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4-(3-Methoxyphenyldiazenyl)-2-methylphenol

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Key indicators

Single-crystal X-ray study
T = 296 K
Mean σ(C–C) = 0.003 Å
R factor = 0.048
wR factor = 0.138
Data-to-parameter ratio = 14.8

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

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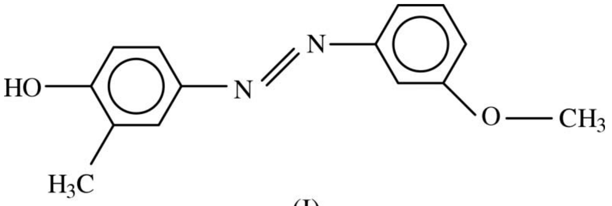
In the molecule of the title compound, $C_{14}H_{14}N_2O_2$, the two rings display a *trans* configuration with respect to the N═N double bond. The molecules are linked by intermolecular O—H···N hydrogen bonds, forming a three-dimensional network.

Comment

Azo compounds are the most widely used class of dyes, due to their versatile application in various fields, such as the dyeing of textiles and fibres, the coloring of different materials, and high-technology areas, such as electro-optical devices and inkjet printers (Peters & Freeman, 1991).



(I)

The molecular structure of the title compound, (I), is shown in Fig. 1. The bond lengths and angles (Table 1) are within normal ranges (Allen *et al.*, 1987). Compound (I) consists of two aromatic groups linked through an azo bridge. The rings *A* (C1–C6) and *B* (C8–C13) adopt a *trans* configuration with respect to the N═N double bond, as observed in other azo compounds (Albayrak *et al.*, 2004). The dihedral angle between the rings is 17.45 (10)°.

The crystal structure is stabilized by the intermolecular O–H···N hydrogen bonds (Table 2), forming a three-dimensional network (Fig. 2).

Experimental

A mixture of *m*-anisidine (4 g, 32.4 mmol), water (50 ml) and concentrated hydrochloric acid (8.14 ml, 97.2 mmol) was stirred until a clear solution was obtained. This solution was cooled to 273–278 K and a nitrite solution (3.13 g, 45.36 mmol) in water was added dropwise, while the temperature was maintained below 278 K. The resulting mixture was stirred for 30 min in an ice bath and *o*-cresol (3.5 g, 32.4 mmol) solution (pH 9) was gradually added by stirring at 273–278 K for 60 min. The product was recrystallized from ethyl alcohol to obtain solid 2-methyl-4-(3-methoxyphenylazo)phenol. The crystals were obtained after 1 d by slow evaporation of an acetonitrile solution (yield 4.1 g, 53%, m.p. 381–384 K).

Crystal data

$C_{14}H_{14}N_2O_2$
$M_r = 242.27$
Monoclinic, $P2_1/n$
$a = 10.2449$ (11) Å
$b = 9.2512$ (7) Å
$c = 13.7955$ (14) Å
$\beta = 107.257$ (8)°
$V = 1248.6$ (2) Å^3
$Z = 4$
$D_x = 1.289$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2829 reflections
$\theta = 2.1$–28.3°
$\mu = 0.09$ mm^{-1}
$T = 296$ (2) K
Prism, orange
0.58 × 0.39 × 0.17 mm

Data collection

Stoe IPDS-II diffractometer
ω scans
Absorption correction: integration (*X-RED32*; Stoe & Cie, 2002)
$T_{\min} = 0.959$, $T_{\max} = 0.985$
12623 measured reflections
2456 independent reflections
1659 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.046$
$\theta_{\max} = 26.0°$
$h = -12 \rightarrow 12$
$k = -11 \rightarrow 11$
$l = -16 \rightarrow 16$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.048$
$wR(F^2) = 0.138$
$S = 1.04$
2456 reflections
163 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0819P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.31$ e Å^{-3}
$\Delta\rho_{\min} = -0.24$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

C1—N1	1.437 (2)	C11—O2	1.360 (2)
C8—N2	1.405 (2)	N1—N2	1.256 (2)
C6—C1—N1	123.40 (16)	C13—C8—N2	126.43 (17)
C2—C1—N1	116.68 (17)	C9—C8—N2	114.95 (16)
O1—C5—C6	115.23 (17)	N2—N1—C1	113.17 (15)
O1—C5—C4	124.24 (18)	N1—N2—C8	116.40 (16)
C14—C10—C11—O2	2.6 (3)	C1—N1—N2—C8	−178.25 (16)
O2—C11—C12—C13	176.8 (2)		

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2···N1$^{\rm i}$	0.82	2.12	2.902 (2)	159

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

H atoms were positioned geometrically [0.82 (OH), 0.93 (CH) and 0.96 (CH$_3$) Å] and constrained to ride on their parent atoms with $U_{\rm iso}$(H) = 1.5 (1.2 for CH) $U_{\rm eq}$(C/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 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

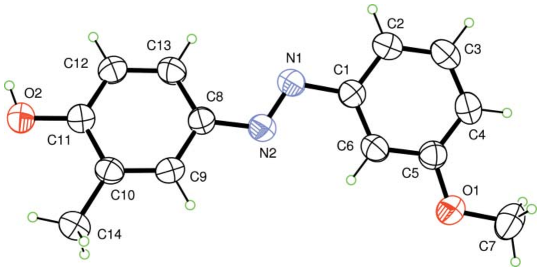


Figure 1
An *ORTEP* drawing of (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

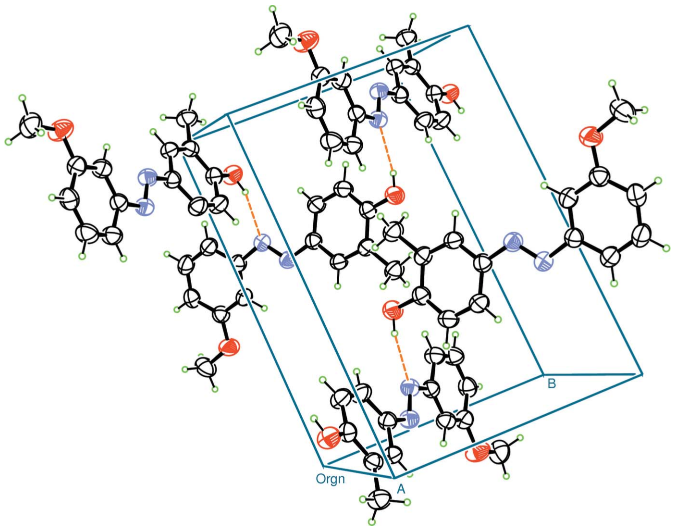


Figure 2
Packing diagram of (I). Hydrogen bonds are indicated by dashed lines.

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