

4-(4-Chlorophenyl)-5-(4-methylphenyl)-
3-(2-pyridyl)-4H-1,2,4-triazoleShu-Ping Zhang, Zhao-Di Liu and
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Key indicators

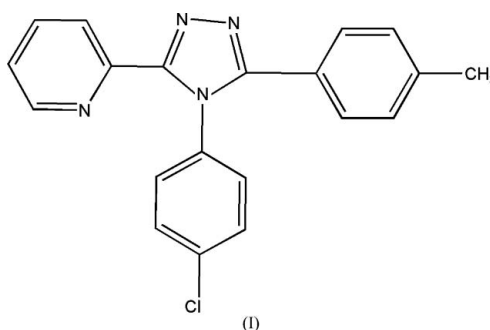
Single-crystal X-ray study
 $T = 298$ K
Mean $\sigma(\text{C}-\text{C}) = 0.003$ Å
 R factor = 0.040
 wR factor = 0.116
Data-to-parameter ratio = 15.7For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.

In the title compound, $\text{C}_{20}\text{H}_{15}\text{ClN}_4$, the two benzene rings form dihedral angles of 30.95 (9) and 70.69 (6)° with the triazole ring, and the dihedral angle between the triazole and the pyridine rings is 43.38 (8)°. Intermolecular $\text{C}-\text{H}\cdots\text{N}$ hydrogen bonds are observed in the crystal structure.

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Comment

1,2,4-Triazole and its derivatives constitute a promising class of ligands that are widely used in the synthesis of various complexes (Haasnoot, 2000). Recently, we have reported the crystal structures of 1,2,4-triazole ligands and their metal complexes (Zhang *et al.*, 2004; Zhang, Liu, Ma *et al.*, 2005; Zhang, Liu, Yang *et al.*, 2005). As an extension of our work on the structural characterization of triazole derivatives, we report here the crystal structure of the title compound, (I).



In (I), the pyridine and benzene rings lie in a propeller arrangement around the central 1,2,4-triazole ring (Fig. 1), thereby minimizing steric effects among these rings. The dihedral angles between the pyridine ring and the two benzene rings (C8–C13 and C15–C20) are 19.39 (8) and 87.81 (6)°, respectively. These two benzene rings form dihedral angles of 30.95 (9) and 70.69 (6)°, respectively, with the triazole ring, and the dihedral angle between the triazole ring and the pyridine ring is 43.38 (8)°. The crystal packing is stabilized by $\text{C}-\text{H}\cdots\text{N}$ hydrogen bonds (Table 1).

Experimental

The title compound was synthesized according to a literature method (Zhu *et al.*, 2000). Equivalent amounts of *p*-methylphosphazoanilide and *N*-pyridyl-*N'*-*p*-methylphenylhydrazine were reacted in ethanol (10 ml) for 1 h. After allowing the resulting solution to stand in air for 15 d, colourless block-shaped crystals were formed on slow evaporation of the solvent. The crystals were isolated, washed with ethanol and dried. Analysis found: C 69.226, H 4.34, N 16.18%; calculated for $\text{C}_{20}\text{H}_{15}\text{ClN}_4$: C 69.26, H 4.36, N 16.15%.

Crystal data

C₂₀H₁₅CIN₄
M_r = 346.81
 Monoclinic, *P*2₁/*c*
a = 18.905 (4) Å
b = 8.4111 (16) Å
c = 11.419 (2) Å
 β = 105.276 (3)°
V = 1751.5 (6) Å³
Z = 4

D_x = 1.315 Mg m⁻³
 Mo *K*α radiation
 Cell parameters from 3824 reflections
 θ = 2.6–28.3°
 μ = 0.23 mm⁻¹
T = 298 (2) K
 Block, colourless
 0.20 × 0.19 × 0.14 mm

Data collection

Bruker SMART CCD area-detector diffractometer
 φ and ω scans
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
T_{min} = 0.956, *T_{max}* = 0.970
 20226 measured reflections

4316 independent reflections
 3093 reflections with *I* > 2σ(*I*)
R_{int} = 0.030
 θ_{max} = 28.3°
h = -24 → 24
k = -11 → 10
l = -15 → 14

Refinement

Refinement on *F*²
R[*F*² > 2σ(*F*²)] = 0.040
wR(*F*²) = 0.116
S = 1.09
 4316 reflections
 275 parameters
 H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.05P)^2 + 0.2731P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 (Δσ)_{max} = 0.011
 Δρ_{max} = 0.17 e Å⁻³
 Δρ_{min} = -0.23 e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

<i>D</i> — <i>H</i> ⋯ <i>A</i>	<i>D</i> — <i>H</i>	<i>H</i> ⋯ <i>A</i>	<i>D</i> ⋯ <i>A</i>	<i>D</i> — <i>H</i> ⋯ <i>A</i>
C17—H17⋯N2 ⁱ	0.984 (17)	2.452 (17)	3.342 (2)	150.3 (14)
C20—H20⋯N1 ⁱⁱ	0.954 (17)	2.554 (17)	3.320 (2)	137.4 (14)

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

The methyl H atoms were placed in calculated positions (C—H = 0.96 Å) and constrained to ride on their parent atom, with *U*_{iso}(H) = 1.5*U*_{eq}(C). The remaining H atoms were located in a difference map and refined freely.

Data collection: SMART (Siemens, 1996); cell refinement: SAINT (Siemens, 1996); data reduction: SAINT; program(s) used to solve

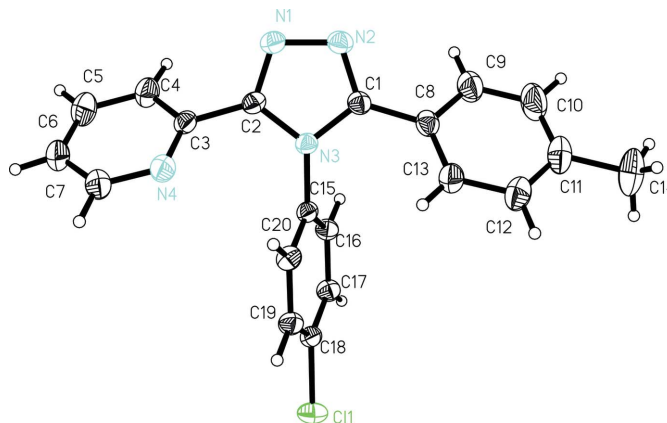


Figure 1

The structure of (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme.

structure: SHELXS97 (Sheldrick, 1997a); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997a); molecular graphics: SHELXTL (Sheldrick, 1997b); software used to prepare material for publication: SHELXTL.

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