

Wei-Xiao Hu,* Lu-Ping Lv, Feng
Xu and Hai-Bo ShiCollege of Pharmaceutical Science, Zhejiang
University of Technology, Hangzhou 310014,
People's Republic of China

Correspondence e-mail: huyang@mail.hz.zj.cn

Key indicators

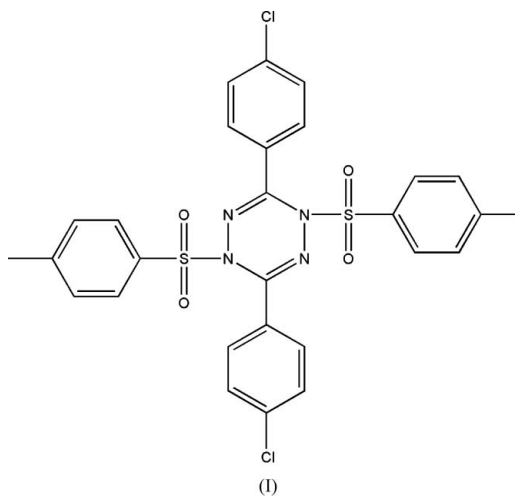
Single-crystal X-ray study
 $T = 292$ K
Mean $\sigma(\text{C}-\text{C}) = 0.002$ Å
 R factor = 0.036
 wR factor = 0.105
Data-to-parameter ratio = 13.4For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.3,6-Bis(*p*-chlorophenyl)-1,4-bis(*p*-tolylsulfonyl)-
1,4-dihydro-1,2,4,5-tetrazine

The title compound, $\text{C}_{28}\text{H}_{22}\text{Cl}_2\text{N}_4\text{O}_4\text{S}_2$, was prepared from triethylamine and *N*-(α ,4-dichlorobenzylideneamino)-*p*-toluenesulfonamide and proved to be a 1,4-dihydro-*s*-tetrazine derivative. In the molecule, which possesses a crystallographically imposed inversion centre, the tetrazine ring is essentially planar.

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Comment

s-Tetrazine derivatives, possessing a wide range of biological activities, are widely used in pesticides and herbicides (Sauer, 1996). In a continuation of our study into the structure–activity relationships of *s*-tetrazine derivatives (Hu *et al.*, 2002, 2004), we have obtained the title compound, (I), as a product of the reaction of triethylamine and *N*-(α ,4-dichlorobenzylideneamino)-*p*-toluenesulfonamide.



The title compound proved to be a 1,4-dihydro-*s*-tetrazine derivative. The molecule of (I) possesses a crystallographically imposed inversion centre (Fig. 1). Selected bond lengths and angles are listed in the Table 1. The central tetrazine ring has an essentially planar conformation, as shown by the minimal deviation [0.0123 (12) Å] of atom N1 from the N2/C7/N2ⁱ/C7ⁱ plane [symmetry code: (i) $-x + 1, -y - 1, -z$].

Experimental

The title compound was obtained by adding *N*-(α ,4-dichlorobenzylideneamino)-*p*-toluenesulfonamide dropwise to triethylamine using tetrahydrofuran as solvent at 265 K. The resulting precipitate was filtered and recrystallized from ethyl acetate to afford the title compound. A solution of the compound in butan-2-one was concentrated gradually at room temperature to afford yellow crystals of (I) suitable for X-ray diffraction (m.p. 453–454.5 K).

Crystal data

$C_{28}H_{22}Cl_2N_4O_4S_2$
 $M_r = 613.52$
 Monoclinic, $C2/c$
 $a = 19.313(8) \text{ \AA}$
 $b = 7.007(4) \text{ \AA}$
 $c = 20.998(4) \text{ \AA}$
 $\beta = 107.50(2)^\circ$
 $V = 2710(2) \text{ \AA}^3$
 $Z = 4$

$D_x = 1.504 \text{ Mg m}^{-3}$
 Mo $K\alpha$ radiation
 Cell parameters from 25 reflections
 $\theta = 9.6\text{--}14.0^\circ$
 $\mu = 0.44 \text{ mm}^{-1}$
 $T = 292(2) \text{ K}$
 Prism, yellow
 $0.35 \times 0.30 \times 0.20 \text{ mm}$

Data collection

Enraf–Nonius CAD-4 diffractometer
 $\omega/2\theta$ scans
 Absorption correction: ψ -scan (North *et al.*, 1968)
 $T_{\min} = 0.862$, $T_{\max} = 0.918$
 2676 measured reflections
 2441 independent reflections
 1847 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.037$
 $\theta_{\text{max}} = 25.2^\circ$
 $h = -1 \rightarrow 22$
 $k = 0 \rightarrow 8$
 $l = -25 \rightarrow 24$
 3 standard reflections
 frequency: 60 min
 intensity decay: none

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.036$
 $wR(F^2) = 0.105$
 $S = 1.06$
 2441 reflections
 182 parameters
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0466P)^2 + 3.219P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} = 0.002$
 $\Delta\rho_{\text{max}} = 0.27 \text{ e \AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.31 \text{ e \AA}^{-3}$

Table 1

Selected geometric parameters (\AA , $^\circ$).

S1–O1	1.4143 (8)	N1–C7	1.4195 (13)
S1–O2	1.4163 (11)	N1–N2	1.4209 (11)
S1–N1	1.7339 (10)	N2–C7 ⁱ	1.2743 (12)
S1–C8	1.7411 (11)	C6–C7	1.4778 (12)
Cl1–C3	1.7333 (12)		
O1–S1–O2	120.51 (5)	N2–N1–S1	106.42 (5)
N1–S1–C8	102.39 (5)	C7 ⁱ –N2–N1	119.49 (7)
C7–N1–N2	116.13 (7)	N2 ⁱ –C7–N1	124.38 (7)
C7–N1–N2–C7 ⁱ	1.08 (10)	N2–N1–C7–N2 ⁱ	−1.14 (11)

Symmetry codes: (i) $-x + 1, -y - 1, -z$.

H atoms were placed in calculated positions and refined using a riding model. They were given isotropic displacement parameters equal to 1.2 (or 1.5 for methyl H atoms) times the equivalent isotropic displacement parameters of their parent atoms, and C–H distances were set to 0.93 \AA for the aromatic H atoms and 0.96 \AA for those of the methyl groups.

Data collection: *CAD4* (Enraf–Nonius, 1994); cell refinement: *CAD4*; data reduction: *XCAD-4*, *PSI* and *EAC* (Enraf–Nonius, 1994); program(s) used to solve structure: *SHELXS97* (Sheldrick,

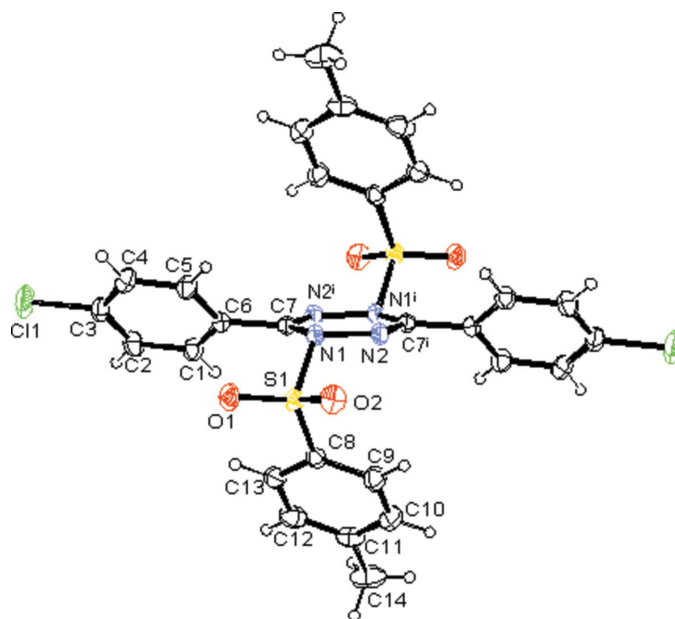


Figure 1

A view of (I), showing the atomic labelling and 30% probability displacement ellipsoids. Unlabelled atoms and atoms labelled with a superscript *i* are related to labelled atoms by the symmetry operator $(-x + 1, -y - 1, -z)$.

1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP3* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

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