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(*E*)-4-(4-Ethylphenyldiazenyl)-2,6-dimethylphenyl acrylate

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The title compound, $C_{19}H_{20}N_2O_2$, has a *trans* configuration with respect to the diazene double bond. The dihedral angle between the planes of the two aromatic rings is 2.92 (3)°.

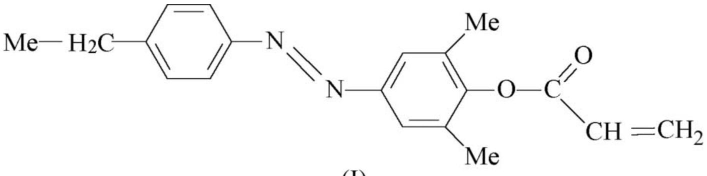
Key indicators

Single-crystal X-ray study
T = 297 K
Mean σ(C–C) = 0.009 Å
Disorder in main residue
R factor = 0.076
wR factor = 0.230
Data-to-parameter ratio = 14.3

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

Comment

Azo dyes have attracted considerable attention due to their versatile application in various fields. Their importance in the dye industry, biochemistry, and in many high-technology areas has been documented over the years (Catino & Farris, 1985; Peter & Freeman, 1991; Ojala *et al.*, 1996). The reversible interconversion between the *cis* and *trans* isomers of azo compounds facilitates the use of these compounds in optical data storage and switching devices (Jeon *et al.*, 2002; Tian *et al.*, 2004). Such optical properties depend on not only the spectroscopic properties of the molecules but also on their crystallographic arrangement (Biswas & Umapathy, 2000). As part of our ongoing research on azo compounds, in order to provide templates for molecular modelling studies, we have synthesized a diazene derivative compound, (I), and determined its crystal structure.



(I)

The molecular structure of compound (I), with the atom-labelling scheme, is shown in Fig. 1, and selected bond lengths and angles are given in Table 1. The aromatic rings are in a *trans* configuration with respect to the diazene double bond. The —N22═N23— azo linkage is disordered over two orientations; in both components the N—C bond lengths indicate single-bond character, whereas the N═N bond lengths are indicative of significant double-bond character. As a result of the disorder, the N═N bond length is slightly different from that observed in other *trans*-azo compounds (Kocaokutgen *et al.*, 2003; Soylu *et al.*, 2004; Kocaokutgen *et al.*, 2005). The C—C—N—N torsion angles suggest delocalization of electron density between the aromatic rings and the azo group. The dihedral angle between the two aromatic rings is 2.92 (3)°.

No significant intra- or intermolecular hydrogen-bonding interactions are observed, and the crystal packing is stabilized by van der Waals forces.

Experimental

Compound (I) was prepared according to the literature method of Kocaokutgen *et al.* (2005). Single crystals of (I) suitable for X-ray difraction analysis were obtained from dimethyl sulfoxide.

Crystal data

$C_{19}H_{20}N_2O_2$
$M_r = 307.47$
Triclinic, $P\overline{1}$
$a = 8.4461$ (15) Å
$b = 8.5053$ (17) Å
$c = 14.260$ (3) Å
$\alpha = 91.860$ (16)°
$\beta = 103.587$ (14)°
$\gamma = 113.006$ (14)°
$V = 907.7$ (3) Å^3
$Z = 2$
$D_x = 1.125$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.07$ mm^{-1}
$T = 297$ (2) K
Prism, orange
0.40 × 0.30 × 0.20 mm

Data collection

STOE IPDS-2 diffractometer
ω scans
Absorption correction: integration (*X-RED32*; Stoe & Cie, 2002)
$T_{min} = 0.975$, $T_{max} = 0.987$
13759 measured reflections
3580 independent reflections
1209 reflections with $I > 2\sigma(I)$
$R_{int} = 0.135$
$\theta_{max} = 26.0°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.076$
$wR(F^2) = 0.231$
$S = 1.02$
3580 reflections
250 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0671P)^2 + 0.1045P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.15$ e Å^{-3}
$\Delta\rho_{min} = -0.12$ e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.018 (4)

Table 1
Selected geometric parameters (Å, °).

C1—N23*B*	1.470 (17)	C10—N22*B*	1.568 (17)
C1—N22*A*	1.541 (17)	N22*A*—N23*A*	1.23 (5)
C9—O2	1.201 (5)	N22*B*—N23*B*	1.27 (5)
C9—O1	1.364 (6)	C23*A*—C22*A*	1.26 (2)
C10—N23*A*	1.453 (16)	C22*B*—C23*B*	1.305 (19)
C2—C1—N22*A*—N23*A*	175.8 (13)	C15—C10—N22*B*—N23*B*	−179.5 (12)
C1—N22*A*—N23*A*—C10	−178.5 (10)	C10—N22*B*—N23*B*—C1	179.3 (11)
C11—C10—N23*A*—N22*A*	−177.1 (12)	C6—C1—N23*B*—N22*B*	−178.7 (12)

H atoms were refined using a riding model, with C—H = 0.93 Å [U_{iso}(H) = 1.2U_{eq}(C)] for aromatic H and C—H = 0.96 Å [U_{iso}(H) = 1.5U_{eq}(C)] for methyl H atoms. The diazene group is disordered over two different orientations (N22*A*/N23*A* and N22*B*/N23*B*) with occupancy factors of 0.52 (3) and 0.48 (2), respectively. Atoms C22 and C23 of the ester group are also disordered over two positions, with occupancies of 0.532 (8) for C22*B*/C23*B* and 0.468 (8) for C22*A*/C23*A*. The C—C and C—N distances involving the disordered atoms were restrained to 1.30 (3) and 1.45 (3) Å, respectively. Rigid-bond and similarity restraints were imposed on disordered atoms.

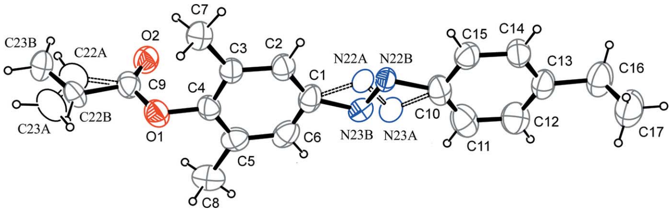


Figure 1
The molecular structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as small spheres of arbitrary radius. All disorder components are shown.

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* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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