

Şehriman Atalay,^a Hande Petek,^a
Nazan Ocak İskeleli,^b Çiğdem
Albayrak^c and Erbil Ağar^{c*}^aDepartment of Physics, Faculty of Arts and Sciences, Ondokuz Mayıs University, Kurupelit, 55139 Samsun, Turkey, ^bDepartment of Science Education, Sinop Faculty of Education, Ondokuz Mayıs University, 57000 Sinop, Turkey, and ^cDepartment of Chemistry, Faculty of Arts and Sciences, Ondokuz Mayıs University, 55139 Samsun, Turkey

Correspondence e-mail: atalays@omu.edu.tr

Key indicators

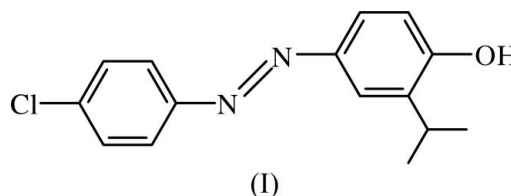
Single-crystal X-ray study
 $T = 296$ K
Mean $\sigma(\text{C}-\text{C}) = 0.002$ Å
 R factor = 0.041
 wR factor = 0.116
Data-to-parameter ratio = 11.9For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.**(E)-4-[(4-Chlorophenyl)diazenyl]-2-isopropylphenol**

In the title compound, $\text{C}_{15}\text{H}_{15}\text{ClN}_2\text{O}$, the aromatic rings adopt a *trans* configuration with respect to the $\text{N}=\text{N}$ bond, as found for other diazene derivatives. The crystal structure is stabilized by intermolecular $\text{O}-\text{H}\cdots\text{N}$ hydrogen bonds, forming a polymeric chain along the c axis.

Received 21 June 2006
Accepted 26 June 2006

Comment

Azo compounds have been used for a long time in industry because of their versatile application in various fields, including dyeing textile fibres, colouring different materials, plastics, biological-medical studies, lasers, liquid crystalline displays, electro-optical devices and ink-jet printers in high-technology areas (Peters & Freeman, 1991).



In the azo groups of (I), the $\text{N1}-\text{C8}$ and $\text{N2}-\text{C10}$ bond lengths (Table 1) indicate significant single-bond character, whereas the $\text{N}=\text{N}$ bond length is indicative of double-bond character. These values are in agreement with those reported for other *trans*-azo compounds (Albayrak *et al.*, 2004). The aromatic rings adopt a *trans* configuration with respect to the azo double bond. The dihedral angle between the chlorophenyl and $\text{C4}-\text{C9}$ benzene rings is $47.81(4)^\circ$. There is an $\text{O}-\text{H}\cdots\text{N}$ intermolecular hydrogen bond in the crystal structure of (I), forming a polymeric chain along the c axis (Fig. 2).

Experimental

A mixture of 4-chloroaniline (1.87 g, 14.7 mmol), water (50 ml) and concentrated hydrochloric acid (3.68 ml, 44 mmol) was stirred until a clear solution was obtained. This solution was cooled to 273–278 K and a solution of sodium nitrite (1.42 g, 20 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-Isopropylphenol (2 g, 14.7 mmol) solution in 50% ethanol (pH 9) was gradually added to the cooled solution of 4-chlorobenzenediazonium chloride, prepared as described above, and the resulting mixture was stirred at 273–278 K for 60 min. The product was recrystallized from ethanol to obtain solid (I). Crystals of (I) were obtained by slow evaporation of a solution in acetic acid (yield 55%, m.p. 352–354 K).

Crystal data

$C_{15}H_{15}ClN_2O$
 $M_r = 274.74$
 Monoclinic, $P2_1/c$
 $a = 10.4856$ (5) Å
 $b = 11.1262$ (6) Å
 $c = 12.0768$ (5) Å
 $\beta = 91.585$ (4)°
 $V = 1408.40$ (12) Å³

$Z = 4$
 $D_x = 1.296$ Mg m⁻³
 Mo $K\alpha$ radiation
 $\mu = 0.27$ mm⁻¹
 $T = 296$ K
 Prism, brown
 $0.70 \times 0.64 \times 0.51$ mm

Data collection

Stoe IPDS-II diffractometer
 ω scans
 Absorption correction: integration
 (*X-RED*; Stoe & Cie, 2002)
 $T_{\min} = 0.842$, $T_{\max} = 0.906$

19848 measured reflections
 2762 independent reflections
 2455 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.032$
 $\theta_{\text{max}} = 26.0^\circ$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.041$
 $wR(F^2) = 0.116$
 $S = 1.10$
 2762 reflections
 233 parameters
 All H-atom parameters refined

$w = 1/[\sigma^2(F_o^2) + (0.0683P)^2 + 0.176P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} < 0.001$
 $\Delta\rho_{\text{max}} = 0.45$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.33$ e Å⁻³
 Extinction correction: *SHELXL97*
 Extinction coefficient: 0.071 (6)

Table 1

Selected geometric parameters (Å, °).

C11—C13	1.7392 (15)	N2—C10	1.4314 (18)
O1—C5	1.3539 (17)	N1—C8	1.4096 (17)
N2—N1	1.2554 (16)	C4—C3	1.5124 (19)
C10—N2—N1—C8	−177.76 (11)	O1—C5—C4—C3	−2.2 (2)
N2—N1—C8—C9	−13.8 (2)	C15—C14—C13—C11	177.82 (12)

Table 2

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1—H1 \cdots N2 ⁱ	0.84 (2)	2.04 (2)	2.8566 (16)	168 (2)

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

All H atoms were refined freely. C—H distances are in the range 0.92 (2)–1.03 (3) Å and $U_{\text{iso}}(\text{H})$ values are in the range 0.057 (4)–0.100 (8) Å².

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED* (Stoe & Cie, 2002); program(s)

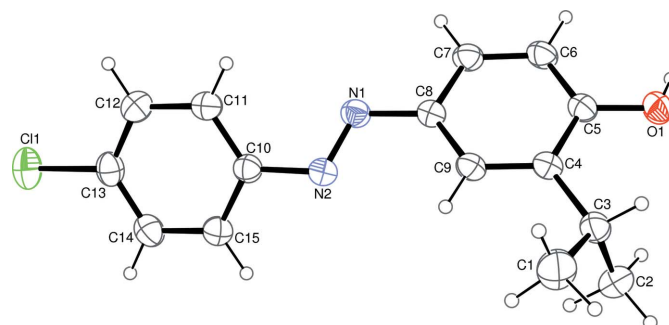


Figure 1

An *ORTEP-3* view of (I), with the atom-numbering scheme and 30% probability displacement ellipsoids.

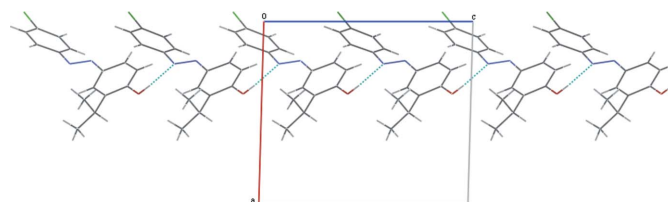


Figure 2

A polymeric chain along the c axis constructed by O—H \cdots N intermolecular hydrogen bonds (broken lines).

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 F.279 of the University Research Fund), and the authors thank the Turkish Government and Ondokuz Mayıs University for research grant F.377.

References

- Albayrak, Ç., Odabaşoğlu, M., Büyükgüngör, O. & Lönnecke, P. (2004). *Acta Cryst.* **C60**, o318–o320.
 Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
 Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
 Peters, A. T. & Freeman, H. S. (1991). *Colour Chemistry*, pp. 193–223. London: Elsevier Science Publishers Ltd.
 Sheldrick, G. M. (1997). *SHELXL97* and *SHELXS97*. University of Göttingen, Germany.
 Stoe & Cie (2002). *X-AREA* and *X-RED*. Stoe & Cie, Darmstadt, Germany.