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(*E*)-2-Acetyl-4-[(3-chlorophenyl)diazenyl]phenol

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.043
wR factor = 0.134
Data-to-parameter ratio = 17.9

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

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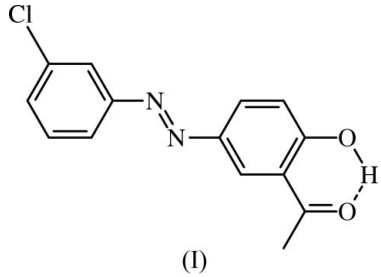
The molecule of the title compound, $C_{13}H_{10}ClN_2O_2$, is essentially planar and displays a *trans* configuration with respect to the central N=N double bond. The dihedral angle between the two aromatic rings is 0.73 (16)°. There is a strong intramolecular O—H···O hydrogen-bonding interaction which stabilizes the molecular structure.

Comment

The extensive application of azo dyes in industry and analytical determinations has attracted attention for decades. Azo dyes incorporating 'push–pull' donor–acceptor aryl rings are of great commercial importance for the dyeing of textiles (Zollinger, 1994).



(I)

The molecular structure of (I) is shown in Fig. 1 with the atom-numbering scheme. Selected bond lengths and angles are listed in Table 1. In the azo group, the N1—C1 and N2—C7 bond lengths indicate significant single-bond character, whereas the N1=N2 bond length is indicative of significant double-bond character.

The molecule is essentially planar, the dihedral angle formed by the aromatic rings being 0.73 (16)°. A strong intramolecular O—H···H hydrogen bond (Table 2) stabilizes the molecular structure.

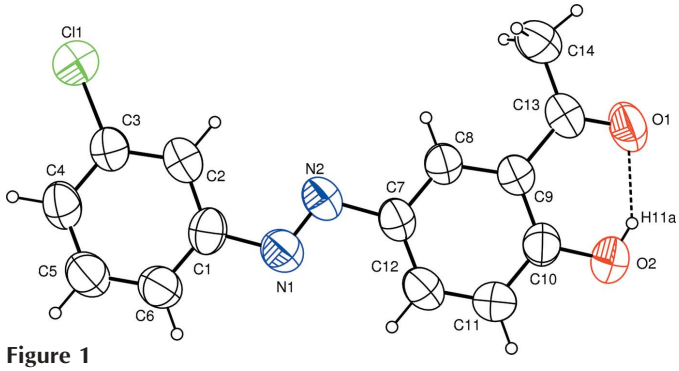


Figure 1
An *ORTEP* view of the title compound, with the atom-numbering scheme and 50% probability displacement ellipsoids. The dashed line indicates a hydrogen bond

Experimental

A mixture of 3-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 sodium nitrite solution (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) aqueous solution (pH 9) was gradually added to a cooled solution of 3-chlorobenzenediazonium chloride, prepared as described above, and the resulting mixture was stirred at 273–278 K for 60 min in an ice bath. Crystals suitable for X-ray analysis were obtained after 1 d by slow evaporation of an ethanol solution (yield 79%, m.p. 385–387 K).

Crystal data

$C_{14}H_{11}ClN_2O_2$
M_r = 274.70
Monoclinic, $P2_1/n$
a = 8.4663 (15) Å
b = 11.236 (3) Å
c = 13.955 (3) Å
β = 103.914 (14)°
V = 1288.6 (5) Å^3
Z = 4
D_x = 1.416 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 17972 reflections
θ = 2.4–27.9°
μ = 0.30 mm^{-1}
T = 293 (2) K
Prism, red
0.40 × 0.35 × 0.29 mm

Data collection

Stoe IPDS-2 diffractometer
ω scans
Absorption correction: integration *X-RED32* (Stoe & Cie, 2002)
T_{min} = 0.887, T_{max} = 0.952
21521 measured reflections
3078 independent reflections
1780 reflections with $I > 2\sigma(I)$
R_{int} = 0.059
θ_{max} = 28.0°
$h = -10 \rightarrow 11$
$k = -14 \rightarrow 14$
$l = -18 \rightarrow 18$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.134
S = 0.97
3078 reflections
172 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0783P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.37 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}

Table 1
Selected bond lengths (Å).

C7—N2	1.460 (2)	C1—N1	1.437 (2)
C13—O1	1.226 (2)	C10—O2	1.335 (2)
C3—Cl1	1.736 (2)	N1—N2	1.233 (2)

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H11A···O1	0.82	1.83	2.547 (2)	146

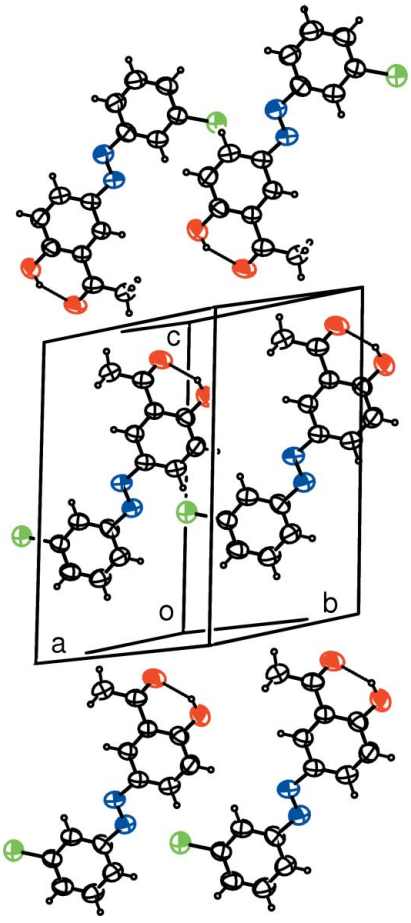


Figure 2
Packing diagram of (I), viewed approximately along the [110] direction. Intramolecular O—H···O hydrogen bonds are shown as dotted lines.

All H atoms were placed in calculated positions and refined using a riding model, with C—H = 0.93–0.96 Å, O—H = 0.82 Å, and with U_{iso}(H) = 1.2–1.5U_{eq}(parent atom).

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED32* (Stoe & Cie, 2002); program(s) used to solve structure: *SHELXS86* (Sheldrick, 1986); 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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