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3,5-Dimethyl-1,4,7-triphenyl-1*H*,7*H*-pyrazolo[3,4-*b*:4′,3′-*e*]pyridine

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Key indicators

Single-crystal X-ray study
T = 120 K
Mean σ(C–C) = 0.002 Å
R factor = 0.040
wR factor = 0.105
Data-to-parameter ratio = 16.2

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

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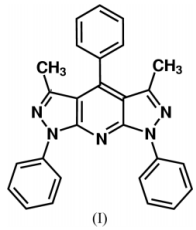
The title compound, $C_{27}H_{21}N_5$, is isomorphous with 3,5-dimethyl-1,7-diphenyl-4-(2-pyridinyl)-1*H*,7*H*-pyrazolo[3,4-*b*:4′,3′-*e*]pyridine.

Comment

The title compound, 3,5-dimethyl-1,4,7-triphenyl-1*H*,7*H*-pyrazolo[3,4-*b*:4′,3′-*e*]pyridine, (I) (Fig. 1, and Tables 1 and 2), is isomorphous with 3,5-dimethyl-1,7-diphenyl-4-(2-pyridinyl)-1*H*,7*H*-pyrazolo[3,4-*b*:4′,3′-*e*]pyridine, (II) (Low *et al.*, 2003), the only difference being that in (I) a phenyl ring replaces the pyridyl ring of (II).



(I)

With the exception of those listed in Table 1, the bonds and angles for this compound are identical to those of (II) within 3σ.

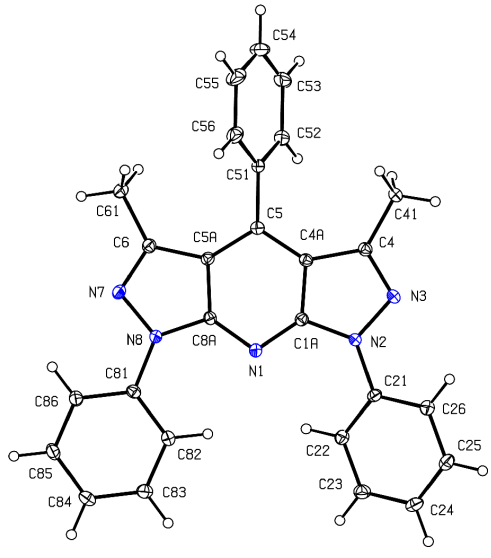


Figure 1
A view of (I), with the atomic numbering scheme. Displacement ellipsoids are drawn at the **30% (50%?)** probability level.

Experimental

A mixture of 5-amino-3-methyl-1-phenylpyrazole (10 mmol) and benzaldehyde (20 mmol) was placed into Pyrex-glass open vessels and irradiated in a domestic microwave oven for 1 min (at 600 W). The solid was filtered, washed with ethanol, dried and recrystallized from ethanol. Yield 65%, m.p. 516 K. Analysis calculated for $C_{27}H_{21}N_5$: C 78.05, H 5.09, N 16.86%; found: C 78.08, H 5.03, N 16.81%.

Crystal data

$C_{27}H_{21}N_5$
M_r = 415.49
Triclinic, $P\overline{1}$
a = 8.5006 (2) Å
b = 10.5829 (3) Å
c = 12.4093 (3) Å
α = 106.078 (1)°
β = 97.615 (2)°
γ = 100.675 (1)°
V = 1033.96 (5) Å^3
Z = 2
D_x = 1.335 Mg m^{-3}
Mo Kα radiation
Cell parameters from 4711 reflections
θ = 3.1–27.5°
μ = 0.08 mm^{-1}
T = 120.0 (2) K
Block, brown
0.40 × 0.26 × 0.20 mm

Data collection

Nonius KappaCCD diffractometer
φ scans and ω scans with κ offsets
Absorption correction: multi-scan (*DENZO–SMN*; Otwinowski & Minor, 1997)
T_{min} = 0.968, T_{max} = 0.984
21256 measured reflections
4711 independent reflections
3815 reflections with $I > 2\sigma(I)$
R_{int} = 0.047
θ_{max} = 27.5°
$h = -11 \rightarrow 10$
$k = -13 \rightarrow 13$
$l = -16 \rightarrow 16$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.105
S = 1.05
4711 reflections
291 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0522P)^2 + 0.2273P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

C51—C52	1.3931 (18)	C52—C53	1.3877 (18)
N3—C4—C41	119.73 (10)	C53—C52—C51	120.38 (13)
C4*A*—C4—C41	129.53 (10)	C54—C53—C52	120.25 (14)
C52—C51—C56	119.11 (11)	C53—C54—C55	119.74 (13)
C52—C51—C5	120.63 (11)	C54—C55—C56	120.60 (14)
C56—C51—C5	120.26 (11)	C55—C56—C51	119.92 (14)
C1*A*—N2—C21—C22	25.02 (18)	C5*A*—C5—C51—C56	62.32 (16)
N3—N2—C21—C22	−153.10 (11)	C4*A*—C5—C51—C56	−118.31 (13)
C1*A*—N2—C21—C26	−155.93 (11)	C8*A*—N8—C81—C82	−4.62 (19)
N3—N2—C21—C26	25.95 (16)	N7—N8—C81—C82	171.84 (10)
C5*A*—C5—C51—C52	−117.76 (13)	C8*A*—N8—C81—C86	175.19 (11)
C4*A*—C5—C51—C52	61.61 (16)	N7—N8—C81—C86	−8.34 (16)

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

D—H···A	D—H	H···A	D···A	D—H···A
C22—H22···N1	0.95	2.44	3.0036 (16)	118
C82—H82···N1	0.95	2.31	2.9674 (16)	126
C85—H85···N3^{i}	0.95	2.54	3.4888 (17)	173

Symmetry code: (i) $x-1, y-1, z$.

H atoms were treated as riding atoms, with C—H distances of 0.95 (aromatic) and 0.98 Å (methyl), and U_{iso}(H) values of 1.2U_{eq}(aromatic C) and 1.5U_{eq}(methyl C).

Data collection: *KappaCCD Server Software* (Nonius, 1997); cell refinement: *DENZO–SMN* (Otwinowski & Minor, 1997); data reduction: *DENZO–SMN*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*II (Johnson, 1976) and *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL*97 and *WordPerfect* macro *PRPKAPPA* (Ferguson, 1999).

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