organic papers

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Key indicators

Single-crystal X-ray study
T = 296 K
Mean σ(C–C) = 0.004 Å
Disorder in main residue
R factor = 0.049
wR factor = 0.144
Data-to-parameter ratio = 14.0

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

(E)-5-(4-Ethylphenyldiazenyl)salicylaldehyde

The molecule of the title compound, $C_{15}H_{14}N_2O_2$, is approximately planar and displays a *trans* configuration with respect to the N═N double bond. The dihedral angle between the two aromatic rings is 10.90 (14)°. The molecules are stacked *via* weak C—H···π interactions.

Comment

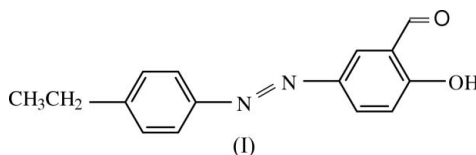Azo compounds are the most widely used class of dyes, due to their versatile applications in various fields, such as the dyeing of textiles and fibres, the colouring of different materials, and high-technology areas, such as electro-optical devices and ink-jet printers (Peters & Freeman, 1991).

The molecule of the title compound, (I), with the atom-labelling scheme, is shown in Fig. 1 and the crystal packing is shown in Fig. 2. The structure of (I) is similar to that of (E)-5-(4-chlorophenyldiazenyl)salicylaldehyde (Şahin et al., 2005), with small differences for some bond lengths, due to the ethyl group attached to the C8–C13 benzene ring. In compound (I), the 4-ethyl group shows disorder and was modelled in two orientations with occupancy factors of 0.478 (9) and 0.522 (9) (Fig. 1). In the azo group, the N1—C5 and N2—C8 bond lengths (Table 1) indicate significant single-bond character, whereas the N1═N2 bond length [1.234 (3) Å] is indicative of significant double-bond character. Similar values have been observed in other *trans*-azo compounds (e.g. Şahin et al., 2005).

Compound (I) consists of benzene rings *A* (C1–C6) and *B* (C8–C13), their substituents, and the azo unit *C* (C5—N1═N2—C8). Benzene rings *A* and *B* adopt a *trans* configuration about the azo functional group, as observed in the crystal structures of the other previously studied azo
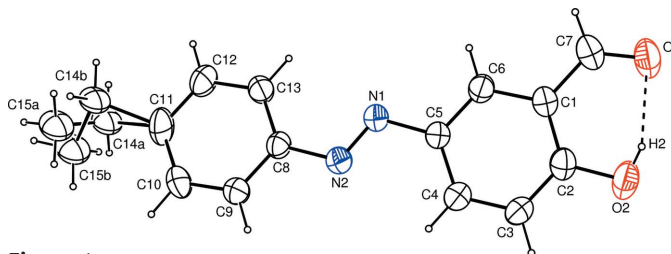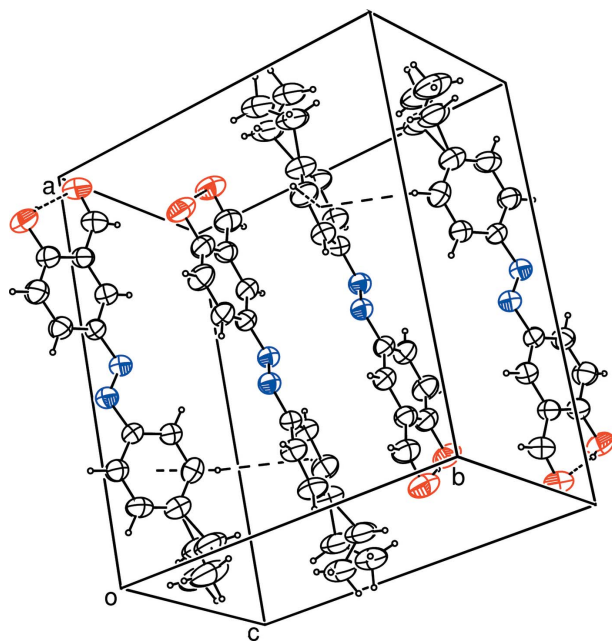

Figure 1
A view of (I), with the atom-numbering scheme and 30% probability displacement ellipsoids for non-H atoms. The intramolecular hydrogen bond is showed as a dashed line. Both disorder components are shown.

Refinement

Refinement on F^2	H atoms treated by a mixture of independent and constrained refinement
$R[F^2 > 2\sigma(F^2)] = 0.049$	
$wR(F^2) = 0.144$	
$S = 0.84$	$w = 1/[\sigma^2(F_o^2) + (0.0616P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
2588 reflections	
185 parameters	$(\Delta/\sigma)_{max} < 0.001$
	$\Delta\rho_{max} = 0.12$ e Å^{-3}
	$\Delta\rho_{min} = -0.10$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

C2—O2	1.380 (3)	C8—N2	1.418 (3)
C5—N1	1.428 (3)	N1—N2	1.234 (3)
C7—O1	1.222 (3)		
O2—C2—C1	120.1 (4)	O1—C7—C1	125.6 (4)
C6—C5—N1	117.2 (3)	C9—C8—N2	114.8 (3)
C4—C5—N1	124.3 (3)		
C5—N1—N2—C8	−178.2 (2)		

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

Cg is the centroid of the C8–C13 benzene ring.

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
O2—H2$\cdots$O1	0.82 (2)	1.83 (3)	2.618 (5)	161 (7)
C12—H12$\cdots Cg(14)^i$	0.93	3.14	3.819 (3)	131

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

The crystal used for data collection was rather thin (0.07 mm) and of not very good quality. As a result, the observed/unique data ratio of *ca* 1/3 is poor. All C-bonded H atoms were refined using a riding model, with C—H distances and U parameters constrained as follows: 0.93 Å and $U_{iso}(H) = 1.2U_{eq}(C)$ for aromatic CH groups; 0.97 Å and $U_{iso}(H) = 1.2U_{eq}(C)$ for methylene CH$_2$; 0.96 Å and $U_{iso}(H) = 1.5U_{eq}(C)$ for methyl CH$_3$. The H atom of the hydroxyl group was found in a difference map and refined with the O—H distance restrained to 0.83 (5) Å and with $U_{iso}(H) = 1.5U_{eq}(O)$.

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).

References

Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
Odabaşoğlu, M., Albayrak, Ç., Büyükgüngör, O. & Goesmann, H. (2003). *Acta Cryst.* C**59**, o234–o236.
Peters, A. T. & Freeman, H. S. (1991). *Colour Chemistry*, pp. 193-223. London: Elsevier Science Publishers Ltd.
Şahin, O., Albayrak, Ç., Odabaşoğlu, M., & Büyükgüngör, O. (2005). *Acta Cryst.* E**61**, o4149–o4150.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Stoe & Cie (2002). *X-AREA* and *X-RED32*. Stoe & Cie, Darmstadt, Germany.

Figure 2
A packing diagram for (I), showing hydrogen bonds as dashed lines. Both disorder components are shown.

compounds. In (I), the dihedral angles are as follows: 10.90 (14)° between *A* and *B*, 6.85 (19)° between *A* and *C*, and 4.3 (2)° between *B* and *C*. Compound (I) also has weak interactions between C12—H12 and the C8–C13(x, $-y - \frac{1}{2}$, $z - \frac{1}{2}$) benzene ring (Table 2). The perpendicular C—H$\cdots$ring contact separation is 3.141 Å and the C—H$\cdots$ring angle is 131.3°. The perpendicular distance between atom H12 and the plane of the benzene ring is 3.02 Å. Compound (I) also presents an intramolecular O—H$\cdots$O hydrogen bond (Fig. 1 and Table 2).

Experimental

Crystal data

$C_{15}H_{14}N_2O_2$	$D_x = 1.282$ Mg m^{-3}
$M_r = 254.28$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 2588 reflections
$a = 14.2617$ (12) Å	$\theta = 2.1–25.2°$
$b = 13.731$ (2) Å	$\mu = 0.09$ mm^{-1}
$c = 6.776$ (3) Å	$T = 296$ K
$\beta = 96.958$ (14)°	Plate, yellow
$V = 1317.2$ (5) Å^3	$0.50 \times 0.31 \times 0.07$ mm
$Z = 4$	

Data collection

Stoe IPDS-2 diffractometer	852 reflections with $I > 2\sigma(I)$
ω scans	$R_{int} = 0.044$
Absorption correction: integration (*X-RED32*; Stoe & Cie, 2002)	$\theta_{max} = 26.0°$
	$h = -17 \rightarrow 17$
$T_{min} = 0.947$, $T_{max} = 0.992$	$k = -16 \rightarrow 16$
9050 measured reflections	$l = -8 \rightarrow 8$
2588 independent reflections	