Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2-Acetyl-4-(4-ethoxyphenyldiazenyl)phenol

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Key indicators

Single-crystal X-ray study
T = 296 K
Mean σ(C–C) = 0.004 Å
R factor = 0.053
wR factor = 0.173
Data-to-parameter ratio = 15.1

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

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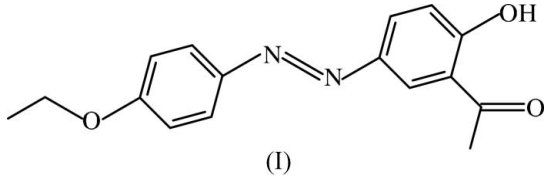
Received 12 July 2005
Accepted 7 September 2005
Online 14 September 2005

In the title structure, $C_{16}H_{16}N_2O_3$, the benzene rings are in a *trans* configuration with respect to the azo double bond and the molecule is essentially planar.

Comment

Azo compounds have been the most widely used class of dyes owing to their versatile application in various fields, such as dyeing textile fibres, colouring different materials, plastics, biological medical studies, lasers, liquid crystalline displays, electrooptical devices and ink-jet printers in high-technology areas (Catino & Farris, 1985; Gregory, 1991). In azo compounds, conversion from the *trans* to the *cis* form can lead to photochromism. Photochromic compounds are of great interest for the control and measurement of radiation intensity, optical computers and display systems (Dürr & Bouas-Laurent, 1990), and for potential applications in molecular electronic devices (Martin *et al.*, 1995). As part of a general study of the crystal chemistry of dyes, and to provide templates for molecular-modelling studies, the crystal structure of the title compound, (I), has been determined.



(I)

The molecular structure of (I) is shown in Fig. 1 and selected geometric parameters are given in Table 1. The bond lengths and angles of the azo group are as expected. The molecule is essentially planar, with dihedral angles between the mean planes of the benzene rings and the C1—N1═N2—C7 azo bridge of 6.19 (6) and 4.12 (4) Å for rings C1–C6 and C7–C12, respectively. The angle between the planes of the two benzene rings is 10.14 (4) Å. Apart from the expected intramolecular O—H···O hydrogen bond (Table 2) there are no other significant hydrogen-bond interactions, the closest contacts being of the types C—H···O and C—H···π, with distances *ca* 2.7 Å for H···O and H···π(ring centroid).

Experimental

The compound was prepared from 4-ethoxyaniline and 2-hydroxyacetophenone (Deveci *et al.*, 2005). Crystals of 2-acetyl-4-(4-ethoxyphenyldiazenyl)phenol were obtained after 1 d by slow evaporation of an acetonitrile solution (yield 56%, m.p. 408–410 K).

Crystal data

$C_{16}H_{16}N_2O_3$
M_r = 284.31
Orthorhombic, *Pbca*
a = 7.2099 (5) Å
b = 13.6448 (9) Å
c = 29.631 (3) Å
V = 2915.0 (4) Å^3
Z = 8
D_x = 1.296 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 13929 reflections
θ = 2.8–27.9°
μ = 0.09 mm^{-1}
T = 296 K
Plate, brown
0.80 × 0.39 × 0.06 mm

Data collection

Stoe IPDS-2 diffractometer
ω scans
Absorption correction: integration (*X-RED32*; Stoe & Cie, 2002)
T_{min} = 0.951, T_{max} = 0.994
19031 measured reflections
2864 independent reflections
1211 reflections with $I > 2\sigma(I)$
R_{int} = 0.111
θ_{max} = 26.0°
$h = -8 \rightarrow 8$
$k = -16 \rightarrow 16$
$l = -36 \rightarrow 36$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.053
$wR(F^2)$ = 0.173
S = 0.89
2864 reflections
190 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0811P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.12 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

C1—C6	1.382 (4)	C8—C9	1.373 (4)
C3—C4	1.403 (4)	C10—O1	1.350 (4)
C4—O3	1.359 (3)	C10—C11	1.397 (4)
C7—C12	1.377 (4)	C13—O2	1.242 (4)
C7—C8	1.398 (4)		
C9—C10—C11	121.1 (3)	O3—C15—C16	107.1 (3)
C12—C11—C13	121.9 (3)	C4—O3—C15	118.4 (2)
C11—C13—C14	121.7 (3)		
C1—N1—N2—C7	178.4 (3)	C3—C4—O3—C15	−173.1 (3)

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

*Cg*1 is the centroid of the C1–C6 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···O2	0.82	1.83	2.555 (4)	146
C14—H14*C*···O1^{i}	0.96	2.70	3.464 (4)	137
C16—H16*C*···*Cg*1^{ii}	0.96	2.75	3.617 (4)	149

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

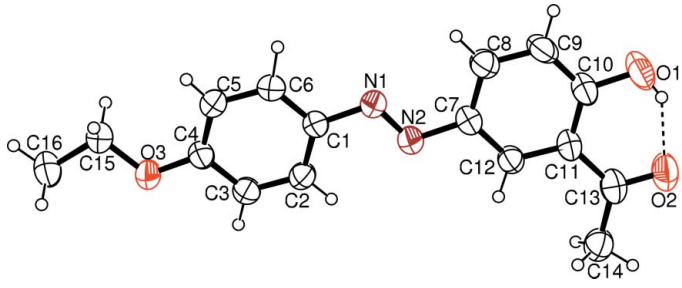


Figure 1
A view of (I), showing the atom-numbering scheme and 50% probability displacement ellipsoids. The dashed line indicates an intramolecular hydrogen bond

All H atoms were positioned geometrically and refined using a riding model, with C—H = 0.93–0.97 Å and O—H = 0.82 Å. U_{iso}(H) values were set at 1.2U_{eq}(C) or 1.5U_{eq}(O or C_{methyl}).

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: *ORTEP3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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