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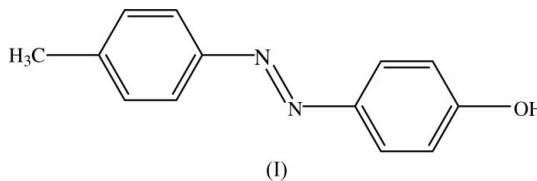
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Key indicators

Single-crystal X-ray study
 $T = 296$ K
Mean $\sigma(C-C) = 0.003$ Å
 R factor = 0.054
 wR factor = 0.160
Data-to-parameter ratio = 18.4For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.**(E)-4-(p-Tolyldiazenyl)phenol**The title compound, $C_{13}H_{12}N_2O$, consisting of two aromatic groups linked through a diazene bridge, exhibits *trans* geometry with respect to the azo double bond and deviates slightly from planarity. The crystal structure is stabilized by intermolecular $O-H \cdots N$ hydrogen bonds.Received 12 October 2006
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Comment

Azo compounds have been the most widely used class of dyes because of their versatile applications in various fields such as dyeing textile fibres, coloring different materials, plastics, biological medical studies, lasers, liquid crystalline displays, electro-optical devices and ink-jet printers in high-technology areas (Catino & Farris, 1985; Gregory, 1991).

Azo compounds are known to exist in two forms, *cis* and *trans*. The *trans*-to-*cis* isomerization occurs by photo-irradiation with UV light and *cis*-to-*trans* isomerization proceeds with blue-light irradiation or by heating, because their *trans* forms are thermodynamically more stable than their *cis* forms (Azuki *et al.*, 2001; Grebenkin & Bolshakov, 1999).In the crystal structure of the title compound, (I), the aromatic rings, which adopt a *trans* configuration around the $N=N$ bond, are inclined with respect to each other by $10.56(13)^\circ$. In the azo groups, the $N1-C4$ and $N2-C7$ bond lengths, which reflect their single-bond character, are 1.428 (3) and 1.439 (3) Å, respectively, whereas the $N1=N2$ bond length of 1.248 (2) Å is indicative of double-bond character. These values are consistent with those reported for other *trans*-azo compounds (Atalay *et al.*, 2006). The crystal structure is stabilized by $O-H \cdots N$ intermolecular hydrogen bonds (Fig. 2).

Experimental

A mixture of 4-methylaniline (2 g, 18.6 mmol), water (50 ml) and concentrated hydrochloric acid (4.71 ml, 55.9 mmol) was stirred until a clear solution was obtained. This solution was cooled to 273–278 K and a solution of sodium nitrite (1.8 g, 26 mmol) in water (15 ml) was added dropwise while the temperature was maintained below 278 K. The resulting mixture was stirred for 30 min in an ice bath. Phenol (1.76 g, 18.6 mmol) solution (pH 9) was gradually added to a cooled solution of 4-methylbenzenediazonium chloride, prepared as

described above, and the resulting mixture was stirred at 273–278 K for 60 min in an ice bath. The product was recrystallized from ethyl alcohol to obtain solid (*E*)-4-(*p*-tolylazo)phenol. Crystals of (*E*)-4-(*p*-tolylazo)phenol were obtained after 1 d by slow evaporation of an acetic acid solution (yield 95%, m.p. 427–428 K).

Crystal data

$C_{13}H_{12}N_2O$	$Z = 4$
$M_r = 212.25$	$D_x = 1.276 \text{ Mg m}^{-3}$
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation
$a = 5.6140 (5) \text{ \AA}$	$\mu = 0.08 \text{ mm}^{-1}$
$b = 17.8226 (14) \text{ \AA}$	$T = 296 \text{ K}$
$c = 11.0657 (10) \text{ \AA}$	Prism, yellow
$\beta = 93.720 (7)^\circ$	$0.34 \times 0.29 \times 0.24 \text{ mm}$
$V = 1104.86 (16) \text{ \AA}^3$	

Data collection

Stoe IPDS-II diffractometer	2519 independent reflections
ω scans	1314 reflections with $I > 2\sigma(I)$
Absorption correction: none	$R_{\text{int}} = 0.107$
13022 measured reflections	$\theta_{\text{max}} = 27.5^\circ$

Refinement

Refinement on F^2	H atoms treated by a mixture of independent and constrained refinement
$R[F^2 > 2\sigma(F^2)] = 0.054$	$w = 1/[\sigma^2(F_o^2) + (0.0743P)^2]$
$wR(F^2) = 0.160$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.03$	$(\Delta/\sigma)_{\text{max}} < 0.001$
2519 reflections	$\Delta\rho_{\text{max}} = 0.19 \text{ e \AA}^{-3}$
137 parameters	$\Delta\rho_{\text{min}} = -0.16 \text{ e \AA}^{-3}$

Table 1

Selected geometric parameters (\AA , $^\circ$).

O1–C1	1.356 (2)	C10–C13	1.507 (3)
C3–C4–N1	115.2 (2)	O1–C1–C2	123.06 (19)
C12–C7–N2	116.3 (2)	C7–N2–N1–C4	178.85 (15)
C7–N2–N1–C4	178.85 (15)	N1–C4–C3–C2	179.61 (18)
N1–C4–C3–C2	179.61 (18)	N2–C7–C12–C11	−179.8 (2)
O1–C1–C2–C3	−179.21 (18)	C13–C10–C11–C12	179.9 (2)

Table 2

Hydrogen-bond geometry (\AA , $^\circ$).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1–H1 \cdots N2 ⁱ	0.93 (4)	1.93 (4)	2.853 (2)	174 (3)

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

Hydroxyl atom H1 was refined freely. All other H atoms were positioned geometrically and refined using a riding model, fixing the aromatic C–H distances at 0.93 \AA and methyl C–H distances at 0.96 \AA . $U_{\text{iso}}(\text{H})$ values were calculated as $1.5U_{\text{eq}}(\text{C})$ (methyl group) or $1.2U_{\text{eq}}(\text{C})$ (other H atoms).

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED* (Stoe & Cie, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular

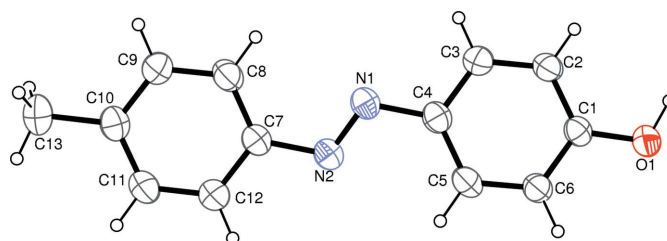


Figure 1

The molecular structure of (I), with the atom-numbering scheme and 30% probability displacement ellipsoids.

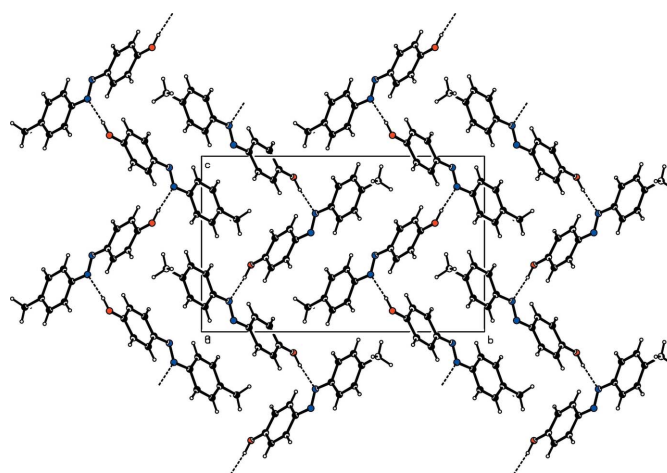


Figure 2

The crystal packing of (I), viewed down the *a* axis. Dashed lines indicate hydrogen bonds.

graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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