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trans-Bis(2-aminophenyl)diazene

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Key indicators

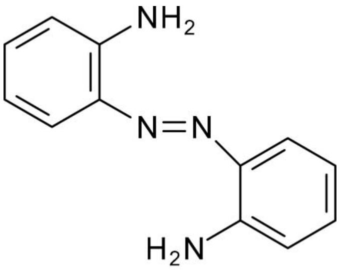
Single-crystal X-ray study
T = 100 K
Mean σ(C–C) = 0.002 Å
R factor = 0.034
wR factor = 0.098
Data-to-parameter ratio = 12.4

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

The title compound, $C_{12}H_{12}N_4$, is a *trans*-azobenzene which crystallizes with an inversion center at the midpoint of the N═N bond.

Comment

The family of azobenzenes has been investigated intensively due to the their remarkable photochemically induced *trans* → *cis* isomerism. Although the structures of many azobenzenes have been determined, some of the fundamental and synthetically important members of this family, such as the title compound, (I), (Fig. 1) have not been characterized. This report describes the 100 K structure of this highly functional member of the azobenzene family.



(I)

In (I) there is an inversion center at the mid-point of the N═N bond. The donating *o*amino substituents of (I) allow for numerous potential derivatives to be prepared (Skrabel & Hohl-Blumer, 1976; de Mendoza *et al.*, 1981) and they are also expected to influence the electronic structure of the azobenzene system. The $N1═N1^i$ [symmetry code: (i) $-x, -y, 1-z$] bond length of 1.2641 (18) Å in (I) is slightly greater than the average value of 1.257 Å for azobenzene N═N bonds found in the Cambridge Structural Database (Version 5.27; Allen, 2002). In addition, the relatively short C1—N1 bond length of 1.4131 (14) Å suggests some delocalization of electron density into the N═N π* orbital, although this needs to be confirmed by spectroscopic measurements. The molecular conformation of (I) appears to be stabilized by a weak intramolecular N—H···N hydrogen bond (Table 1).

Experimental

The title compound was prepared by surfactant-mediated aerial oxidation of *o*-phenylenediamine in toluene by literature methods (de Mendoza *et al.*, 1981). Crystals of (I) suitable for X-ray diffraction were obtained by slow evaporation of a toluene solution.

Crystal data

$C_{12}H_{12}N_4$
$M_r = 212.26$
Monoclinic, $C2/c$
$a = 22.278$ (6) Å
$b = 5.8647$ (16) Å
$c = 8.254$ (2) Å
$\beta = 106.357$ (3)°
$V = 1034.8$ (5) Å^3
$Z = 4$
$D_x = 1.362$ Mg m^{-3}
$D_m = 1.32$ Mg m^{-3}
D_m measured by flotation **in ????**
Mo $K\alpha$ radiation
$\mu = 0.09$ mm^{-1}
$T = 100$ (2) K
Block, orange–red
0.20 × 0.10 × 0.07 mm

Data collection

Siemens SMART CCD diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Siemens, 1996)
$T_{\min} = 0.983$, $T_{\max} = 0.990$
3927 measured reflections
1003 independent reflections
929 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.021$
$\theta_{\max} = 25.9°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.034$
$wR(F^2) = 0.098$
$S = 1.03$
1003 reflections
81 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0584P)^2 + 0.6927P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.27$ e Å^{-3}
$\Delta\rho_{\min} = -0.18$ e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2A···N1	0.884 (18)	2.330 (17)	2.7064 (15)	105.7 (13)

The N-bound H atoms were located in difference maps and their positions and $U_{\rm iso}$ values were freely refined. The C-bound H atoms were located in difference maps and then repositioned in idealized locations (C—H = 0.93 Å) and refined as riding, with $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}({\rm C})$.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Siemens, 1996); software used to prepare material for publication: *SHELXTL*.

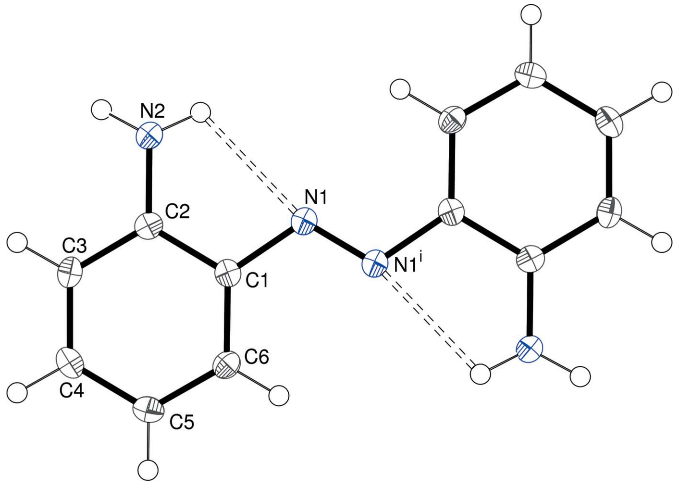


Figure 1
View of the molecular structure of (I), showing 50% displacement ellipsoids (arbitrary spheres for the H atoms). [Symmetry code: (i) $-x$, $-y$, $1 - z$.]

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