Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

3,6-Diethyl-*N*,*N*′-bis(3-methylphenyl)-1,6-dihydro-1,2,4,5-tetrazine-1,4-dicarboxamide

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.035
wR factor = 0.110
Data-to-parameter ratio = 13.6

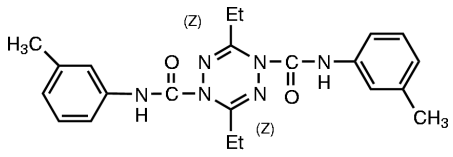
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 10 May 2004
Accepted 18 May 2004
Online 29 May 2004

The title compound, $C_{22}H_{26}N_6O_2$, was prepared from 3-tolyl isocyanate and 3,6-diethyl-1,6-dihydro-*s*-tetrazine. The central six-membered ring has a boat conformation.

Comment

s-Tetrazine derivatives have a high potential for biological activity, possessing a wide range of antiviral and antitumour properties, and these derivatives have been widely used in pesticides and herbicides (Sauer, 1996). As a continuation of our work on the structure–activity relationships of *s*-tetrazine derivatives (Hu *et al.*, 2002, 2004), we have obtained a colourless crystalline compound that was the product of the reaction of 3-tolyl isocyanate and 3,6-diethyl-1,6-dihydro-*s*-tetrazine. The structure of our product, (I), was established 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), atoms N4, C10, N6 and C9 are coplanar [deviations within 0.0347 (7) Å] and atoms N3 and N5 deviate from the plane by 0.412 (2) and 0.420 (2) Å, respectively, *i.e.* the central six-membered ring of (I), the tetrazine ring, has a boat conformation.

Experimental

The title compound was prepared according to the procedure of Hu *et al.* (2002). A solution of the compound in acetone was concentrated gradually at room temperature to afford colourless blocks (m.p. 363–364 K).

Crystal data

$C_{22}H_{26}N_6O_2$
M_r = 406.49
Triclinic, $P\overline{1}$
a = 8.425 (4) Å
b = 11.357 (2) Å
c = 11.489 (2) Å
α = 104.56 (2)°
β = 80.66 (2)°
γ = 95.19 (3)°
V = 1048.5 (6) Å^3
Z = 2
D_x = 1.288 Mg m^{-3}
Mo *Kα* radiation
Cell parameters from 25 reflections
θ = 9.9–14.3°
μ = 0.09 mm^{-1}
T = 293 (2) K
Block, colourless
0.30 × 0.30 × 0.20 mm

Data collection

Enraf–Nonius CAD-4 diffractometer	R_{int} = 0.013
$\omega/2\theta$ scans	θ_{max} = 25.2°
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)	$h = -10 \rightarrow 10$
T_{min} = 0.975, T_{max} = 0.983	$k = -13 \rightarrow 13$
4371 measured reflections	$l = -1 \rightarrow 13$
3762 independent reflections	3 standard reflections
2707 reflections with $I > 2\sigma(I)$	frequency: 60 min
	intensity decay: 0.3%

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0591P)^2 + 0.2187P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.035	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2)$ = 0.110	$\Delta\rho_{max}$ = 0.22 e Å^{-3}
S = 1.03	$\Delta\rho_{min}$ = −0.17 e Å^{-3}
3762 reflections	Extinction correction: *SHELXL*97
276 parameters	Extinction coefficient: 0.016 (3)
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

N3—C10	1.402 (2)	N5—C9	1.400 (2)
N3—N4	1.418 (2)	N5—N6	1.425 (2)
N4—C9	1.273 (2)	N6—C10	1.272 (2)
C10—N3—N4	116.4 (1)	C9—N5—N6	116.4 (1)
C10—N3—N4—C9	40.5 (2)	N6—N5—C9—N4	−36.1 (2)
C9—N5—N6—C10	41.3 (2)	N4—N3—C10—N6	−35.3 (2)

H atoms were placed at calculated positions (N—H = 0.86 Å, C—H = 0.93 Å for phenyl H atoms, 0.96 Å for methyl H atoms and 0.97 Å for all other H atoms) and refined using a riding model, with U_{iso} = 1.2 (or 1.5 for methyl H atoms) times U_{eq}(parent atom).

Data collection: *CAD*-4 *EXPRESS* (Enraf–Nonius, 1994); cell refinement: *CAD*-4 *EXPRESS*; data reduction: *XCAD*4 (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*-3 for Windows (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

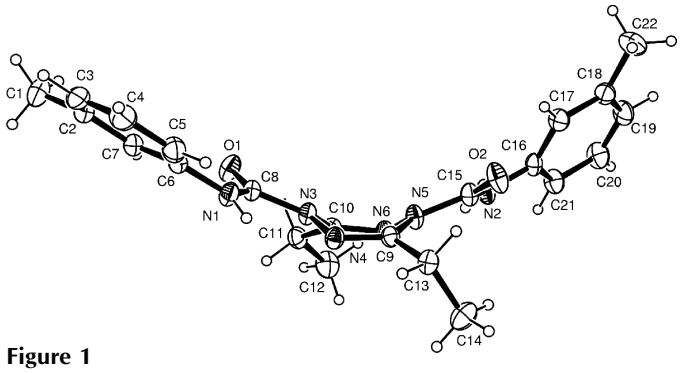


Figure 1
The structure of (I), shown with 30% probability displacement ellipsoids.

We are grateful to the National Natural and Scientific Foundation (grant No. 20272053) and Zhejiang Science and Technology Bureau (grant No. 011101937) for financial support.

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3,6-Diethyl-*N*,*N*′-bis(3-methylphenyl)-1,6-dihydro-1,2,4,5-tetrazine-1,4-dicarboxamide. Erratum

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In the paper by Shi, Hu & Rao [*Acta Cryst.* (2004), E**60**, o1065–o1066], the title is given incorrectly. The chemical name should appear as '3,6-Diethyl-*N*,*N*′-bis(3-methylphenyl)-1,4-dihydro-1,2,4,5-tetrazine-1,4-dicarboxamide'.