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4-(4-Methylphenylazo)-2-allylphenol monohydrate

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.008 Å
Disorder in main residue
R factor = 0.068
wR factor = 0.180
Data-to-parameter ratio = 13.0

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

In the title compound, $C_{16}H_{16}N_2O\cdot H_2O$, the azobenzene moiety has a *trans* configuration, and the two phenyl rings are inclined with respect to each other by 14.23 (17)°. There are intermolecular O—H···O and O—H···N hydrogen bonds involving the water molecule.

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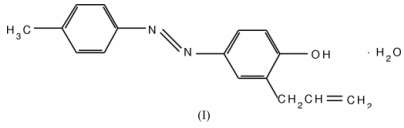
Comment

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 fibers, the coloring of different materials, and high-technology areas, such as electro-optical devices and ink-jet printers (Peters & Freeman, 1991).



(I)

The molecular structure of (I) is shown in Fig. 1 with the atom numbering scheme. The compound contains two benzene rings (C1–C6 and C7–C12), and an azo linkage (C4—N1—N2—C7). The benzene rings adopt a *trans*-configuration about the azo functional group, as observed in the crystal structure of other azo compounds. Atom C15 of the allyl group shows a positional disorder over two sites, C15*A* and C15*B*. The allyl C14—C15*A*—C16 moiety is twisted out of the plane of its attached benzene ring by 74.08 (2)°. All the C—C bond distances in the benzene rings have typical Csp^2—Csp^2 values. The average C—C bond distances within these two

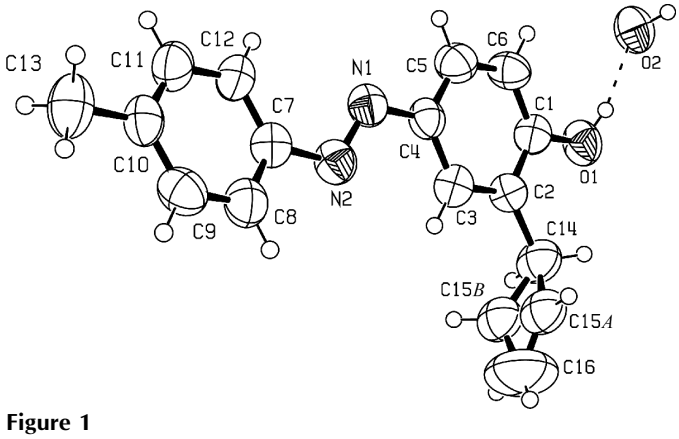


Figure 1
The molecular structure of (I), showing the atom-numbering scheme. Displacement ellipsoids for non-H atoms are shown at the 50% probability level. The hydrogen bond is indicated by a dashed line. The site-occupancy factors of C15*A* and C15*B* are 0.677 (10) and 0.323 (10), respectively.

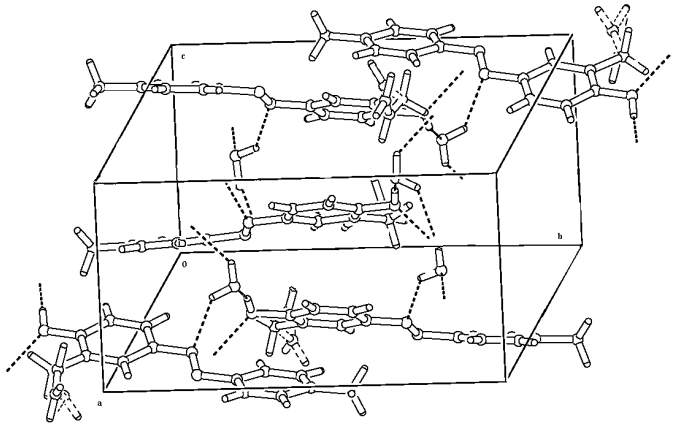


Figure 2
The crystal structure of (I). Hydrogen bonds are indicated by dashed lines.

rings are 1.370 (7) and 1.410 (7) Å. The N1═N2 bond length of 1.272 (5) Å is typical for a double bond and this is approximately equal to a previously reported N═N double-bond length (Odabaşoğlu, *et al.*, 2003; Domański *et al.*, 2001; Yatsenko & Paseshnichenko, 2001). The C—O bond length is 1.378 (6) Å and agrees with the literature value (Jottier *et al.*, 1991; Stomberg *et al.*, 1998). There are intermolecular O—H···O and O—H···N hydrogen bonds involving the water molecule (Fig. 2 and Table 2).

Experimental

The title compound (I) was obtained as described previously (Odabaşoğlu, *et al.*, 1999). Single crystals of (I) suitable for X-ray diffraction analysis were obtained by slow evaporation of an ethyl alcohol solution over 2 d (yield 85%; m.p. 357–358 K).

Crystal data

$C_{16}H_{16}N_2O\cdot H_2O$
M_r = 270.32
Orthorhombic, *Pbcn*
a = 27.2961 (9) Å
b = 14.4293 (17) Å
c = 7.568 (4) Å
V = 2980.8 (16) Å^3
Z = 8
D_x = 1.205 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 3655 reflections
θ = 1.5–21.6°
μ = 0.08 mm^{-1}
T = 293 K
Prism, light brown
0.30 × 0.17 × 0.10 mm

Data collection

Stoe IPDS 2 diffractometer
ω rotation scans
Absorption correction: none
17874 measured reflections
2629 independent reflections
806 reflections with $I > 2\sigma(I)$
R_{int} = 0.175
θ_{max} = 25.0°
$h = -32 \rightarrow 32$
$k = -17 \rightarrow 17$
$l = -8 \rightarrow 8$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.069
$wR(F^2)$ = 0.180
S = 0.88
2629 reflections
202 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.062P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.030
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}
Extinction correction: *SHELXL*
Extinction coefficient: 0.0040 (6)

Table 1
Selected geometric parameters (Å, °).

O1—C1	1.378 (6)	C2—C3	1.403 (7)
N1—N2	1.272 (5)	C2—C14	1.520 (7)
N1—C4	1.441 (6)	C3—C4	1.410 (7)
N2—C7	1.450 (6)	C4—C5	1.348 (7)
C1—C6	1.374 (7)	C5—C6	1.383 (7)
C1—C2	1.392 (7)		
N2—N1—C4	114.8 (5)	C5—C4—C3	120.1 (5)
N1—N2—C7	111.9 (5)	C5—C4—N1	117.0 (5)
C6—C1—O1	120.9 (6)	C8—C7—N2	114.8 (6)
O1—C1—C2	116.9 (5)	C12—C7—N2	124.4 (6)
C4—N1—N2—C7	−178.1 (5)		

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···O2	0.82	1.91	2.674 (6)	154.8
O2—H1A···N1^{i}	0.87 (2)	2.22 (12)	2.908 (7)	136 (14)
O2—H1B···O1^{ii}	0.84 (2)	2.17 (9)	2.864 (6)	140 (12)

Symmetry codes: (i) $\frac{1}{2}-x, y-\frac{1}{2}, z$; (ii) $\frac{1}{2}-x, \frac{1}{2}-y, z-\frac{1}{2}$.

The R_{int} was relatively poor (0.17). As a result of the long unit-cell dimension, a = 27.2961 (9) Å, the diffraction spots were close to each other and their integration might introduce some error in the intensity data. Atom C15 of the allyl group shows positional disorder over two sites, C15*A* and C15*B*, with occupation factors of 0.677 (10) and 0.323 (10), respectively. The positions of the H atoms bonded to C14 and C16 were calculated, neglecting the minor component (C15*B*). The atomic displacement parameters of C15*A* and C15*B* were restrained to be equal to those of C14. The H atoms of the water molecule were found and refined. All other H atoms were placed in calculated positions and refined using a riding model, with fixed C—H distances of 0.93 Å for Csp^2—H bonds and 0.96 Å for methyl C—H bonds and 0.93–0.97 for methylene C—H, and an O—H distance of 0.82 Å. Their U_{iso} parameters were fixed at 1.2U_{eq}(C—H and O—H) and 1.5U_{eq}(methyl groups) of the parent atoms.

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED*32 (Stoe & Cie, 2002); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*III (Burnett & Johnson, 1996); *PLUTON* (Spek, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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