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2,3-Diphenyl-6,7-dihydro-5*H*-1,4-diazepine

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.003 Å
R factor = 0.041
wR factor = 0.140
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.

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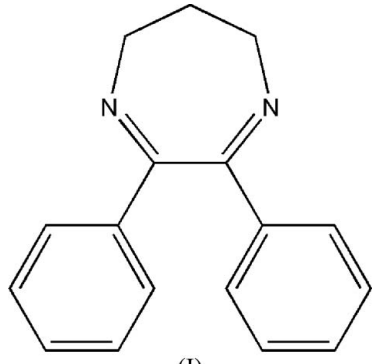
In the title compound, $C_{17}H_{16}N_2$, the 1,4-diazepine ring adopts a distorted boat conformation, in which the sum of the internal angles is 809°. The molecules are linked by a pair of C—H···N hydrogen bonds into a $C_2^2(14)$ chain along the $[10\bar{1}]$ direction.

Comment

1,4-Diazepine derivatives are known to have a broad range of biological activities, such as selective inhibition of Rho-kinase (Tamura *et al.*, 2005), and as HDM2 antagonists used in the treatment of certain cancers (Raboisson *et al.*, 2005). The crystal structures of some 1,4-diazepine derivatives have been reported (Nesterov, 2002; Clark *et al.*,1999). We here report the crystal structure of a 1,4-diazepine derivative, 6,7-hydro-2,3-diphenyl-1,4-diazepine, (I).



(I)

In the molecule of compound (I) (Fig. 1), the 1,4-diazepine ring adopts a distorted boat conformation, in which the sum of the internal angles is 809° (Table 1). The two phenyl rings are located on opposite sides of the seven-membered ring and they enclose a dihedral angle of 82.58 (6)°.

In the crystal structure of (I), the molecules are linked by a pair of C—H···N hydrogen bonds into a $C_2^2(14)$ chain (Bernstein *et al.*, 1995) along the $[10\bar{1}]$ direction (Fig. 2 and Table 2). Atom C16 in the molecule at (*x*, *y*, *z*) act as hydrogen-bond donor to atom N1 in the molecule at $(\frac{1}{2} + x, \frac{1}{2} - y, -\frac{1}{2} + z)$. There are no significant intermolecular interaction between the chains.

Experimental

The title compound, (I), was synthesized by the condensation reaction between propane-1,3-diamine and benzoin in ethanol. Colourless crystals of (I) suitable for X-ray structure analysis were obtained by recrystallizing the crude product from ethanol (m.p. 392–393 K).

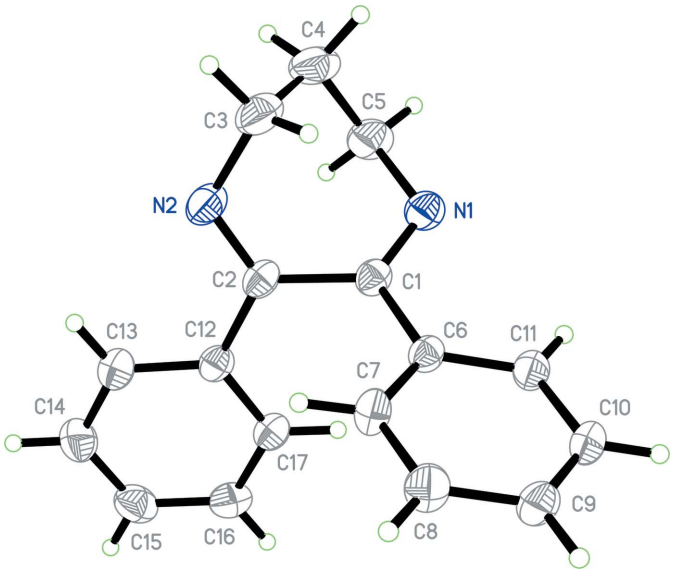


Figure 1
The molecular structure of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level.

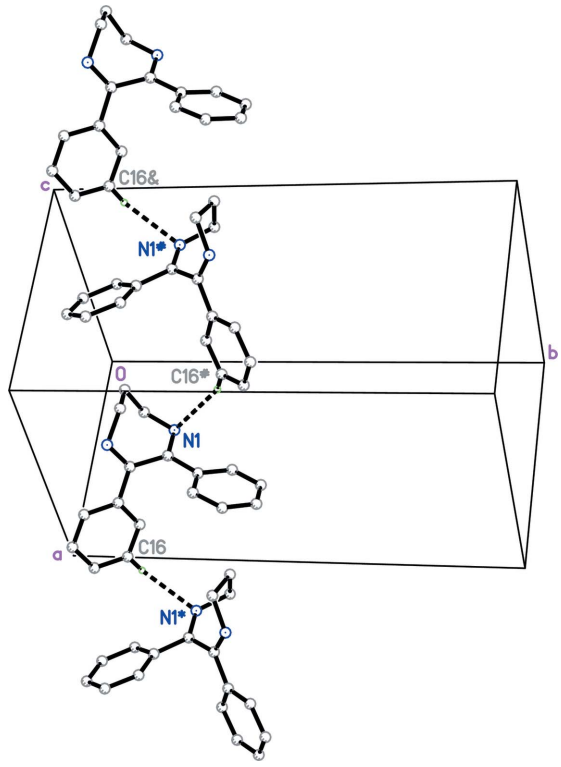


Figure 2
Part of the crystal structure of (I), showing the formation of a $C_2^2(14)$ chain along the [10$\bar{1}$] direction. For clarity, H atoms not involved in the motifs shown have been omitted. [Symmetry codes: (*) $\frac{1}{2}+x, \frac{1}{2}-y, -\frac{1}{2}+z$; (#) $-\frac{1}{2}+x, \frac{1}{2}-y, \frac{1}{2}+z$; (&) $-1+x, y, 1+z$]. Dashed lines indicate hydrogen bonds.

Crystal data

$C_{17}H_{16}N_2$
$M_r = 248.32$
Monoclinic, $P2_1/n$
$a = 8.708$ (2) Å
$b = 17.649$ (3) Å
$c = 9.171$ (2) Å
$\beta = 105.115$ (2)°
$V = 1360.7$ (5) Å^3
$Z = 4$
$D_x = 1.212$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.07$ mm^{-1}
$T = 298$ (2) K
Block, colourless
0.63 × 0.58 × 0.52 mm

Data collection

Siemens SMART 1000 CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.956$, $T_{max} = 0.964$
6849 measured reflections
2375 independent reflections
1671 reflections with $I > 2\sigma(I)$
$R_{int} = 0.054$
$\theta_{max} = 25.0°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.041$
$wR(F^2) = 0.140$
$S = 1.01$
2375 reflections
173 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0742P)^2 + 0.1494P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.11$ e Å^{-3}
$\Delta\rho_{min} = -0.15$ e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.44 (3)

Table 1
Selected geometric parameters (Å, °).

N1—C1	1.276 (2)	N2—C2	1.274 (2)
C1—N1—C5	116.47 (16)	C3—C4—C5	112.24 (16)
C2—N2—C3	116.18 (16)	N1—C5—C4	111.32 (16)
N2—C3—C4	110.48 (17)		
N2—C3—C4—C5	−47.0 (2)	C3—C4—C5—N1	−43.1 (2)

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C16—H16···N1^{i}	0.93	2.62	3.454 (2)	149

Symmetry code: (i) $x+\frac{1}{2}, -y+\frac{1}{2}, z-\frac{1}{2}$.

All H atoms were positioned geometrically and refined as riding on their parent atoms, with C—H = 0.93 Å for aromatic H atoms, C—H = 0.97 Å for methylene H atoms and U_{iso}(H) = 1.2U_{eq}(C) for all H atoms.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

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