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4-(4-Chlorophenyl)-3-phenyl-5-(4-pyridyl)-4*H*-1,2,4-triazole

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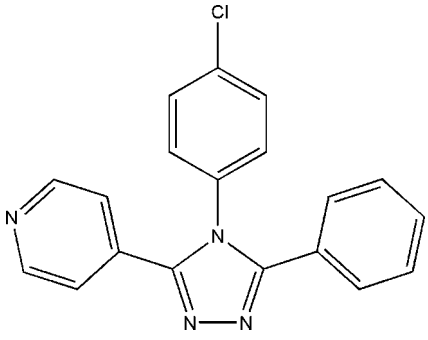
Key indicators: single-crystal X-ray study; T = 113 K; mean σ(C–C) = 0.002 Å; R factor = 0.045; wR factor = 0.104; data-to-parameter ratio = 18.1.

The title compound, $C_{19}H_{13}ClN_4$, was synthesized by the condensation of isonicotinohydrazide and *N*-(4-clorophenyl)-benzimidoyl chloride in *N*,*N*-dimethylacetamide. In the title molecule, the triazole ring is oriented at dihedral angles of 34.64 (2), 30.97 (3) and 71.82 (3)° with respect to the pyridyl, phenyl and chlorophenyl rings, respectively.

Related literature

For related literature, see: Kido *et al.* (1993); Li *et al.* (2006); Zhu *et al.* (2000); Zhu *et al.* (2001). For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_{19}H_{13}ClN_4$
M_r = 332.78
Monoclinic, $P2_1/n$
a = 5.6436 (8) Å
b = 16.730 (2) Å
c = 16.239 (2) Å
β = 95.193 (7)°
V = 1527.0 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.26 mm^{-1}
T = 113 (2) K
0.32 × 0.28 × 0.10 mm

Data collection

Rigaku Saturn diffractometer
Absorption correction: multi-scan (Jacobson; 1998)
T_{min} = 0.912, T_{max} = 0.975
19621 measured reflections
3939 independent reflections
3204 reflections with $I > 2\sigma(I)$
R_{int} = 0.041

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.104
S = 1.09
3939 reflections
218 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.31 e Å^{-3}
$\Delta\rho_{min}$ = −0.49 e Å^{-3}

Data collection: *CrystalClear* (Rigaku/MSC, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *CrystalStructure* (Rigaku/MSC, 2004); software used to prepare material for publication: *CrystalStructure*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HK2371).

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supplementary materials

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4-(4-Chlorophenyl)-3-phenyl-5-(4-pyridyl)-4*H*-1,2,4-triazole

J. Hu, G. Ma, G. Chen and W. Zhang

Comment

In recent years, the 1,2,4-triazole derivatives have appealed much attention by their structures, specific magnetic (Zhu *et al.*, 2000; Zhu *et al.*, 2001) and electron-transporting properties (Kido *et al.*, 1993; Li *et al.*, 2006). We report herein the crystal structure of the title compound, (I), in order to elucidate its molecular conformation.

In the molecule of (I) (Fig. 1), the bond lengths and angles are within normal ranges (Allen *et al.*, 1987). Rings A (C1—C6), B (N1/N2/N3/C7/C8), C (N4/C9—C13) and D (C14—C19) are, of course, planar and the dihedral angles between them are A/B = 71.82 (3)°, A/C = 62.87 (3)°, A/D = 68.98 (2)°, B/C = 34.64 (2)°, B/D = 30.97 (3)° and C/D = 62.71 (3)°.

Experimental

The title compound was synthesized by the reaction of isonicotinohydrazide (274.0 mg, 2.0 mmol) and *N*-(4-clorophenyl)-benzimidoyl chloride (500.0 mg, 2.0 mmol) in *N*,*N*-dimethyl-acetamide (10 ml). The mixture was stirred and refluxed for 5 h. After cooling, the product crystallized from the orange reaction mixture. It was filtered off, washed with *N*,*N*-dimethyl-acetamide and dried *in vacuo* to give the product as fine colorless needles. Single crystals of (I) were obtained by slow evaporation of the ethanol solution in 15 d (yield; 385.0 mg, 57%, m.p. 488–489 K).

Refinement

H atoms were positioned geometrically, with C—H = 0.95 Å for aromatic H atoms and constrained to ride on their parent atoms, with $U_{iso}(H) = 1.2U_{eq}(C)$.

Figures

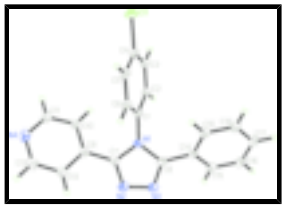


Fig. 1. The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

4-(4-Chlorophenyl)-3-phenyl-5-(4-pyridyl)-4*H*-1,2,4-triazole

Crystal data

$C_{19}H_{13}ClN_4$	F_{000} = 688
M_r = 332.78	D_x = 1.448 Mg m^{-3}
Monoclinic, $P2_1/n$	Melting point: 488 K

Hall symbol: -P 2yn	Mo $K\alpha$ radiation $\lambda = 0.71070$ Å
$a = 5.6436$ (8) Å	Cell parameters from 3105 reflections
$b = 16.730$ (2) Å	$\theta = 1.8–25.0°$
$c = 16.239$ (2) Å	$\mu = 0.26$ mm^{-1}
$\beta = 95.193$ (7)°	$T = 113$ (2) K
$V = 1527.0$ (3) Å^3	Prism, colorless
$Z = 4$	0.32 × 0.28 × 0.10 mm

Data collection

Rigaku Saturn diffractometer	3204 reflections with $I > 2\sigma(I)$
Radiation source: rotating anode	$R_{int} = 0.041$
Monochromator: confocal	$\theta_{max} = 28.7°$
$T = 113(2)$ K	$\theta_{min} = 1.8°$
ω scans	$h = -7 \rightarrow 7$
Absorption correction: multi-scan (Jacobson; 1998)	$k = -22 \rightarrow 22$
$T_{min} = 0.912$, $T_{max} = 0.975$	$l = -21 \rightarrow 21$
19621 measured reflections	Standard reflections: ?
3939 independent reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.045$	H-atom parameters constrained
$wR(F^2) = 0.104$	$w = 1/[\sigma^2(F_o^2) + (0.0442P)^2 + 0.487P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.09$	$(\Delta/\sigma)_{max} < 0.001$
3939 reflections	$\Delta\rho_{max} = 0.31$ e Å^{-3}
218 parameters	$\Delta\rho_{min} = -0.49$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit S are based on F^2, conventional *R*-factors *R* are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2$sigma(F^2) is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on F, and R– factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cl1	0.04399 (10)	0.03869 (2)	−0.12216 (3)	0.03717 (14)
N1	0.0462 (2)	0.27192 (7)	0.15171 (7)	0.0170 (3)
N2	0.1492 (2)	0.37831 (8)	0.22700 (8)	0.0217 (3)
N3	−0.0129 (2)	0.33435 (8)	0.26789 (8)	0.0219 (3)
N4	0.6710 (3)	0.41964 (8)	−0.01248 (9)	0.0261 (3)
C1	0.0402 (3)	0.21366 (8)	0.08607 (9)	0.0168 (3)
C2	−0.1579 (3)	0.20819 (9)	0.02902 (9)	0.0193 (3)
H2	−0.2925	0.2413	0.0342	0.023*
C3	−0.1572 (3)	0.15387 (9)	−0.03561 (10)	0.0225 (3)
H3	−0.2911	0.1493	−0.0752	0.027*
C4	0.0415 (3)	0.10650 (9)	−0.04141 (9)	0.0228 (3)
C5	0.2388 (3)	0.11159 (9)	0.01555 (10)	0.0242 (4)
H5	0.3732	0.0784	0.0104	0.029*
C6	0.2378 (3)	0.16572 (9)	0.08021 (10)	0.0203 (3)
H6	0.3713	0.1698	0.1200	0.024*
C7	0.1828 (3)	0.34010 (8)	0.15814 (9)	0.0180 (3)
C8	−0.0723 (3)	0.27118 (9)	0.22224 (9)	0.0179 (3)
C9	0.3466 (3)	0.36720 (9)	0.09792 (9)	0.0185 (3)
C10	0.2993 (3)	0.35674 (9)	0.01233 (10)	0.0207 (3)
H10	0.1561	0.3319	−0.0098	0.025*
C11	0.4652 (3)	0.38327 (9)	−0.03956 (10)	0.0222 (3)
H11	0.4319	0.3754	−0.0974	0.027*
C12	0.7103 (3)	0.43173 (9)	0.07007 (10)	0.0231 (3)
H12	0.8514	0.4589	0.0905	0.028*
C13	0.5552 (3)	0.40652 (9)	0.12651 (10)	0.0210 (3)
H13	0.5911	0.4160	0.1840	0.025*
C14	−0.2430 (3)	0.21041 (9)	0.24557 (9)	0.0181 (3)
C15	−0.4253 (3)	0.23521 (9)	0.29282 (9)	0.0216 (3)
H15	−0.4386	0.2899	0.3075	0.026*
C16	−0.5866 (3)	0.17960 (10)	0.31825 (10)	0.0242 (3)
H16	−0.7085	0.1967	0.3509	0.029*
C17	−0.5729 (3)	0.10054 (10)	0.29707 (10)	0.0229 (3)
H17	−0.6851	0.0633	0.3145	0.028*
C18	−0.3944 (3)	0.07550 (10)	0.25005 (10)	0.0236 (3)
H18	−0.3855	0.0209	0.2347	0.028*
C19	−0.2272 (3)	0.12954 (9)	0.22487 (9)	0.0203 (3)
H19	−0.1030	0.1115	0.1937	0.024*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0690 (4)	0.0219 (2)	0.0225 (2)	−0.0056 (2)	0.0144 (2)	−0.00746 (16)
N1	0.0189 (7)	0.0167 (6)	0.0154 (6)	0.0013 (5)	0.0018 (5)	−0.0014 (5)
N2	0.0240 (7)	0.0208 (6)	0.0204 (7)	0.0018 (5)	0.0026 (6)	−0.0020 (5)

N3	0.0239 (7)	0.0215 (6)	0.0203 (6)	0.0017 (5)	0.0032 (5)	−0.0029 (5)
N4	0.0258 (8)	0.0235 (7)	0.0295 (8)	0.0034 (6)	0.0058 (6)	0.0021 (6)
C1	0.0215 (8)	0.0152 (6)	0.0141 (7)	−0.0013 (6)	0.0048 (6)	−0.0006 (5)
C2	0.0205 (8)	0.0193 (7)	0.0183 (7)	0.0015 (6)	0.0028 (6)	0.0018 (6)
C3	0.0286 (9)	0.0220 (8)	0.0165 (7)	−0.0068 (6)	0.0004 (6)	0.0021 (6)
C4	0.0376 (10)	0.0159 (7)	0.0164 (7)	−0.0045 (7)	0.0099 (7)	−0.0018 (6)
C5	0.0283 (9)	0.0194 (7)	0.0267 (8)	0.0029 (6)	0.0111 (7)	0.0003 (6)
C6	0.0199 (8)	0.0207 (7)	0.0208 (7)	0.0012 (6)	0.0042 (6)	0.0010 (6)
C7	0.0208 (8)	0.0160 (7)	0.0170 (7)	0.0016 (6)	0.0002 (6)	−0.0001 (5)
C8	0.0193 (8)	0.0198 (7)	0.0145 (7)	0.0056 (6)	0.0020 (6)	0.0003 (5)
C9	0.0211 (8)	0.0144 (7)	0.0199 (7)	0.0025 (6)	0.0019 (6)	0.0003 (5)
C10	0.0217 (8)	0.0201 (7)	0.0200 (7)	0.0001 (6)	0.0010 (6)	−0.0002 (6)
C11	0.0247 (9)	0.0225 (8)	0.0196 (7)	0.0034 (6)	0.0024 (6)	0.0006 (6)
C12	0.0199 (8)	0.0192 (7)	0.0303 (9)	0.0025 (6)	0.0020 (7)	0.0019 (6)
C13	0.0232 (8)	0.0178 (7)	0.0215 (8)	0.0019 (6)	−0.0012 (6)	0.0002 (6)
C14	0.0179 (8)	0.0219 (7)	0.0145 (7)	0.0025 (6)	0.0010 (6)	0.0010 (6)
C15	0.0233 (9)	0.0245 (8)	0.0171 (7)	0.0063 (6)	0.0031 (6)	−0.0002 (6)
C16	0.0208 (8)	0.0333 (9)	0.0191 (8)	0.0054 (7)	0.0060 (6)	0.0024 (6)
C17	0.0197 (8)	0.0282 (8)	0.0212 (8)	−0.0014 (7)	0.0034 (6)	0.0072 (6)
C18	0.0255 (9)	0.0232 (8)	0.0221 (8)	0.0014 (6)	0.0015 (7)	0.0037 (6)
C19	0.0220 (8)	0.0211 (7)	0.0180 (7)	0.0050 (6)	0.0038 (6)	0.0017 (6)

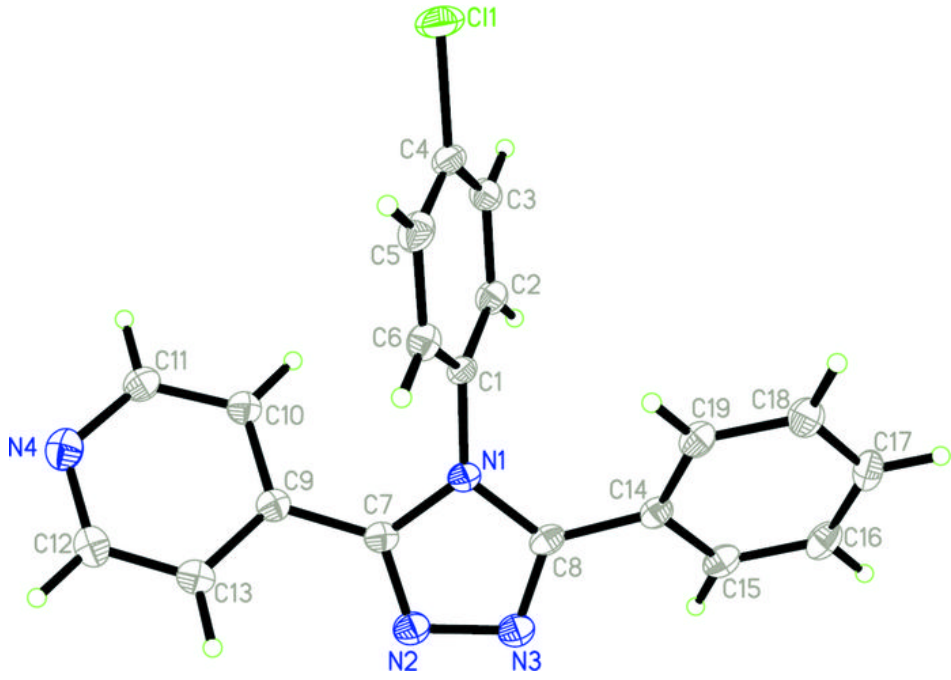
Geometric parameters (Å, °)

Cl1—C4	1.7350 (15)	C8—C14	1.473 (2)
N1—C7	1.3756 (19)	C9—C13	1.391 (2)
N1—C8	1.3776 (19)	C9—C10	1.402 (2)
N1—C1	1.4425 (18)	C10—C11	1.388 (2)
N2—C7	1.3166 (19)	C10—H10	0.9500
N2—N3	1.3887 (18)	C11—H11	0.9500
N3—C8	1.3169 (19)	C12—C13	1.389 (2)
N4—C11	1.349 (2)	C12—H12	0.9500
N4—C12	1.354 (2)	C13—H13	0.9500
C1—C6	1.384 (2)	C14—C19	1.399 (2)
C1—C2	1.389 (2)	C14—C15	1.401 (2)
C2—C3	1.389 (2)	C15—C16	1.390 (2)
C2—H2	0.9500	C15—H15	0.9500
C3—C4	1.384 (2)	C16—C17	1.371 (2)
C3—H3	0.9500	C16—H16	0.9500
C4—C5	1.384 (2)	C17—C18	1.383 (2)
C5—C6	1.387 (2)	C17—H17	0.9500
C5—H5	0.9500	C18—C19	1.394 (2)
C6—H6	0.9500	C18—H18	0.9500
C7—C9	1.476 (2)	C19—H19	0.9500
C7—N1—C8	104.79 (12)	C10—C9—C7	122.95 (14)
C7—N1—C1	126.29 (12)	C11—C10—C9	118.93 (15)
C8—N1—C1	128.88 (12)	C11—C10—H10	120.5
C7—N2—N3	107.49 (12)	C9—C10—H10	120.5
C8—N3—N2	107.53 (12)	N4—C11—C10	123.67 (15)

C11—N4—C12	116.69 (14)	N4—C11—H11	118.2
C6—C1—C2	121.40 (14)	C10—C11—H11	118.2
C6—C1—N1	118.50 (14)	N4—C12—C13	123.46 (15)
C2—C1—N1	120.07 (13)	N4—C12—H12	118.3
C3—C2—C1	119.37 (15)	C13—C12—H12	118.3
C3—C2—H2	120.3	C12—C13—C9	119.22 (15)
C1—C2—H2	120.3	C12—C13—H13	120.4
C4—C3—C2	118.93 (15)	C9—C13—H13	120.4
C4—C3—H3	120.5	C19—C14—C15	118.95 (14)
C2—C3—H3	120.5	C19—C14—C8	123.24 (13)
C3—C4—C5	121.82 (14)	C15—C14—C8	117.78 (13)
C3—C4—Cl1	119.20 (13)	C16—C15—C14	119.83 (14)
C5—C4—Cl1	118.97 (13)	C16—C15—H15	120.1
C4—C5—C6	119.22 (15)	C14—C15—H15	120.1
C4—C5—H5	120.4	C17—C16—C15	121.20 (15)
C6—C5—H5	120.4	C17—C16—H16	119.4
C1—C6—C5	119.25 (15)	C15—C16—H16	119.4
C1—C6—H6	120.4	C16—C17—C18	119.42 (15)
C5—C6—H6	120.4	C16—C17—H17	120.3
N2—C7—N1	110.14 (13)	C18—C17—H17	120.3
N2—C7—C9	124.07 (13)	C17—C18—C19	120.77 (15)
N1—C7—C9	125.78 (13)	C17—C18—H18	119.6
N3—C8—N1	110.04 (13)	C19—C18—H18	119.6
N3—C8—C14	123.24 (13)	C18—C19—C14	119.81 (14)
N1—C8—C14	126.71 (13)	C18—C19—H19	120.1
C13—C9—C10	117.97 (14)	C14—C19—H19	120.1
C13—C9—C7	119.06 (14)		
C7—N2—N3—C8	−0.17 (17)	C1—N1—C8—C14	−2.4 (2)
C7—N1—C1—C6	69.64 (19)	N2—C7—C9—C13	33.6 (2)
C8—N1—C1—C6	−107.64 (18)	N1—C7—C9—C13	−145.59 (15)
C7—N1—C1—C2	−108.42 (17)	N2—C7—C9—C10	−144.90 (16)
C8—N1—C1—C2	74.3 (2)	N1—C7—C9—C10	35.9 (2)
C6—C1—C2—C3	−0.4 (2)	C13—C9—C10—C11	2.2 (2)
N1—C1—C2—C3	177.58 (13)	C7—C9—C10—C11	−179.20 (14)
C1—C2—C3—C4	0.0 (2)	C12—N4—C11—C10	−1.6 (2)
C2—C3—C4—C5	0.3 (2)	C9—C10—C11—N4	−0.6 (2)
C2—C3—C4—Cl1	−179.82 (11)	C11—N4—C12—C13	2.1 (2)
C3—C4—C5—C6	−0.1 (2)	N4—C12—C13—C9	−0.5 (2)
Cl1—C4—C5—C6	179.97 (12)	C10—C9—C13—C12	−1.7 (2)
C2—C1—C6—C5	0.6 (2)	C7—C9—C13—C12	179.66 (13)
N1—C1—C6—C5	−177.46 (13)	N3—C8—C14—C19	−147.90 (16)
C4—C5—C6—C1	−0.3 (2)	N1—C8—C14—C19	32.6 (2)
N3—N2—C7—N1	0.34 (17)	N3—C8—C14—C15	30.2 (2)
N3—N2—C7—C9	−179.00 (14)	N1—C8—C14—C15	−149.32 (15)
C8—N1—C7—N2	−0.37 (17)	C19—C14—C15—C16	0.0 (2)
C1—N1—C7—N2	−178.18 (14)	C8—C14—C15—C16	−178.22 (14)
C8—N1—C7—C9	178.95 (14)	C14—C15—C16—C17	−0.8 (2)
C1—N1—C7—C9	1.1 (2)	C15—C16—C17—C18	0.5 (2)
N2—N3—C8—N1	−0.06 (17)	C16—C17—C18—C19	0.7 (2)

N2—N3—C8—C14	−179.67 (13)	C17—C18—C19—C14	−1.5 (2)
C7—N1—C8—N3	0.26 (17)	C15—C14—C19—C18	1.2 (2)
C1—N1—C8—N3	177.99 (14)	C8—C14—C19—C18	179.28 (15)
C7—N1—C8—C14	179.85 (14)		

Fig. 1


Cl1
C4
C3
C5
C2
C6
C1
C11
C10
C19
C18
N4
N1
C17
C9
C7
C14
C12
C16
C8
C13
C15
N2
N3