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1-Phenyl-5-(piperidinomethyl)-1*H*-tetrazole

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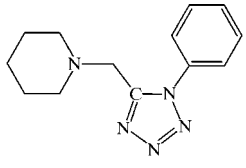
In the molecule of the title 1,5-disubstituted tetrazole, $C_{13}H_{17}N_5$, the tetrazole and benzene rings are not coplanar, having a dihedral angle of 42.96 (5)° between them. The piperidine fragment adopts a chair conformation, and there is a non-classical intramolecular contact between the benzene H atom and the piperidine N atom. Intermolecular C—H···π interactions involving the piperidine C—H groups and the benzene rings are responsible for the formation of two-dimensional networks, extending parallel to the *ab* plane. These networks are linked together into a three-dimensional polymeric structure *via* π–π stacking interactions between the tetrazole rings of two adjacent molecules.

Comment

This work forms part of a systematic investigation of the molecular and crystal structures of 5-(α-aminoalkyl)tetrazoles, which are of great interest in the field of bioorganic and medicinal chemistry. We previously reported the structures of 5-(piperidiniomethyl)-1*H*-tetrazolide (Lyakhov *et al.*, 2003) and the copper(II) chloride complex of *N*,*N*-dimethyl-1-(1-methyl-1*H*-tetrazol-5-yl)methanamine (Ivashkevich *et al.*, 2002). We present here the crystal structure of 1-phenyl-5-(piperidinomethyl)-1*H*-tetrazole, (I) (Fig. 1).



(I)

The tetrazole and benzene rings are planar to within 0.0012 (7) and 0.0051 (9) Å, respectively, but they are not coplanar, their mean planes being inclined at 42.96 (5)° to one another.

The formal N2═N3 [1.2928 (15) Å] and N4═C5 double bonds [1.3169 (14) Å] are the shortest in the tetrazole ring, while the three remaining ring bonds have lengths in the narrow range 1.3510 (15)–1.3553 (17) Å (Table 1). This geometry is typical of 1,5-disubstituted tetrazoles with alkyl or aryl substitutents. An analysis performed using the Cambridge Structural Database (Version 5.25 of November 2003; Allen, 2002) gave the following mean values of the tetrazole ring

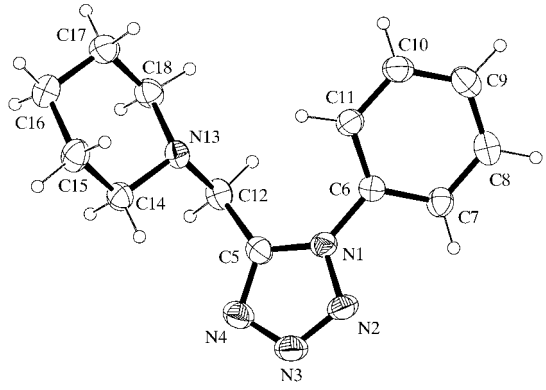


Figure 1
A view of (I), with the atom-numbering scheme and displacement ellipsoids at the 30% probability level. H atoms are shown as spheres of arbitrary radii.

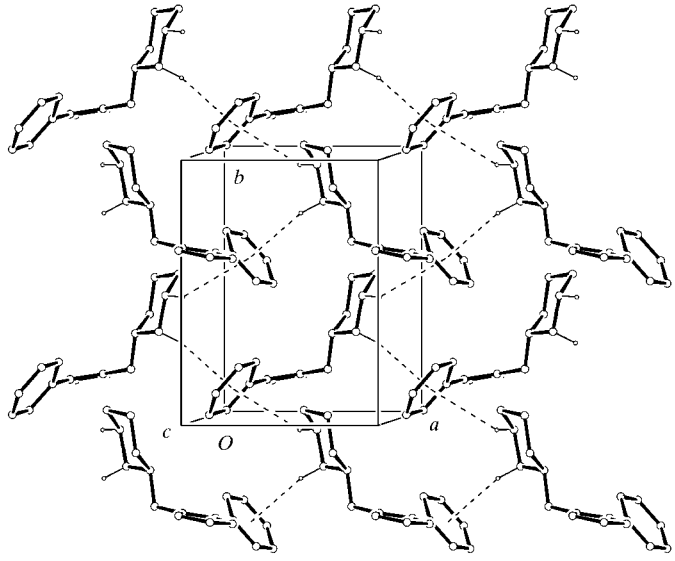


Figure 2
A fragment of the crystal structure of (I), showing the two-dimensional network parallel to the *ab* plane. Dashed lines indicate C—H···π interactions (Table 2). H atoms, with the exception of atoms H17*A* and H18*A*, have been omitted.

bond lengths for such compounds (14 hits): N1—N2 1.355 (2) Å, N2═N 1.295 (1) Å, N3—N4 1.357 (2) Å, N4═C5 1.320 (2) Å and N1—C5 1.340 (2) Å. The tetrazole ring bond lengths of (I) are consistent with these values.

The piperidine fragment has a chair conformation (bond lengths are listed in Table 1).

There is a short intramolecular C11—H11···N13 contact (Table 2), which may be responsible for the conformation adopted by the molecule in the solid state.

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Because of the lack of classical hydrogen-bond donors in the structure of (I), the packing is determined by weaker interactions, namely C—H···π and π–π contacts.

C—H···π interactions arise, firstly, between piperidine atom H17*A* of one molecule and the benzene ring of another molecule at $(\frac{3}{2}-x,\ \frac{1}{2}+y,\ \frac{3}{2}-z)$, and, secondly, between piperidine atom H18*A* and the benzene ring of the molecule at $(1+x,\ y,\ z)$ (Table 2). These interactions form two-dimensional networks, extending parallel to the *ab* plane (Fig. 2).

π–π stacking interactions exist between the tetrazole rings of two molecules related by the symmetry transformation $(1-x,\ -y,\ 1-z)$, the centroid–centroid distance being 3.7015 (13) Å. These interactions connect the two-dimensional networks into a three-dimensional polymeric structure.

Experimental

The title compound was prepared by aminomethylation of 1-phenyltetrazole with piperidine and formaldehyde according to the method described by Karavai & Gaponik (1991). A solution of 1-phenyltetrazole (5.8 g, 40 mmol), piperidine (3.5 ml, 40 mmol) and paraform (3 g) in trifluoroacetic acid (50 ml) was heated under reflux for 5 h. The solvent was removed *in vacuo* and the residue was treated with an aqueous solution of sodium hydroxide (30%, 20 ml). The title compound was isolated by extraction of the resulting solution with diethyl ether (3 × 30 ml), evaporation of the diethyl ether and recrystallization of the residue from ethanol (yield 64%, 6.2 g; m.p. 361 K). ^{1}H NMR (100 MHz, DMSO-d_6): δ 1.43–1.64 (*m*, 6H, $3CH_2$), 2.40 (*t*, 4H, $2CH_2$), 3.82 (*s*, 2H, CH_2), 7.58–7.66 (*m*, 3H, Ph), 7.80–7.88 (*m*, 2H, Ph). Single crystals of (I) suitable for analysis were grown by slow evaporation from a 2-propanol solution at room temperature in air.

Crystal data

$C_{13}H_{17}N_5$
M_r = 243.32
Monoclinic, $P2_1/n$
a = 7.7537 (13) Å
b = 10.436 (3) Å
c = 15.937 (3) Å
β = 96.142 (13)°
V = 1282.2 (5) Å^3
Z = 4
D_x = 1.260 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
θ = 12.4–20.3°
μ = 0.08 mm^{-1}
T = 293 (2) K
Prism, colourless
0.54 × 0.50 × 0.46 mm

Table 1
Selected intermolecular distances (Å).

N1—C5	1.3510 (15)	C12—N13	1.4613 (15)
N1—N2	1.3546 (12)	N13—C14	1.4637 (13)
N1—C6	1.4296 (13)	N13—C18	1.4724 (14)
N2—N3	1.2928 (15)	C14—C15	1.5158 (18)
N3—N4	1.3553 (17)	C15—C16	1.5136 (19)
N4—C5	1.3169 (14)	C16—C17	1.5116 (19)
C5—C12	1.4878 (16)	C17—C18	1.508 (2)

Data collection

Nicolet *R*3*m* four-circle diffractometer
$\omega/2\theta$ scans
4125 measured reflections
3746 independent reflections
2759 reflections with $I > 2\sigma(I)$
R_{int} = 0.019
θ_{max} = 30.1°
$h = 0 \rightarrow 10$
$k = 0 \rightarrow 14$
$l = -22 \rightarrow 22$
3 standard reflections every 100 reflections
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.120
S = 1.06
3746 reflections
232 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0582P)^2 + 0.0879P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}
Extinction correction: *SHELXL*97
Extinction coefficient: 0.480 (16)

Table 2
Hydrogen-bonding and C—H···π interaction geometry (Å, °).

CgBz is the centroid of the benzene ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C11—H11···N13	0.978 (14)	2.648 (13)	3.4395 (15)	138.3 (10)
C17—H17*A*···*CgBz*^{i}	1.012 (16)	3.246 (15)	4.0673 (19)	139.2 (11)
C18—H18*A*···*CgBz*^{ii}	1.028 (16)	2.726 (15)	3.6679 (17)	152.1 (11)

Symmetry codes: (i) $\frac{3}{2}-x,\ \frac{1}{2}+y,\ \frac{3}{2}-z$; (ii) $1+x,\ y,\ z$.

H-atom positions were found from a difference Fourier map and all associated parameters were refined freely [C—H = 0.96 (1)–1.05 (2) Å].

Data collection: *R*3*m Software* (Nicolet, 1980); cell refinement: *R*3*m Software*; data reduction: *R*3*m Software*; program(s) used to solve structure: *SIR*97 (Altomare *et al.*, 1999); 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: *SHELXL*97 and *PLATON* (Spek, 2003).

Supplementary data for this paper are available from the IUCr electronic archives (Reference: AV1171). Services for accessing these data are described at the back of the journal.

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