Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

3,6-Diphenyl-1,4-bis(*p*-tolylsulfonyl)-1,4-dihydro-1,2,4,5-tetrazine

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Received 25 January 2005
Accepted 9 March 2005
Online 18 March 2005

Key indicators

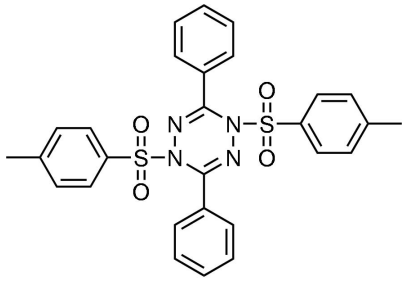
Single-crystal X-ray study
T = 296 K
Mean σ(C–C) = 0.005 Å
R factor = 0.037
wR factor = 0.118
Data-to-parameter ratio = 14.1

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

The central six-membered ring of the title compound, $C_{28}H_{24}N_4O_4S_2$, has a boat conformation, in which the N atoms bonded to sulfonyl groups deviate from the plane of the other four atoms by 0.389 (4) and 0.343 (4) Å.

Comment

s-Tetrazine derivatives have a high potential for biological activity, possessing a wide range of antiviral and antitumor properties, and these derivatives have been widely used in pesticides and herbicides (Sauer, 1996). In a continuation of our work on the structure–activity relationship of *s*-tetrazine derivatives (Hu *et al.*, 2002, 2004), we have obtained a yellow crystalline compound produced according to the procedure of Wawzonek & James (1973). The structural identity of our product, (I), was resolved using single-crystal X-ray diffraction.



(I)

The molecular structure of (I) is illustrated in Fig. 1. Selected bond lengths and angles are listed in Table 1. In (I),

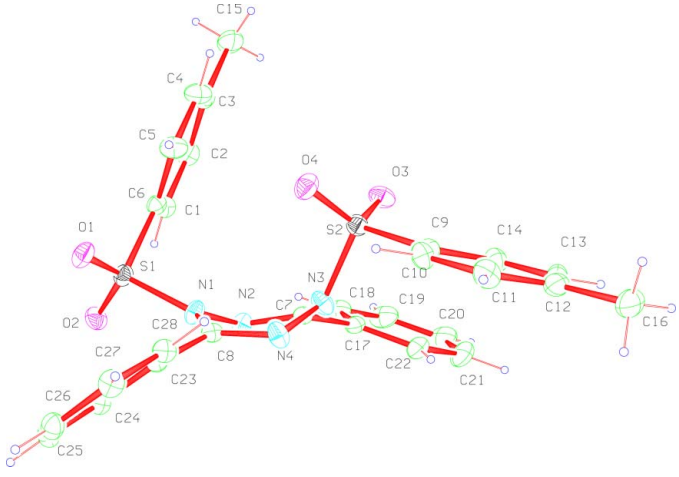


Figure 1
The structure of (I), shown with 30% probability displacement ellipsoids.

atoms N2, C7, N4 and C8 are coplanar [deviations within 0.0534 (12) Å], and atoms N1 and N3 deviate from the plane by 0.389 (4) and 0.343 (4) Å, respectively, indicating a boat conformation.

Experimental

The title compound was prepared according to the procedure of Wawzonek & James (1973). A solution of the compound in butanone was concentrated gradually at room temperature to afford yellow blocks (m.p. 430–432 K).

Crystal data

$C_{28}H_{24}N_4O_4S_2$
M_r = 544.63
Monoclinic, $P2_1/n$
a = 10.8010 (17) Å
b = 14.279 (4) Å
c = 18.074 (3) Å
β = 103.230 (13)°
V = 2713.5 (10) Å^3
Z = 4
D_x = 1.333 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
θ = 11.4–16.0°
μ = 0.24 mm^{-1}
T = 296 (2) K
Prism, colorless
0.35 × 0.30 × 0.25 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.890, T_{max} = 0.943
5598 measured reflections
4877 independent reflections
2870 reflections with $I > 2\sigma(I)$
R_{int} = 0.016
θ_{max} = 25.2°
$h = 0 \rightarrow 12$
$k = -1 \rightarrow 17$
$l = -21 \rightarrow 21$
3 standard reflections
frequency: 60 min
intensity decay: <1%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.118
S = 1.01
4877 reflections
346 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0506P)^2 + 0.7918P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.23 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.0024 (5)

Table 1
Selected geometric parameters (Å, °).

N1—C8	1.391 (3)	N3—C7	1.406 (3)
N1—N2	1.415 (3)	N3—N4	1.440 (3)
N2—C7	1.265 (3)	N4—C8	1.284 (3)
C8—N1—N2	118.41 (19)	C8—N4—N3	112.8 (2)
C7—N2—N1	113.4 (2)	N2—C7—N3	120.6 (2)
C7—N3—N4	116.16 (19)		
C8—N1—N2—C7	−36.6 (3)	N4—N3—C7—N2	30.4 (3)
C7—N3—N4—C8	−38.9 (3)	N2—N1—C8—N4	27.5 (3)

H atoms were included in calculated positions and refined using a riding model. H atoms were given isotropic displacement parameters equal to 1.2 (or 1.5 for methyl H atoms) times U_{eq} of their parent atoms and C—H distances were set at 0.93 Å for the aromatic H atoms and 0.96 Å for those of the methyl groups.

Data collection: *CAD-4 EXPRESS* (Enraf–Nonius, 1994); cell refinement: *CAD-4 EXPRESS*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Version 1.05; Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

We are very grateful to the National Natural and Scientific Foundation (grant No. 20272053) for financial support.

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