Acta Crystallographica Section C
Crystal Structure Communications
ISSN 0108-2701

1-(2,4,6-Trimethylphenyl)-1*H*-1,2,3,4-tetrazole

Alexander S. Lyakhov,* Dmitri O. Ivashkevich, Pavel N. Gaponik, Yuri V. Grigoriev and Ludmila S. Ivashkevich

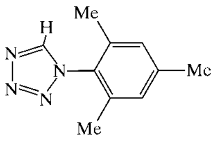
Research Institute for Physical Chemical Problems, Belarussian State University, Leningradskaya Str., 14 Minsk 220080, Belarus
Correspondence e-mail: lyakhov@fhp.bsu.unibel.by

Received 27 August 1999
Accepted 15 November 1999

In the title compound, $C_{10}H_{12}N_4$, the tetrazole and phenyl rings are planar to within 0.001 (2) and 0.006 (2) Å, respectively. The two rings are not coplanar and have a dihedral angle of 69.07 (9)° between them. Each molecule is connected with two adjacent ones by C—H···N bridges between atoms of tetrazole rings forming chains parallel with the *y* axis of the unit cell.

Comment

The increasing interest in 1-monosubstituted tetrazoles is due to the possible application of them in the synthesis of medicines (Wittenberger, 1994), as ligands for complexes with thermal and light-induced spin transitions (Lavrenova & Larionov, 1998) and for ferromagnetic ordering (Gaponik, 1998). However, a rather small number of structures of this type have been described so far: 1-methyltetrazole (Palmer & Parsons, 1996), 1-phenyltetrazole (Matsunaga *et al.*, 1999) and hydrated 1-(3-pyrazolyl)tetrazole (Reimlinger *et al.*, 1970). The crystal structure of a new compound, (I), has been determined and is presented here.



(I)

Bond distances within the tetrazole ring show significant differences. The shortest bond is between the atoms N2 and N3 [1.294 (3) Å]. This value in question is close to the N4—C5 bond distance of 1.303 (3) Å. The N3—N4 and N1—N2 bonds are the longest and similar [1.351 (2) and 1.349 (2) Å, respectively]. These data are consistent with the formulation of formal double bonds between N4—C5 and N2—N3. The tetrazole ring is planar – the r.m.s. deviation of ring atoms from the least-squares plane through them is 0.001 (2) Å.

The bond distances and angles in the phenyl fragment are consistent with those observed previously for the phenyl ring. It is planar to within 0.006 (2) Å (Fig. 1).

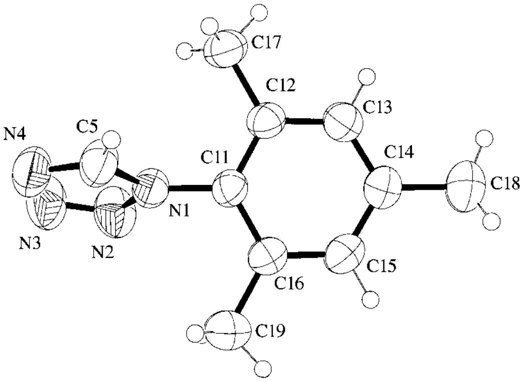


Figure 1
The molecular structure of (I) with the atom-numbering scheme.

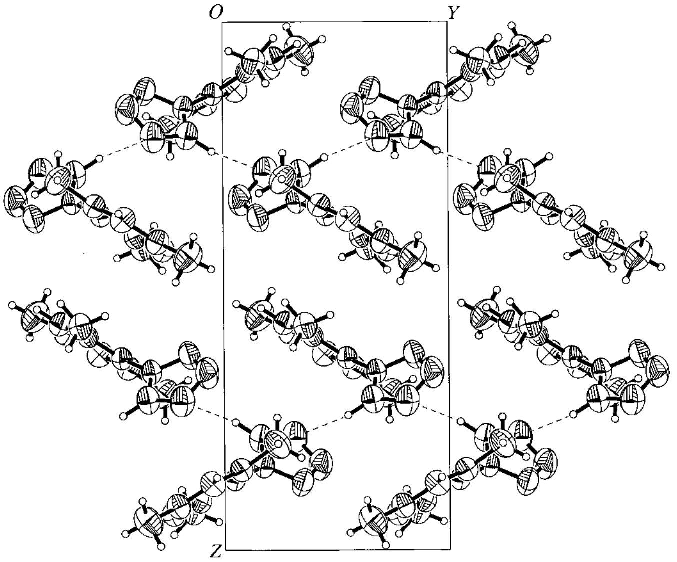


Figure 2
Packing diagram of (I).

The tetrazole and phenyl rings are not coplanar with the mean planes inclined at 69.07 (9)° to each other. Such conformation is due to a steric interaction between the tetrazole ring H(—C5) atom and the C17 methyl group of the phenyl ring. The N1—C11 bond length is 1.437 (2) Å, which is almost the same as a normal N—C(phenyl) single-bond length. These facts indicate that the conjugation effects between the phenyl and tetrazole rings in (I) are negligible.

Inspection of the packing of the molecules (Fig. 2) reveals that they are linked by C—H···N bridges between tetrazole rings forming chains parallel with the *y* axis of the unit cell. The dihedral angle between the adjacent tetrazole rings is 41.1°.

Experimental

The title compound was prepared by heterocyclization of 2,4,6-trimethylaniline with ethyl orthoformate and sodium azide in acetic acid (Gaponik *et al.*, 1985). Single crystals of (I) used for analysis were grown by recrystallization from an ethanol solution.

Crystal data

$C_{10}H_{12}N_4$
$M_r = 188.24$
Monoclinic, $P2_1/n$
$a = 8.220\ (2)$ Å
$b = 7.2950\ (10)$ Å
$c = 17.470\ (4)$ Å
$\beta = 100.97\ (2)^\circ$
$V = 1028.4\ (4)$ Å^3
$Z = 4$
$D_x = 1.216$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 22 reflections
$\theta = 10.14$–16.87°
$\mu = 0.078$ mm^{-1}
$T = 293\ (2)$ K
Prism, colourless
0.55 × 0.50 × 0.35 mm

Data collection

Nicolet *R*3*m* four-circle diffractometer
$\omega/2\theta$ scans
2642 measured reflections
2386 independent reflections
1357 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.023$
$\theta_{\rm max} = 27.56^\circ$
$h = -2 \rightarrow 10$
$k = 0 \rightarrow 9$
$l = -22 \rightarrow 22$
3 standard reflections every 100 reflections intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.053$
$wR(F^2) = 0.190$
$S = 1.059$
2386 reflections
168 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0849P)^2 + 0.3158P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} = 0.004$
$\Delta\rho_{\rm max} = 0.27$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.21$ e Å^{-3}
Extinction correction: *SHELXL*97 (Sheldrick, 1997)
Extinction coefficient: 0.074 (9)

Table 1
Selected geometric parameters (Å, °).

N1—C5	1.332 (3)	C11—C12	1.395 (3)
N1—N2	1.349 (2)	C11—C16	1.395 (3)
N1—C11	1.437 (2)	C12—C13	1.390 (3)
N2—N3	1.294 (3)	C13—C14	1.384 (3)
N3—N4	1.351 (3)	C14—C15	1.386 (3)
N4—C5	1.303 (3)	C15—C16	1.384 (3)
C5—N1—N2	107.5 (2)	N2—N3—N4	111.1 (2)
C5—N1—C11	130.6 (2)	C5—N4—N3	105.3 (2)
N2—N1—C11	121.9 (2)	N4—C5—N1	110.0 (2)
N3—N2—N1	106.2 (2)		

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

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
C5—H5$\cdots$N4$^{\rm i}$	0.98 (3)	2.43 (3)	3.290 (3)	147 (2)

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

H atom positions were found from the ΔF map. Refinement of methyl-H atom positions was performed with fixed displacement parameters. Other H atoms were refined isotropically. The C—H bond lengths are in the range 0.89 (3)–1.00 (3) 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: *SHELXS*97 (Sheldrick, 1990); 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.

The authors would like to thank Dr V. S. Poplavsky for providing the 2,4,6-trimethylaniline used in the synthesis of the title compound.

Supplementary data for this paper are available from the IUCr electronic archives (Reference: AV1031). Services for accessing these data are described at the back of the journal.

References

Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Gaponik, P. N. (1998). *Chemical Problems of Development of New Materials and Technologies*, edited by V. V. Sviridov, pp. 185–214. Minsk: BSU Press.
Gaponik, P. N., Karavai, V. P. & Grigoriev, Y. V. (1985). *Khim. Geterotsikl. Soedin.* **11**, 1521–1524. (In Russian.)
Lavrenova, L. G. & Larionov, S. V. (1998). *Russ. J. Coord. Chem.* **24**, 379–395.
Matsunaga, T., Ohno, Y., Akutsu, Y., Arai, M., Tamura, M. & Iida, M. (1999). *Acta Cryst.* C**55**, 129–131.
Nicolet (1980). *R3m Software*. Nicolet XRD Corporation, Cupertino, USA.
Palmer, M. H. & Parsons, S. (1996). *Acta Cryst.* C**52**, 2818–2822.
Reimlinger, H., King, G. S. D. & Peiren, M. A. (1970). *Chem. Ber.* **103**, 2821–2827.
Sheldrick, G. M. (1990). *Acta Cryst.* A**46**, 467–473.
Sheldrick, G. M. (1997). *SHELXL97*. University of Göttingen, Germany.
Wittenberger, S. F. (1994). *Org. Prep. Proced. Int.* **26**, 499–531.

Acta Cryst. (2000). C**56**, 256–257 Alexander S. Lyakhov *et al.* • $C_{10}H_{12}N_4$ **257**