Acta Crystallographica Section E
**Structure Reports Online**
ISSN 1600-5368

# *trans*-3,6-Dibenzyl-1,2,4,5-tetrazine

**John C. Barnes**

Division of Physical and Inorganic Chemistry, School of Life Sciences, Carnelley Building, University of Dundee, Dundee DD1 4HN, Scotland

Correspondence e-mail: j.c.barnes@dundee.ac.uk

Received 2 May 2002
Accepted 20 May 2002
Online 31 May 2002

In *trans*-3,6-dibenzyl-1,2,4,5-tetrazine, $C_{16}H_{14}N_4$, with crystallographic inversion symmetry, there is an angle of 84.73 (4)° between the phenyl and tetrazine planes. Close contacts between H atoms on each phenyl group with phenyl rings in adjacent molecules (3.353 and 3.382 Å) give rise to weak layers parallel to the *bc* plane, but there are no intermolecular $\pi$ interactions.

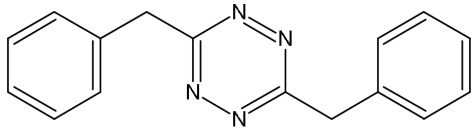
**Key indicators**

Single-crystal X-ray study
*T* = 150 K
Mean $\sigma$(C–C) = 0.002 Å
*R* factor = 0.052
*wR* factor = 0.141
Data-to-parameter ratio = 16.8

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

## Comment

The s-tetrazine group occurs in about 90 reported structures. In most of these, the tetrazine core is highly substituted or else complexed. Many of the less substituted s-tetrazines prepared by Watson & Neilson (1975) and their students crystallize either as very fine needles or extremely thin plates. Attempts to collect data from these have not succeeded. However, the title compound, (I), yielded substantial plates which gave adequate X-ray data.



(I)

Compound (I) is centrosymmetric and thus has *trans* geometry (Fig. 1), whereas 3,6-bis[1-hydroxy-1-(4-methylphenyl)ethyl]-1,2,4,5-tetrazine, previously examined in this laboratory (Low *et al.*, 1986), proved to be the *cis* isomer with no internal symmetry. There are no unusual bond lengths or angles in (I). The torsion angle C1—C7—C8—N9 is 122.01 (15)°, giving an angle of 84.73 (4)° between the phenyl and tetrazine planes. There are no intermolecular $\pi$ interactions between phenyl rings, but the packing allows for short contacts between phenyl H atoms and phenyl rings on neighbouring molecules [H3$\cdots Cg_{Ph}(x, 3/2-y, 1/2+z)$ = 3.353 Å; H6$\cdots Cg_{Ph}(x, 1/2-y, -1/2+z)$ = 3.382 Å; $Cg_{Ph}$ is a phenyl-ring centroid]. Thus, each phenyl group is involved in four interactions, which create weak layers parallel to the *bc* plane.

## Experimental

For the general preparative method used, see Neilson *et al.* (1973). No specific details have been located for the prepararion of the crystals used (legacy crystals), by an unidentified student of Dr Neilson.

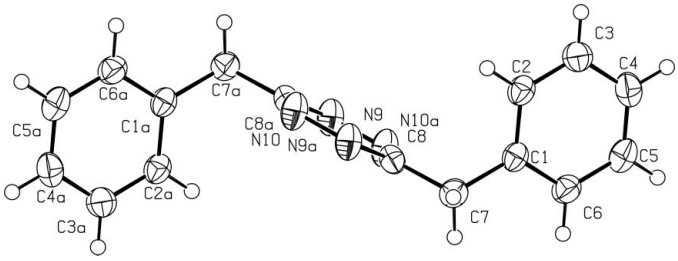



**Figure 1**
The structure of (I), showing 50% probability displacement ellipsoids.

*Crystal data*

$C_{16}H_{14}N_4$
$M_r = 262.32$
Monoclinic, $P2_1/c$
$a = 14.3350\ (4)$ Å
$b = 5.0304\ (8)$ Å
$c = 9.5755\ (13)$ Å
$\beta = 104.571\ (4)^\circ$
$V = 668.29\ (14)$ Å$^3$
$Z = 2$
$D_x = 1.304$ Mg m$^{-3}$
Mo $K\alpha$ radiation
Cell parameters from 7750 reflections
$\theta = 1.5$–$27.5^\circ$
$\mu = 0.08$ mm$^{-1}$
$T = 150\ (2)$ K
Plate, red
0.22 × 0.20 × 0.02 mm

*Data collection*

Nonius KappaCCD area-detector diffractometer
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SORTAV*; Blessing, 1995)
$T_{min} = 0.982$, $T_{max} = 0.998$
7750 measured reflections
1533 independent reflections
902 reflections with $I > 2\sigma(I)$
$R_{int} = 0.063$
$\theta_{max} = 27.5^\circ$
$h = -18 \rightarrow 18$
$k = -6 \rightarrow 6$
$l = -12 \rightarrow 12$

*Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)] = 0.052$
$wR(F^2) = 0.141$
$S = 0.97$
1533 reflections
91 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0808P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.002$
$\Delta\rho_{max} = 0.27$ e Å$^{-3}$
$\Delta\rho_{min} = -0.22$ e Å$^{-3}$

Data collection: *DENZO* (Otwinowski & Minor, 1997) and *COLLECT* (Hooft, 1998); cell refinement: *DENZO* and *COLLECT*; data reduction: *DENZO* and *COLLECT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 1999); software used to prepare material for publication: *SHELXL*97.

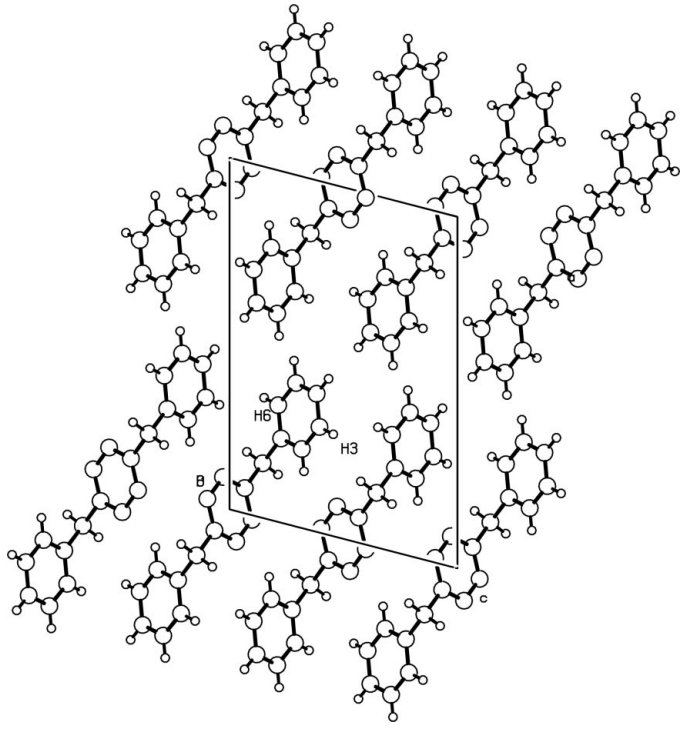



**Figure 2**
The packing of (I), viewed down the *b* axis, showing the alignment of atoms H3 and H6 with phenyl rings on adjacent molecules.

The authors thank the EPSRC X-ray Crystallographic Service and Professor M. B. Hursthouse for the data collection.

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