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

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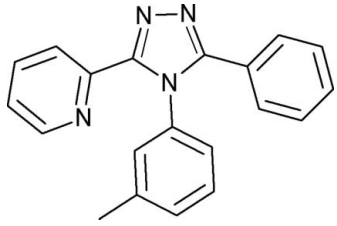
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.057; wR factor = 0.162; data-to-parameter ratio = 17.2.

In the title compound, $C_{20}H_{16}N_4$, the *m*-tolyl and phenyl substituents form dihedral angles of 74.20 (6) and 36.94 (8)°, respectively, with the 1,2,4-triazole ring and the dihedral angle between the triazole and pyridine rings is 36.06 (9)°. In the crystal, molecules are linked by C—H···N and C—H···π interactions.

Related literature

For the synthesis of the title compound, see: Klingsberg (1958). For related structures, see: Wang *et al.* (2005); Huang *et al.* (2008).



Experimental

Crystal data

$C_{20}H_{16}N_4$
M_r = 312.37
Monoclinic, $P2_1/c$
a = 11.246 (3) Å
b = 9.377 (2) Å
c = 18.956 (5) Å
β = 124.655 (16)°
V = 1644.3 (7) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 293 K
0.65 × 0.50 × 0.27 mm

Data collection

Rigaku SCXmini diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
T_{min} = 0.787, T_{max} = 1.000
16277 measured reflections
3751 independent reflections
2691 reflections with $I > 2\sigma(I)$
R_{int} = 0.040

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.057
$wR(F^2)$ = 0.162
S = 1.06
3751 reflections
218 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.31 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C12—H12···N2^{i}	0.93	2.60	3.375 (3)	142
C20—H20A···N2^{ii}	0.96	2.62	3.549 (4)	163
C10—H10···$Cg1^{ii}$	0.93	2.72	3.646 (3)	175

Symmetry codes: (i) $-x+1, y+\frac{1}{2}, -z+\frac{3}{2}$; (ii) $-x+2, y+\frac{1}{2}, -z+\frac{3}{2}$. $Cg1$ is the centroid of the C3–C8 ring.

Data collection: *CrystalClear* (Rigaku, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *PRPKAPPA* (Ferguson, 1999).

We are grateful to Jingye Pharmochemical Pilot Plant for financial assistance through project 8507041056.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: GK2238).

References

Ferguson, G. (1999). *PRPKAPPA*. University of Guelph, Canada.
Huang, L., Wang, Z., Zhang, X. & Wu, P. (2008). *Acta Cryst.* E**64**, m741–m742.
Klingsberg, E. (1958). *J. Org. Chem.* **23**, 1086–1087.
Rigaku (2005). *CrystalClear*. Rigaku Corporation, Tokyo, Japan.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Wang, Z.-X., Lan, Y., Yuan, L.-T. & Liu, C.-Y. (2005). *Acta Cryst.* E**61**, o2033–o2034.

supporting information

Acta Cryst. (2009). E**65**, o3214 [doi:10.1107/S1600536809049174]

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

Xiaoning Gong, Zuoxiang Wang and Yan Liu

S1. Comment

Recently we have prepared some new 1,2,4-triazoles and their complexes (Wang *et al.*, 2005; Huang *et al.*, 2008). We report here the crystal structure of the title compound.

S2. Experimental

The title compound was prepared by the reaction of 3,3′– dimethylphenylphosphazoanilide (2.90, 12 mmol) with *N*-benzoyl-N′-(2-pyridoyl)hydrazine (2.41 g, 10 mmol) in *N*,*N*-dimethylaniline at 463–473 K for 5 hrs (Klingsberg, 1958). Single crystals suitable for X-ray diffraction were obtained by recrystallization from water.

S3. Refinement

Positional parameters of all the H atoms were calculated geometrically. The H atoms were allowed to ride on the C atoms to which they were bonded, riding with C—H = 0.93 Å (aromatic) and 0.96 Å (methyl); U_{iso}(H) = 1.2 or 1.5 times U_{eq}(C).

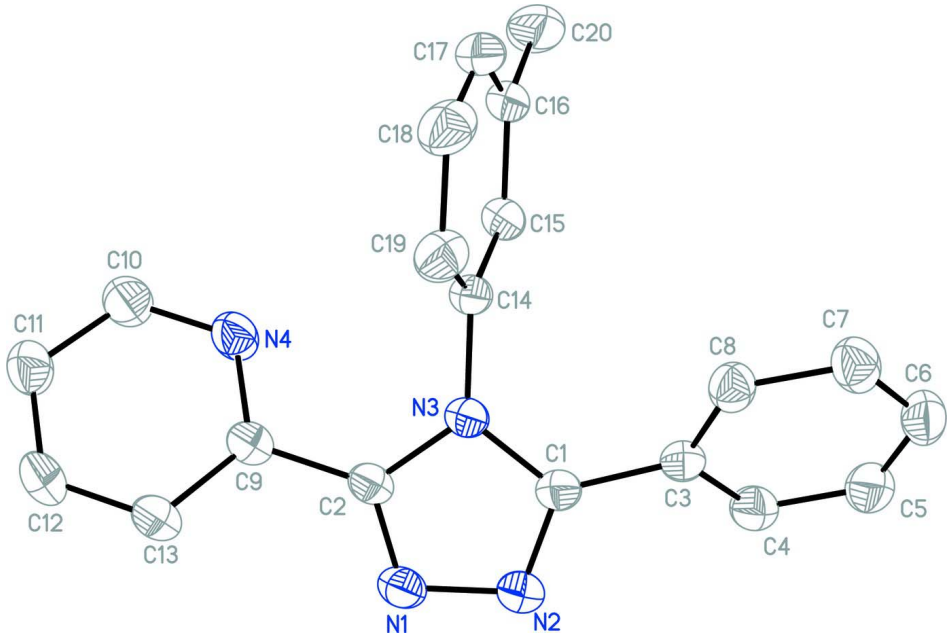


Figure 1

The molecular structure of the title compound with the atom labelling. Displacement ellipsoids are shown at the 30% probability level.

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Crystal data

$C_{20}H_{16}N_4$
$M_r = 312.37$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 11.246$ (3) Å
$b = 9.377$ (2) Å
$c = 18.956$ (5) Å
$\beta = 124.655$ (16)°
$V = 1644.3$ (7) Å^3
$Z = 4$
$F(000) = 656$
$D_x = 1.262$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3426 reflections
$\theta = 2.3$–27.5°
$\mu = 0.08$ mm^{-1}
$T = 293$ K
Block, white
0.65 × 0.50 × 0.27 mm

Data collection

Rigaku SCXmini diffractometer
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Graphite monochromator
ω scan
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
$T_{min} = 0.787$, $T_{max} = 1.000$
16277 measured reflections
3751 independent reflections
2691 reflections with $I > 2\sigma(I)$
$R_{int} = 0.040$
$\theta_{max} = 27.5°$, $\theta_{min} = 2.3°$
$h = -14 \rightarrow 14$
$k = -12 \rightarrow 12$
$l = -24 \rightarrow 24$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.057$
$wR(F^2) = 0.162$
$S = 1.06$
3751 reflections
218 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0823P)^2 + 0.1727P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.31$ e Å^{-3}
$\Delta\rho_{min} = -0.23$ e Å^{-3}

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 $F^2 > \sigma(F^2)$ 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}
C1	0.91724 (18)	−0.14398 (19)	0.88581 (11)	0.0461 (4)
C2	0.74890 (17)	−0.02378 (18)	0.77576 (11)	0.0447 (4)
C3	1.05742 (18)	−0.1952 (2)	0.95950 (11)	0.0481 (4)
C4	1.0759 (2)	−0.3404 (2)	0.97830 (14)	0.0603 (5)

H4	1.0017	−0.4038	0.9427	0.072*
C5	1.2038 (2)	−0.3906 (2)	1.04945 (15)	0.0703 (6)
H5	1.2151	−0.4876	1.0619	0.084*
C6	1.3143 (2)	−0.2978 (3)	1.10189 (14)	0.0684 (6)
H6	1.4005	−0.3317	1.1498	0.082*
C7	1.2969 (2)	−0.1545 (2)	1.08313 (12)	0.0618 (5)
H7	1.3719	−0.0917	1.1186	0.074*
C8	1.16981 (19)	−0.1029 (2)	1.01265 (11)	0.0513 (4)
H8	1.1594	−0.0058	1.0007	0.062*
C9	0.67146 (17)	0.07496 (19)	0.70258 (10)	0.0457 (4)
C10	0.6617 (2)	0.1881 (3)	0.59246 (13)	0.0687 (6)
H10	0.7040	0.2101	0.5636	0.082*
C11	0.5267 (2)	0.2440 (2)	0.56156 (13)	0.0679 (6)
H11	0.4792	0.3009	0.5127	0.081*
C12	0.4644 (2)	0.2140 (2)	0.60434 (13)	0.0625 (5)
H12	0.3740	0.2507	0.5852	0.075*
C13	0.53747 (18)	0.1287 (2)	0.67597 (12)	0.0529 (5)
H13	0.4973	0.1074	0.7062	0.063*
C14	1.00456 (17)	0.05403 (19)	0.83598 (10)	0.0445 (4)
C15	1.08632 (18)	−0.0030 (2)	0.80966 (11)	0.0510 (4)
H15	1.0713	−0.0967	0.7903	0.061*
C16	1.19103 (19)	0.0793 (2)	0.81200 (13)	0.0595 (5)
C17	1.2116 (2)	0.2171 (3)	0.84272 (14)	0.0676 (6)
H17	1.2815	0.2735	0.8447	0.081*
C18	1.1320 (2)	0.2735 (2)	0.87042 (13)	0.0693 (6)
H18	1.1494	0.3660	0.8917	0.083*
C19	1.0255 (2)	0.1913 (2)	0.86644 (12)	0.0583 (5)
H19	0.9695	0.2283	0.8840	0.070*
C20	1.2756 (3)	0.0194 (3)	0.7795 (2)	0.1004 (10)
H20A	1.2660	0.0814	0.7363	0.151*
H20B	1.2390	−0.0734	0.7555	0.151*
H20C	1.3757	0.0120	0.8262	0.151*
N1	0.68517 (15)	−0.12089 (17)	0.79297 (10)	0.0527 (4)
N2	0.79217 (16)	−0.19790 (17)	0.86336 (10)	0.0536 (4)
N3	0.89575 (14)	−0.03337 (15)	0.83260 (9)	0.0441 (3)
N4	0.73453 (16)	0.1044 (2)	0.66152 (10)	0.0615 (5)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0450 (9)	0.0508 (9)	0.0478 (9)	−0.0015 (8)	0.0295 (8)	0.0013 (8)
C2	0.0375 (9)	0.0539 (9)	0.0450 (9)	−0.0015 (7)	0.0247 (8)	−0.0039 (8)
C3	0.0455 (9)	0.0578 (10)	0.0489 (9)	0.0031 (8)	0.0316 (8)	0.0057 (8)
C4	0.0523 (11)	0.0593 (12)	0.0703 (12)	−0.0002 (9)	0.0354 (10)	0.0096 (10)
C5	0.0653 (13)	0.0683 (13)	0.0807 (15)	0.0140 (11)	0.0436 (12)	0.0243 (12)
C6	0.0563 (12)	0.0908 (16)	0.0562 (11)	0.0201 (11)	0.0308 (10)	0.0193 (11)
C7	0.0533 (11)	0.0786 (14)	0.0473 (10)	0.0022 (10)	0.0250 (9)	−0.0035 (10)
C8	0.0529 (10)	0.0559 (10)	0.0445 (9)	0.0026 (8)	0.0273 (9)	0.0014 (8)

C9	0.0408 (9)	0.0534 (10)	0.0433 (9)	−0.0030 (7)	0.0242 (8)	−0.0071 (7)
C10	0.0587 (12)	0.0980 (16)	0.0542 (11)	0.0093 (12)	0.0349 (10)	0.0124 (11)
C11	0.0525 (12)	0.0875 (15)	0.0519 (11)	0.0106 (10)	0.0226 (10)	0.0141 (11)
C12	0.0395 (10)	0.0748 (13)	0.0626 (12)	0.0098 (9)	0.0227 (9)	0.0021 (10)
C13	0.0409 (9)	0.0652 (11)	0.0542 (10)	−0.0010 (8)	0.0280 (8)	−0.0045 (9)
C14	0.0375 (9)	0.0542 (10)	0.0400 (8)	−0.0046 (7)	0.0210 (7)	0.0040 (7)
C15	0.0403 (9)	0.0629 (11)	0.0487 (10)	−0.0006 (8)	0.0245 (8)	0.0053 (8)
C16	0.0403 (10)	0.0791 (14)	0.0584 (11)	0.0024 (9)	0.0277 (9)	0.0208 (10)
C17	0.0481 (11)	0.0823 (15)	0.0605 (12)	−0.0146 (10)	0.0237 (10)	0.0190 (11)
C18	0.0746 (14)	0.0596 (12)	0.0589 (12)	−0.0203 (10)	0.0292 (11)	−0.0003 (10)
C19	0.0645 (12)	0.0581 (11)	0.0536 (11)	−0.0049 (9)	0.0344 (10)	0.0005 (9)
C20	0.0799 (17)	0.123 (2)	0.132 (2)	0.0221 (16)	0.0802 (18)	0.047 (2)
N1	0.0420 (8)	0.0610 (9)	0.0584 (9)	−0.0034 (7)	0.0304 (7)	−0.0005 (8)
N2	0.0450 (8)	0.0583 (9)	0.0599 (9)	−0.0028 (7)	0.0314 (8)	0.0045 (7)
N3	0.0379 (7)	0.0515 (8)	0.0450 (7)	−0.0017 (6)	0.0249 (6)	0.0015 (6)
N4	0.0491 (9)	0.0881 (12)	0.0516 (9)	0.0111 (8)	0.0313 (8)	0.0086 (8)

Geometric parameters (Å, º)

C1—N2	1.317 (2)	C11—C12	1.368 (3)
C1—N3	1.369 (2)	C11—H11	0.9300
C1—C3	1.470 (2)	C12—C13	1.375 (3)
C2—N1	1.310 (2)	C12—H12	0.9300
C2—N3	1.368 (2)	C13—H13	0.9300
C2—C9	1.472 (2)	C14—C19	1.375 (3)
C3—C8	1.383 (3)	C14—C15	1.379 (2)
C3—C4	1.393 (3)	C14—N3	1.444 (2)
C4—C5	1.379 (3)	C15—C16	1.388 (2)
C4—H4	0.9300	C15—H15	0.9300
C5—C6	1.373 (3)	C16—C17	1.381 (3)
C5—H5	0.9300	C16—C20	1.504 (3)
C6—C7	1.375 (3)	C17—C18	1.375 (3)
C6—H6	0.9300	C17—H17	0.9300
C7—C8	1.375 (3)	C18—C19	1.390 (3)
C7—H7	0.9300	C18—H18	0.9300
C8—H8	0.9300	C19—H19	0.9300
C9—N4	1.346 (2)	C20—H20A	0.9600
C9—C13	1.384 (2)	C20—H20B	0.9600
C10—N4	1.335 (3)	C20—H20C	0.9600
C10—C11	1.383 (3)	N1—N2	1.387 (2)
C10—H10	0.9300		
N2—C1—N3	110.12 (15)	C13—C12—H12	120.5
N2—C1—C3	123.56 (16)	C12—C13—C9	119.16 (18)
N3—C1—C3	126.29 (15)	C12—C13—H13	120.4
N1—C2—N3	110.15 (15)	C9—C13—H13	120.4
N1—C2—C9	123.91 (15)	C19—C14—C15	121.67 (16)
N3—C2—C9	125.86 (15)	C19—C14—N3	119.22 (16)

C8—C3—C4	118.92 (17)	C15—C14—N3	119.10 (16)
C8—C3—C1	122.00 (17)	C14—C15—C16	120.07 (19)
C4—C3—C1	119.04 (17)	C14—C15—H15	120.0
C5—C4—C3	120.3 (2)	C16—C15—H15	120.0
C5—C4—H4	119.9	C17—C16—C15	117.99 (19)
C3—C4—H4	119.9	C17—C16—C20	121.9 (2)
C6—C5—C4	120.2 (2)	C15—C16—C20	120.1 (2)
C6—C5—H5	119.9	C18—C17—C16	122.09 (18)
C4—C5—H5	119.9	C18—C17—H17	119.0
C5—C6—C7	119.64 (19)	C16—C17—H17	119.0
C5—C6—H6	120.2	C17—C18—C19	119.6 (2)
C7—C6—H6	120.2	C17—C18—H18	120.2
C8—C7—C6	120.8 (2)	C19—C18—H18	120.2
C8—C7—H7	119.6	C14—C19—C18	118.5 (2)
C6—C7—H7	119.6	C14—C19—H19	120.7
C7—C8—C3	120.15 (19)	C18—C19—H19	120.7
C7—C8—H8	119.9	C16—C20—H20A	109.5
C3—C8—H8	119.9	C16—C20—H20B	109.5
N4—C9—C13	122.49 (17)	H20A—C20—H20B	109.5
N4—C9—C2	116.73 (15)	C16—C20—H20C	109.5
C13—C9—C2	120.72 (16)	H20A—C20—H20C	109.5
N4—C10—C11	123.52 (19)	H20B—C20—H20C	109.5
N4—C10—H10	118.2	C2—N1—N2	107.66 (14)
C11—C10—H10	118.2	C1—N2—N1	107.09 (14)
C12—C11—C10	118.65 (19)	C2—N3—C1	104.97 (13)
C12—C11—H11	120.7	C2—N3—C14	127.64 (14)
C10—C11—H11	120.7	C1—N3—C14	127.40 (13)
C11—C12—C13	119.03 (18)	C10—N4—C9	117.14 (16)
C11—C12—H12	120.5		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C12—H12···N2^{i}	0.93	2.60	3.375 (3)	142
C20—H20*A*···N2^{ii}	0.96	2.62	3.549 (4)	163
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