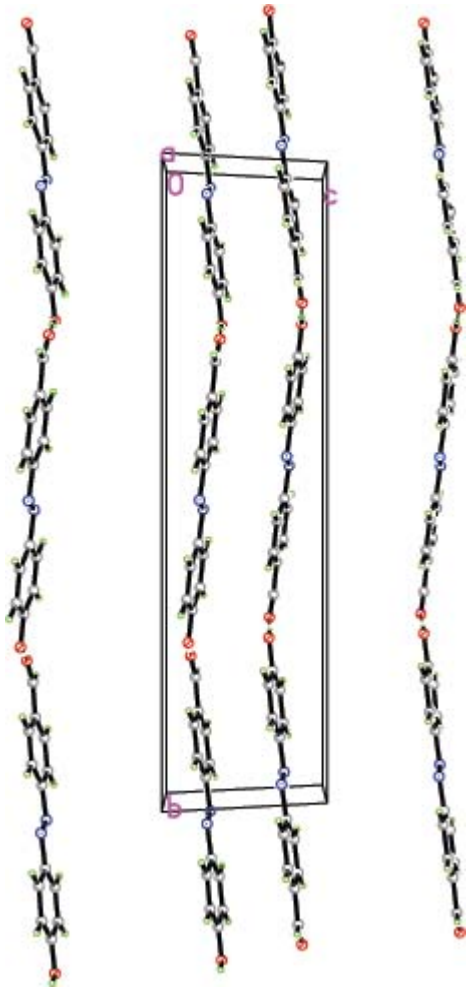


Figure 2
The crystal packing, viewed along the *a* axis, showing the polymeric chains.

precipitate of (I) was filtered and washed with water. ^{1}H NMR ($CDCl_3$): δ 5.21 (*s*, 1H), 6.97–6.99 (*d*, 2H), 7.92–8.05 (*m*, 6H), 10.10 (*s* 1H). Recrystallization from acetone over 10 d at ambient temperature gave colourless single crystals of (I).

Crystal data

$C_{13}H_{10}N_2O_2$
M_r = 226.23
Monoclinic, $P2_1/c$
a = 6.405 (2) Å
b = 25.820 (9) Å
c = 7.197 (2) Å
β = 114.140 (6)°
V = 1086.2 (6) Å^3
Z = 4
D_x = 1.383 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1178 reflections
θ = 3.2–23.6°
μ = 0.10 mm^{-1}
T = 293 (2) K
Block, colourless
0.20 × 0.14 × 0.08 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)
T_{min} = 0.972, T_{max} = 0.991
6049 measured reflections
2206 independent reflections
1083 reflections with $I > 2\sigma(I)$
R_{int} = 0.046
θ_{max} = 26.4°
$h = -7 \rightarrow 7$
$k = -32 \rightarrow 31$
$l = -8 \rightarrow 5$

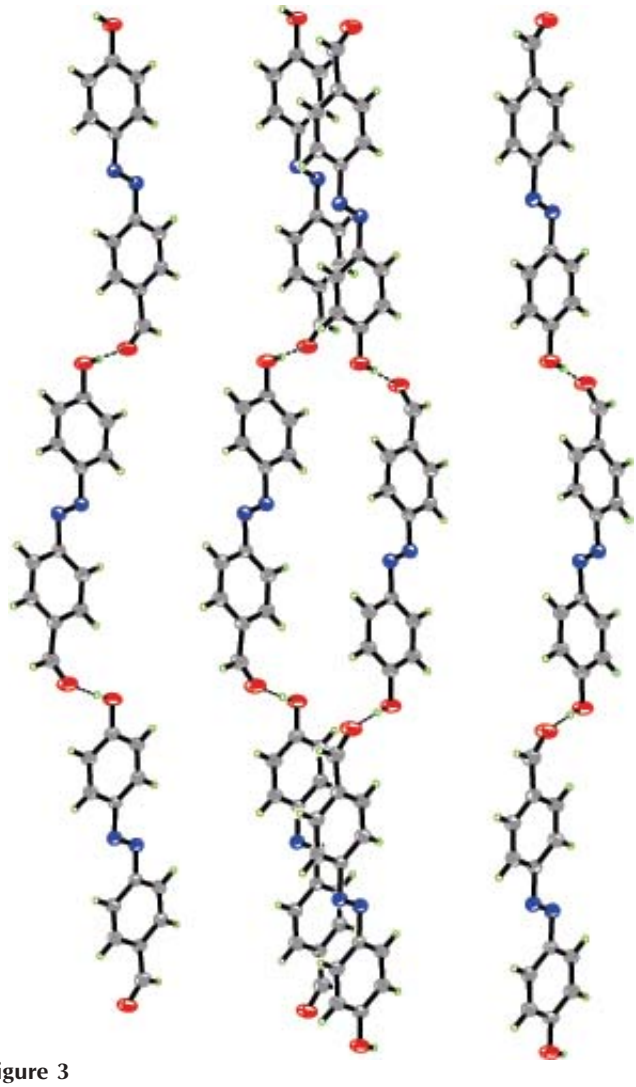


Figure 3
O—H···O hydrogen bonds (dashed lines), forming polymeric chains.

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.129
S = 1.00
2206 reflections
158 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0555P)^2 + 0.0666P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.14 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1A···O2^{i}	0.91 (3)	1.80 (3)	2.711 (3)	176 (3)

Symmetry code: (i) $1-x, y-\frac{1}{2}, \frac{3}{2}-z$.

The hydroxy H atom was located in a difference map and its coordinates and isotropic displacement parameter were freely refined. Other H atoms were positioned geometrically (C—H = 0.93 Å) and refined with a riding model, U_{iso}(H) = 1.2U_{eq}(carrier).

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

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