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4′-Methylazobenzene-2-sulfenyl cyanide

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Key indicators

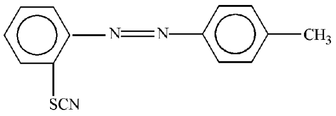
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.006 Å
R factor = 0.074
wR factor = 0.231
Data-to-parameter ratio = 13.7

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

The title compound [systematic name: 2-(*p*-tolyldiazenyl)-phenyl isothiocyanate], $C_{14}H_{11}N_3S$, is non-ionic in nature. Highly electronegative atoms like Br or Cl in sulfenyl halides make the S atom sufficiently electron deficient for strong *ortho* azo–sulfur interaction in sulfenyl bromides or chlorides of *ortho* mercaptoazo compounds; this leads to a planar thiadiazolium structure, in which the S atom interacts with the *ortho* azo group. However, in case of the 4′-Me title compound, the S atom is not sufficiently electron deficient, and no intramolecular *ortho* azo–sulfur interaction exists. The molecule is almost planar. There are no hydrogen bonds and the crystal structure is stabilized by van der Waals interactions.

Comment

With a view to investigating the effect of an electron-releasing group in the 4′-position, and an electron-withdrawing group on the S atom of azobenzene-2-sulfenyl compounds in the formation of thiadiazolium structures by intramolecular *ortho* azo-sulfur interaction, the present study of the title compound, (I), was undertaken. Investigation shows that the sulfenyl group does not approach the azo group of the *trans*-azobenzene plane [S1···N1 2.698 (4) Å]. Such a situation was also found in azobenzene-2-sulfenyl cyanide (Kakati & Chaudhuri, 1968). On the other hand, electron-releasing groups at the 2′- or 4′-positions of the arylazo moiety will increase the electron density at the azo group, and will favour the formation of a thiadiazolium structure (Karmakar *et al.*, 2001), due to *ortho* azo-sulfur interaction. Both the Csp^2—S and S—Csp bond lengths are in the expected ranges [C2—S1 = 1.785 (4) and S1—C7 = 1.690 (6) Å] whereas, in the structure of azobenzene-2-sulfenyl cyanide (Kakati & Chaudhuri, 1968), these bond lengths were 1.68 (2) and 1.89 (2) Å, respectively.



(I)

The two aromatic rings in azobenzene-2-sulfenyl cyanide (Kakati & Chaudhuri, 1968) are not coplanar, but in the title compound they are almost coplanar [dihedral angle 3.3 (2)°]. The coplanarity is presumed to be due to the electron-releasing effect of the methyl group, which is present in the title compound, and the electron-withdrawing effect of the —SCN group. Atom S1 is coplanar with the attached aromatic ring, whereas atoms C7 and N3 deviate from it by 0.113 (6) and 0.152 (6) Å, respectively.

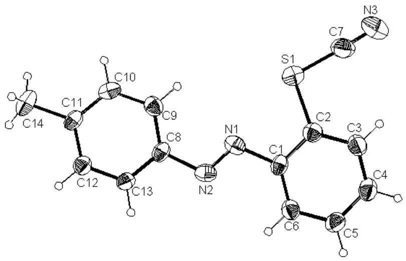


Figure 1
ORTEP-3 (Farrugia, 1997) diagram of (I), with 30% probability displacement ellipsoids. H atoms are shown as circles of arbitrary radius.

Experimental

Crystal data

$C_{14}H_{11}N_3S$
$M_r = 253.33$
Monoclinic, $P2_1/c$
$a = 14.516\ (2)$ Å
$b = 4.784\ (2)$ Å
$c = 19.194\ (4)$ Å
$\beta = 107.62\ (1)°$
$V = 1270.4\ (6)$ Å^3
$Z = 4$
$D_x = 1.324$ Mg m^{-3}
Cu $K\alpha$ radiation
Cell parameters from 25 reflections
$\theta = 55–65°$
$\mu = 2.13$ mm^{-1}
$T = 293\ (2)$ K
Block, yellow
0.53 × 0.40 × 0.20 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
2ω scans
Absorption correction: ψ scan (North *et al.*, 1968)
$T_{min} = 0.414$, $T_{max} = 0.654$
2342 measured reflections
2266 independent reflections
1509 reflections with $I > 2\sigma(I)$
$R_{int} = 0.053$
$\theta_{max} = 70.1°$
$h = 0 \rightarrow 17$
$k = 0 \rightarrow 5$
$l = -23 \rightarrow 22$
4 standard reflections every 600 reflections intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.074$
$wR(F^2) = 0.231$
$S = 1.08$
2266 reflections
166 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1132P)^2 + 1.0209P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.048$
$\Delta\rho_{max} = 0.41$ e Å^{-3}
$\Delta\rho_{min} = -0.40$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

S1—C7	1.690 (6)	N1—C1	1.452 (5)
S1—C2	1.785 (4)	N2—C8	1.475 (5)
N1—N2	1.208 (4)		
C7—S1—C2	100.0 (2)	C6—C1—N1	128.3 (4)
N2—N1—C1	112.2 (3)	C2—C1—N1	111.4 (4)
N1—N2—C8	111.2 (3)	C12—C11—C10	117.8 (4)
C13—C8—N2	114.8 (3)	C12—C11—C14	122.0 (4)
C9—C8—N2	124.8 (4)		
C1—N1—N2—C8	179.7 (3)	N2—N1—C1—C6	2.7 (6)
N1—N2—C8—C13	−179.1 (4)	N2—N1—C1—C2	−178.3 (4)
N1—N2—C8—C9	2.0 (6)	N1—C1—C2—S1	0.9 (5)

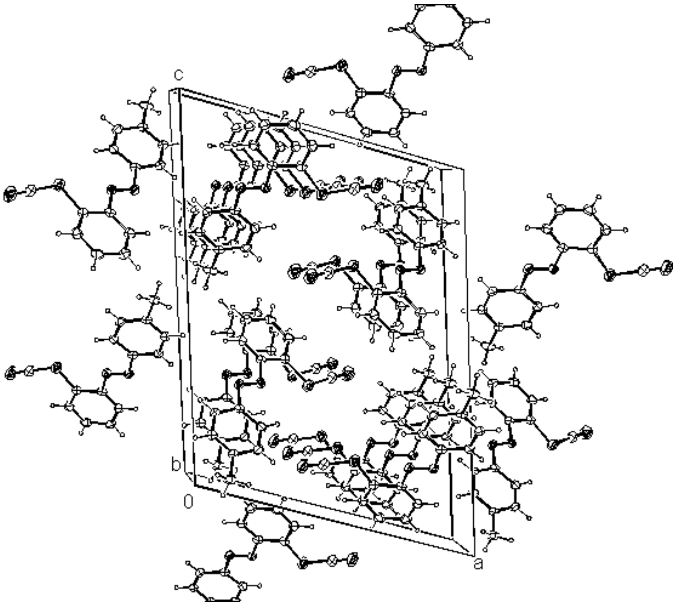


Figure 2
The packing of (I), viewed down the *b* axis.

H atoms were placed in calculated positions, with C—H distances in the range 0.93–0.96 Å. The U_{iso}(H) values of the ring H atoms were refined as a common value. Similarly, the U_{iso}(H) values of the methyl H atoms were set equal and refined as a separate common value.

Data collection: *CAD*-4 *EXPRESS* (Enraf–Nonius, 1994); cell refinement: *CAD*-4 *EXPRESS*; data reduction: *CAD*-4 *EXPRESS*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*-3 (Farrugia, 1997); software used to prepare material for publication: *SHELXL*97.

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References

Enraf–Nonius (1994). *CAD*-4 *EXPRESS*. Enraf–Nonius, Delft, The Netherlands.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Kakati, K. K. & Chaudhuri, B. (1968). *Acta Cryst.* B**24**, 1645–1652.
Karmakar, S., Talukdar, A. N., Barman, P. & Bhattacharjee, S. (2001). *Indian J. Pure Appl. Phys.* **39**, 357–360.
North, A. C. T., Phillips, D. C. & Mathews, F. S. (1968). *Acta Cryst.* A**24**, 351–359.
Sheldrick, G. M. (1997). *SHELXS*97 and *SHELXL*97. University of Göttingen, Germany.

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