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2-Acetyl-4-(2-chorophenyldiazenyl)phenol

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Key indicators

Single-crystal X-ray study
T = 296 K
Mean σ(C–C) = 0.002 Å
R factor = 0.038
wR factor = 0.111
Data-to-parameter ratio = 15.9

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

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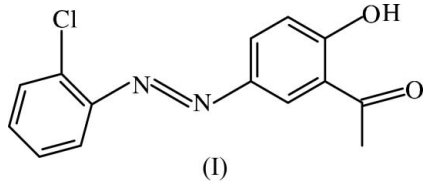
In the title structure, $C_{14}H_{11}N_2O_2Cl$, the benzene rings are in a *trans* configuration with respect to the azo double bond and the molecule is essentially planar.

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, a conversion from the *trans* to *cis* form can be effected by exposure to UV radiation and 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), was determined.



(I)

The molecular structure of (I) is shown in Fig. 1 and selected geometric parameters are given in Table 1. The bond

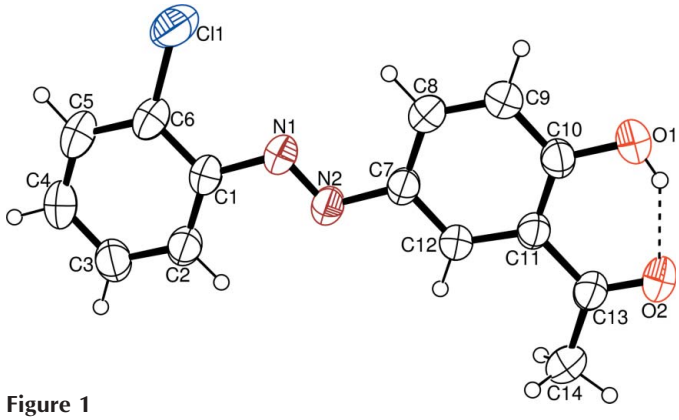


Figure 1
A view of (I), showing the atom-numbering scheme and 50% probability displacement ellipsoids. A dashed line indicates the intramolecular hydrogen bond.

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 7.34 (19) and 4.3 (2)° for C1–C6 and C7–C12, respectively. The angle between the planes of the two bezene rings is 3.73 (9)°. Apart from an expected intramolecular O—H···O hydrogen bond (Table 2) there are no other significant hydrogen-bond interactions.

Experimental

A mixture of 2-chloroaniline (1 g, 7.8 mmol), water (20 ml) and concentrated hydrochloric acid (1.97 ml, 23.4 mmol) was stirred until a clear solution was obtained. This solution was cooled to 273–278 K and a solution of sodium nitrite (0.75 g, 7.8 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. 2-Hydroxyacetophenone (1.067 g, 7.8 mmol) solution (pH 9) was gradually added to a cooled solution of 2-chlorobenzenediazonium 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 2-acetyl-4-(2-chorophenyldiazenyl)phenol. Crystals of (I) were obtained after 1 d by slow evaporation of a methanol solution (yield 80%, m.p. 424–426 K).

Crystal data

$C_{14}H_{11}ClN_2O_2$
M_r = 274.70
Monoclinic, $C2/c$
a = 10.8170 (9) Å
b = 9.3912 (6) Å
c = 25.3745 (18) Å
β = 95.576 (6)°
V = 2565.5 (3) Å^3
Z = 8
D_x = 1.422 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 8416 reflections
θ = 1.6–28.0°
μ = 0.30 mm^{-1}
T = 296 K
Plate, brown
0.40 × 0.29 × 0.11 mm

Data collection

Stoe IPDS-2 diffractometer
ω scans
Absorption correction: integration (*X-RED32*; Stoe & Cie, 2002)
T_{min} = 0.888, T_{max} = 0.972
10193 measured reflections
3074 independent reflections
1746 reflections with $I > 2\sigma(I)$
R_{int} = 0.049
θ_{max} = 28.0°
$h = -14 \rightarrow 14$
$k = -12 \rightarrow 12$
$l = -33 \rightarrow 33$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.111
S = 0.92
3074 reflections
193 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0615P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.0024 (6)

Table 1
Selected geometric parameters (Å, °).

C1—C2	1.385 (2)	C10—C11	1.400 (2)
C1—C6	1.394 (2)	C11—C12	1.397 (2)
C4—C5	1.361 (3)	C13—O2	1.226 (2)
C7—C8	1.396 (2)	N1—N2	1.2475 (18)
C10—O1	1.3391 (19)		
C2—C1—N1	124.39 (14)	C12—C11—C13	121.83 (15)
C1—C6—Cl1	120.10 (14)	O2—C13—C11	119.89 (16)
C8—C7—N2	124.65 (14)	C11—C13—C14	120.70 (16)
O1—C10—C11	122.29 (14)	N2—N1—C1	113.87 (13)
C1—N1—N2—C7	−179.37 (12)		

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1*O*···O2	0.82	1.81	2.5327 (19)	146

All H atoms, except for H2, H4, H5, H8 and H9, were treated using a riding model, with C—H = 0.93–0.96 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}). The remaining H atoms were refined isotropically [C—H = 0.82 (2)–0.96 (2) Å and U_{iso}(H) = 0.058 (5)–0.126 (9) Å^2].

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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