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4-[(Phenyldiazenyl)amino]benzaldehyde

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Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.004 Å
R factor = 0.037
wR factor = 0.094
Data-to-parameter ratio = 9.1

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

The title compound, $C_{13}H_{11}N_3O$, is essentially planar in the solid state and displays a *trans* configuration with respect to the azo double bond. The dihedral angle between the planes of the two aromatic rings is 4.9 (4)°. Molecules form infinite chains *via* N—H···O and C—H···O hydrogen bonds.

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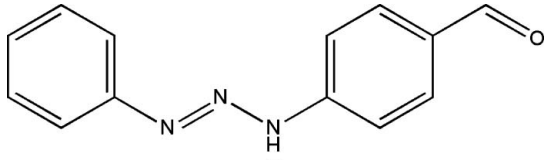
Comment

Aldehydes are important building blocks for pharmaceuticals and performance materials. Azo compounds are among the largest group of dyes, with over one thousand compounds commercially available. Azo dyes have been developed for coloring fibers, both natural and synthetic, and for the coloration of solvents and a wide range of nontextile substrates (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).



(I)

We report here the synthesis and structure of the title compound, (I) (Fig. 1). The bond lengths and angles have normal values and the N2═N3 bond length of 1.267 (3) Å compares well with the values (1.250–1.268 Å) found in (*E*)-4-[(4-hydroxyphenyl)diazenyl]benzaldehyde (Liu *et al.*, 2005), 2,6-dimethyl-4-(phenyldiazenyl)phenol (Soylu *et al.*, 2004) and 2-*tert*-butyl-4-methyl-6-(phenyldiazenyl)phenol (Kocaokutgen *et al.*, 2003), The molecule is essentially planar, the mean deviation being 0.0306 (2) Å. The dihedral angle between the planes of the two aromatic rings is 4.9 (4)°. Moreover, the title compound displays the expected *trans* configuration with respect to the azo double bond.

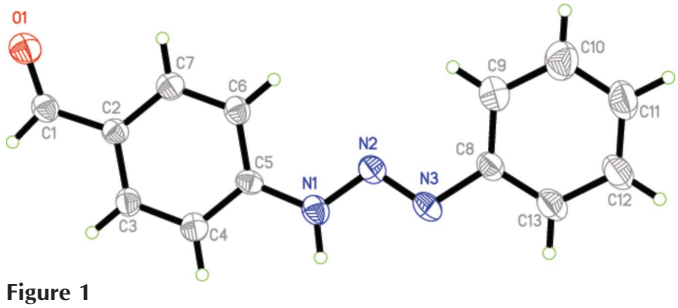


Figure 1
The molecular structure of (I), with atom labels and 30% probability ellipsoids. H atoms are drawn as spheres of arbitrary radius.

The molecules are linked into chains by N—H···O and C—H···O hydrogen bonds (Table 1 and Fig. 2).

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 min. The resulting solution was added dropwise to sodium acetate (10 mmol) and aniline (5 mmol) in water (40 ml) and stirred for 30 min. The brown 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 colorless single crystals of (I).

Crystal data

$C_{13}H_{11}N_3O$
M_r = 225.25
Orthorhombic, $P2_12_12_1$
a = 4.9916 (9) Å
b = 6.2388 (11) Å
c = 37.342 (7) Å
V = 1162.9 (4) Å^3
Z = 4
D_x = 1.287 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1750 reflections
θ = 3.3–25.3°
μ = 0.09 mm^{-1}
T = 294 (2) K
Block, brown
0.26 × 0.20 × 0.12 mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)
T_{min} = 0.970, T_{max} = 0.990
6580 measured reflections
1445 independent reflections
1016 reflections with $I > 2\sigma(I)$
R_{int} = 0.039
θ_{max} = 26.4°
$h = -6 \rightarrow 4$
$k = -7 \rightarrow 7$
$l = -42 \rightarrow 46$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.094
S = 1.08
1445 reflections
158 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0383P)^2 + 0.132P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.14 e Å^{-3}
$\Delta\rho_{min}$ = −0.15 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···O1^{i}	0.91 (3)	2.07 (3)	2.934 (3)	157 (3)
C4—H4···O1^{i}	0.93	2.56	3.286 (3)	135

Symmetry code: (i) $x+1, y-1, z$.

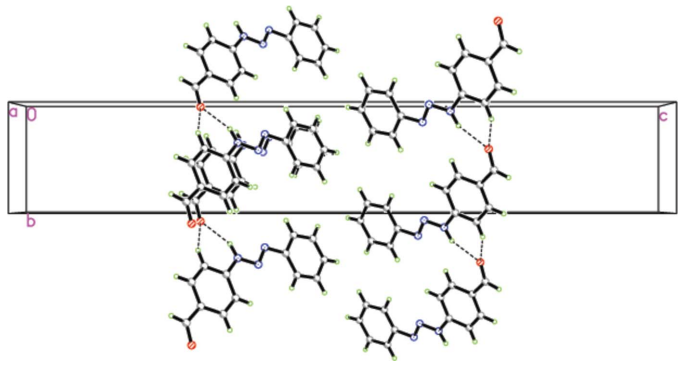


Figure 2
The crystal packing, viewed along the *a* axis. Hydrogen bonds are shown as dashed lines.

The N-bound H atom was located in a difference Fourier map and its coordinates and isotropic displacement parameter were freely refined. Other H atoms were positioned geometrically, with C—H = 0.93 Å and refined with a riding model; U_{iso}(H) = 1.2U_{eq}(carrier atom). In the absence of significant anomalous dispersion effects, Friedel pairs were averaged.

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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