Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

1-Methyl-3,5-diphenyl-1*H*-1,2,4-triazole

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.005 Å
R factor = 0.051
wR factor = 0.141
Data-to-parameter ratio = 14.9

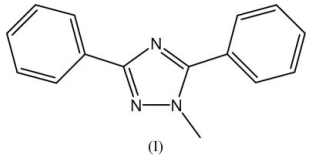
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 10 March 2004
Accepted 13 April 2004
Online 24 April 2004

Two independent but virtually identical molecules comprise the asymmetric unit in the title compound, $C_{15}H_{13}N_3$, in each of which the triazole ring is planar.

Comment

Triazole ring systems are typically planar six-π-electron partially aromatic systems. Several articles have been devoted to the synthesis and pharmacological investigation of triazole compounds (*e.g.* Lønning *et al.*, 1998); for example, the title compound, (I), displays antibacterial activity against various bacteria (Yüksek *et al.*, 1997).



(I)

Two independent molecules comprise the asymmetric unit in the title compound, (I) (Fig. 1 and Table 1), and these are virtually identical. In each molecule, the non-H atoms are effectively coplanar. The N3*a*═C7*a* and N1*a*═C8*a* bonds displays double-bond character, with bond lengths of 1.326 (3) and 1.333 (3) Å, respectively; for the second molecule, the values are 1.331 (3) and 1.339 (3) Å, respectively. In a closely related compound, 4-(*p*-methoxyphenyl)-3,5-bis(2-pyridyl)-4*H*-1,2,4-triazole [(II); Fun *et al.*, 1999], the equivalent bond lengths are 1.311 (2) and 1.316 (2) Å, respectively. The modest elongations of the bond lengths in (I) can be traced to the presence of the methyl and phenyl groups, which are absent in (II).

The dihedral angles between the triazole and ring C1*a*–C6*a* is 15.5 (7)°, that between triazole and ring C9*a*–C14*a* is 33.6 (9)° and that between rings C1*a*–C6*a* and C9*a*–C14*a* is 46.1 (8)°; for molecule *b* these are similar at 13.0 (5), 33.5 (1) and 44.5 (9)°, respectively.

Experimental

N-Benzoyl ethylimidobenzoate (0.01 mol) and methylhydrazine (0.01 mol) in ethanol (50 ml) were refluxed for 8 h. The resulting solution was evaporated at 313–323 K under reduced pressure and dried *in vacuo*. The solid residue was recrystallized from ethanol–water (3:1) to give the desired compound in 86% yield (m.p. 361–362 K).

Crystal data

$C_{15}H_{13}N_3$	$Z = 4$
$M_r = 235.28$	$D_x = 1.260$ Mg m^{-3}
Triclinic, $P\overline{1}$	Mo $K\alpha$ radiation
$a = 7.0796$ (12) Å	Cell parameters from 7029 reflections
$b = 7.0238$ (11) Å	$\theta = 1.6$–$22.0°$
$c = 25.238$ (4) Å	$\mu = 0.08$ mm^{-1}
$\alpha = 86.954$ (14)°	$T = 293$ K
$\beta = 85.952$ (14)°	Prism, colourless
$\gamma = 82.653$ (13)°	0.32 × 0.22 × 0.08 mm
$V = 1240.3$ (4) Å^3	

Data collection

Stoe IPDS-II diffractometer	4846 independent reflections
ω scans	1571 reflections with $I > 2\sigma(I)$
Absorption correction: by integration (*X-RED*32; Stoe & Cie, 2002)	$R_{int} = 0.088$
	$\theta_{max} = 26.0°$
$T_{min} = 0.975$, $T_{max} = 0.993$	$h = -8 \rightarrow 8$
17588 measured reflections	$k = -7 \rightarrow 8$
	$l = -30 \rightarrow 30$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0647P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.051$	$(\Delta/\sigma)_{max} = 0.001$
$wR(F^2) = 0.141$	$\Delta\rho_{max} = 0.19$ e Å^{-3}
$S = 0.72$	$\Delta\rho_{min} = -0.19$ e Å^{-3}
4846 reflections	Extinction correction: *SHELXL*97
326 parameters	Extinction coefficient: 0.030 (2)
H-atom parameters constrained	

Table 1
Selected interatomic distances (Å).

N2*a*—N3*a*	1.367 (3)	N2*b*—N3*b*	1.368 (3)
N1*a*—C7*a*	1.368 (3)	N1*b*—C7*b*	1.360 (4)
N1*a*—C8*a*	1.333 (3)	N1*b*—C8*b*	1.339 (3)
N2*a*—C8*a*	1.351 (4)	N2*b*—C8*b*	1.347 (4)
N2*a*—C15*a*	1.469 (3)	N2*b*—C15*b*	1.465 (3)
N3*a*—C7*a*	1.326 (3)	N3*b*—C7*b*	1.331 (3)

H atoms were included in calculated positions and refined using the riding-model approximation, with aromatic C—H = 0.93 Å and methyl C—H = 0.96 Å, and with U_{iso}(H) = 1.5U_{eq}(parent C atom).

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED*32 (Stoe & Cie, 2002); 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).

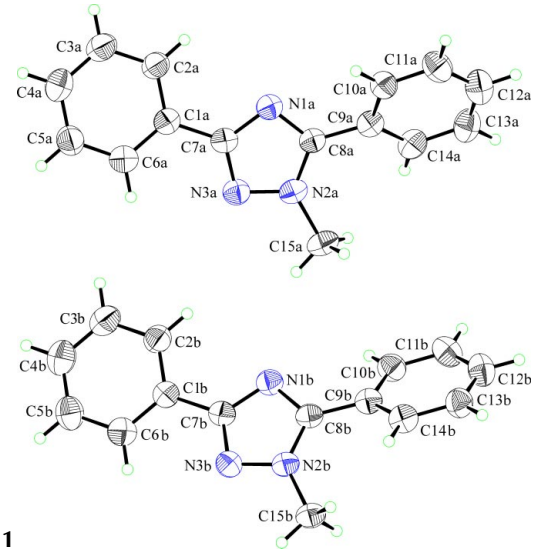


Figure 1
A view of the asymmetric unit of the title compound, showing the atomic numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

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