Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

(*E*)-5-(4-Chlorophenyldiazenyl)salicylaldehyde

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Key indicators

Single-crystal X-ray study
T = 296 K
Mean σ(C–C) = 0.004 Å
R factor = 0.055
wR factor = 0.149
Data-to-parameter ratio = 17.7

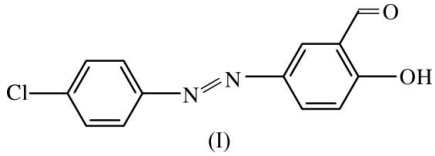
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 23 September 2005
Accepted 9 November 2005
Online 16 November 2005

The molecule of the title compound, $C_{13}H_9ClN_2O_2$, is approximately planar and displays a *trans* configuration with respect to the central N=N double bond. The dihedral angle between the two aromatic rings is 3.69 (14)°. The molecules are linked by intermolecular O—H···O hydrogen bonds, forming a two-dimensional network.

Comment

The extensive application of azo dyes in industry and in analytical determinations has attracted attention for decades. Some arylazo compounds derived from resorcinol or β-naphthol have been widely used in the spectrophotometric determination of traces of metals (Betteridge & John, 1973; Pollard *et al.*, 1959). Optically active azobenzene polymers are very important functional materials because of their photo-responsive properties.



(I)

Fig. 1 shows the structure of the title compound, (I), with the atom-numbering scheme. Selected bond distances and angles are listed in Table 1. In the azo group, the N1—C5 and N2—C8 bond lengths indicate significant single-bond character, whereas the N1=N2 bond length is indicative of significant double-bond character. The C7=O1 and C2—O2 bond lengths agree with the corresponding distances in 3-methoxy-5-(4-methylphenyldiazenyl)salicylaldehyde and 3-methoxy-5-(2-methylphenyldiazenyl)salicylaldehyde [1.224 (2) and 1.350 (2) Å, respectively; Ersanli *et al.*, 2004].

Compound (I) consists of benzene rings *A* (C1–C6) and *B* (C8–C13), their substituents and the azo unit *C* (C5—

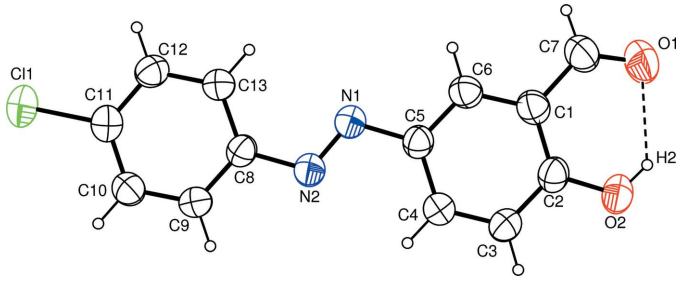


Figure 1
A view of (I), with the atom-numbering scheme and 50% probability displacement ellipsoids for non-H atoms. The intramolecular hydrogen bond is shown as a dashed line.

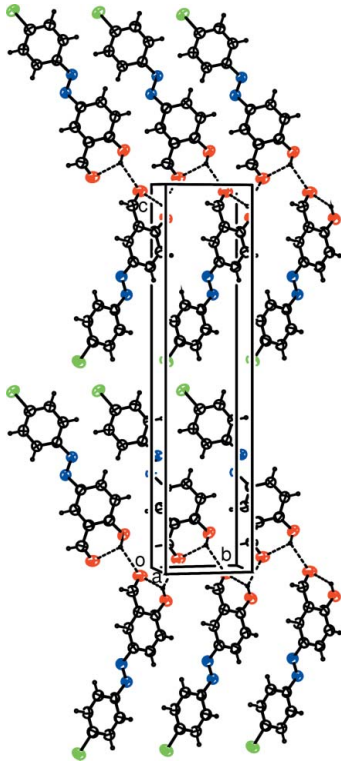


Figure 2
A packing diagram for (I), showing hydrogen bonds as dashed lines.

N1═N2—C8). Benzene rings *A* and *B* adopt a *trans* configuration about the azo functional group, as observed in the crystal structures of other previously studied azo compounds. In (I), dihedral angles are as follows: 3.69 (14)° between *A* and *B*, 3.4 (3)° between *A* and *C*, and 0.8 (3)° between *B* and *C*. Compound (I) also presents intramolecular O—H···O and weak intermolecular O—H···O hydrogen bonds (Table 2), forming a two-dimensional network (Fig. 2).

Experimental

The title compound was prepared according to the literature method of Odabaşoğlu *et al.* (2003), using *p*-chloroaniline and salicylaldehyde as starting materials. The product was crystallized from toluene to obtain well shaped crystals (yield 83%; m.p. 484–485 K).

Crystal data

$C_{13}H_9ClN_2O_2$
M_r = 260.67
Monoclinic, $P2_1$
a = 3.8486 (5) Å
b = 5.818 (1) Å
c = 25.437 (4) Å
β = 91.408 (12)°
V = 569.39 (15) Å^3
Z = 2
D_x = 1.520 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 5345 reflections
θ = 1.6–29.4°
μ = 0.33 mm^{-1}
T = 296 K
Plate, colourless
0.50 × 0.32 × 0.03 mm

Data collection

Stoe IPDS-2 diffractometer
ω scans
Absorption correction: integration (*X-RED32*; Stoe & Cie, 2002)
T_{min} = 0.882, T_{max} = 0.990
5538 measured reflections
2974 independent reflections
2346 reflections with $I > 2\sigma(I)$
R_{int} = 0.078
θ_{max} = 29.2°
$h = -4 \rightarrow 5$
$k = -7 \rightarrow 7$
$l = -34 \rightarrow 34$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.055
$wR(F^2)$ = 0.149
S = 0.98
2974 reflections
168 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0964P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.29 e Å^{-3}
$\Delta\rho_{min}$ = −0.41 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.046 (12)
Absolute structure: Flack (1983), with 1335 Friedel pairs
Flack parameter = 0.27 (10)

Table 1
Selected geometric parameters (Å, °).

C1—C2	1.414 (4)	C7—O1	1.223 (4)
C2—O2	1.347 (3)	C8—N2	1.417 (3)
C5—N1	1.419 (3)	N1—N2	1.267 (3)
O2—C2—C3	117.3 (3)	O1—C7—C1	124.6 (3)
O2—C2—C1	123.3 (2)	C9—C8—N2	116.1 (2)
C6—C5—N1	117.3 (2)	C13—C8—N2	124.7 (2)
C4—C5—N1	123.7 (2)		
C5—N1—N2—C8	−179.3 (2)		

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2···O1	0.85 (2)	2.08 (4)	2.702 (4)	130 (5)
O2—H2···O1^{i}	0.85 (2)	2.29 (4)	2.923 (3)	132 (5)

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

All C-bonded H atoms were refined using a riding model, with C—H distances constrained to 0.93 Å and with $U_{iso} = 1.2U_{eq}$(C). The H atom of the hydroxyl group was found in a difference map and refined with the O—H distance restrained to 0.83 (2) Å and U_{iso}(H) = $1.5U_{eq}$(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).

The authors acknowledge the Faculty of Arts and Sciences, Ondokuz Mayıs University, Turkey, for the use of the Stoe IPDS-II diffractometer (purchased under grant No. F279 of the University Research Fund).

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